Variational Simulation of Continuous Quantum Systems

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Declaration of Authorship

I, Sarah Kim Harrison-Schmidt, hereby declare that this thesis and the work presented in it is entirely my own. Where I have consulted the work of others, this is always clearly stated.

Signed:

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Abstract

As the realisation of a fully scalable quantum computer remains distant, the simulation of many-body quantum systems becomes an intermediate goal of great practical importance. This thesis focusses on the simulation of continuous quantum systems by application of variational methods. Such methods rely on a choice of variational ansatz states, which when constructed appropriately can be used to successfully determine properties of physical systems and simulate their dynamics. Applications of variational methods in this thesis employ the family of continuous matrix product states (cMPS) for quantum field theories and continuum models in one spatial dimension as a variational class.

We develop a variational method exploiting the natural physics of cavity quantum electrodynamics (cavity QED) architectures to simulate interacting quantum fields. The natural interpretation of the output of cavity QED apparatuses as a cMPS is exploited, allowing for an analogue quantum simulation procedure using current technology. We demonstrate that the paradigmatic cavity QED system comprising a single trapped atom coupled to a single cavity mode is capable of simulating the ground state physics of an equally paradigmatic quantum field, namely the Lieb-Liniger model. We find that varying the adjustable parameters of the cavity QED system within an experimentally feasible parameter regime, and in the presence of losses, allows for the quantum simulation of Lieb-Liniger ground state physics. The scheme can also be extended to simulate systems of entangled multi-component fields, beyond the reach of existing classical simulation methods.

Furthermore, we develop an algorithm that allows for the simulation of the dynamics of a continuous quantum system under the action of a random potential. The exact simulation of the dynamics of such a continuous quantum random system (cQRS) would usually require an infinite number of evolutions, corresponding to each realisation of the random potential. We avoid this impracticable task by introducing an auxiliary system, such that a mapping between the cQRS and an interacting, non-random, system is established. By means of an extension of the time-dependent variational principle using multi-component cMPS, we explicitly derive the equations of motion determining the time evolution of the cMPS variational parameters, allowing for numerical simulation of the dynamics of the interacting quantum fields. In a simple one-dimensional case we obtain the Gross Pitaevskii equation and thereby verify our results.

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Chapter 1

Introduction

Interesting phenomena in the natural sciences often involve a large number of interacting particles. Classically, the simulation of such systems is challenging, since the number of variables required to exactly specify the time evolution of each component easily grows beyond the reach of existing computational power. In the quantum regime the situation is worse, due to the dramatic increase in the number of variables required to specify the state. To describe the dynamics of a collection of n quantum particles one requires a system of differential equations scaling exponentially in n. However, the study and understanding of interacting particle systems in the quantum regime is of great importance, since such systems exhibit behaviour beyond that of classical systems and their properties have led to a host of applications. A prominent example is the development of electronic control devices such as diodes and transistors, built out of semiconductors, whose conducting properties require a quantum mechanical description, and which lead to the development of integrated circuits, the cornerstone for modern chip industry.

The sheer complexity of modelling many-particle quantum systems commonly requires clever approximation methods to reduce the amount of information required to specify the state of the system, yet still preserving certain physical quantities of interest. An alternative approach to the study of such systems was proposed by R. P. Feynman [Feynman, 1982]. Feynman emphasised the complexity of simulating quantum systems using classical computers and proposed that the size of a quantum state's state space might be the problem and the solution at the same time. He suggested using quantum systems in order to simulate other quantum systems, resulting in the field of quantum simulation. With the realisation of a fully operational quantum computer a distant hope, the simulation of complex many-body quantum systems has become an intermediate goal of great practical importance.

This thesis is concerned with variational simulations of continuous quantum systems, where variational methods are used to calculate the ground state and dynamical properties of quantum fields. Variational methods have proven to be powerful tools in the study of quantum systems when used in conjunction with an appropriate variational class. Indeed, the

success and power of a variational method is highly contingent on the choice of variational class. Finding a class of quantum states that captures certain physical effects whilst also providing efficient computation of physical quantities of interest is a much sought after, but difficult, task.

One example of a successful application of variational methods arose from the introduction of the matrix product state (MPS) representation [Fannes et al., 1992, Vidal, 2003] for one dimensional quantum lattice systems. It was then observed that the already acclaimed numerical renormalisation group (NRG) of Wilson [Wilson, 1975] and density matrix renormalisation group (DMRG) of White [White, 1992] could be reformulated as variational methods within the class of MPS [Östlund and Rommer, 1995, Rommer and Östlund, 1997]. This insight led to a huge increase in the power of the DMRG approach. The method was no longer restricted to computing ground state physics of finite, one-dimensional quantum lattice systems with open boundary conditions, but extended to periodic boundary conditions, infinite chains, higher dimensional systems and non-equilibrium physics (see, for example, [Schollwock, 2011, Verstraete et al., 2008, Verstraete et al., 2004]). The DMRG is arguably the most powerful tool available for the study of one-dimensional strongly interacting quantum lattice systems due to the prolific variational class of MPS.

Lying at the heart of the power of the DMRG method, the class of MPS form the basis of a large number of recent developments in quantum information theory and condensed matter theory. It is therefore unsurprising that the MPS formalism was extended to describe one-dimensional quantum field theories by F. Verstraete and J. I. Cirac in 2010 [Verstraete and Cirac, 2010]. This class of states, known as continuous matrix product states (cMPS) have shown to be capable of the classical simulation of relativistic and nonrelativistic quantum fields [Haegeman et al., 2010, Osborne et al., 2010, Verstraete and Cirac, 2010]. We consider applications of variational methods using the family of cMPS as a variational class of quantum field states to approximate the ground state and simulate the dynamics of continuous quantum systems.

This thesis is organised as follows. Part I provides preliminary material required for the understanding of the results presented in Part II. Chapter 2 discusses the variational methods that form the basis of applications of Part II, and Chapter 4 describes in detail the corresponding variational class of cMPS. Also included in this chapter is a review of the paradigmatic Lieb-Liniger model for one-dimensional continuous quantum systems, which features heavily in Part II. Chapter 3 gives some quantum optics preliminaries essential to the understanding of one of the schemes proposed in Part II.

The second part of the thesis develops two new approaches to the variational simulation of continuous quantum systems. In Chapter 5 we propose a cMPS-inspired analogue algorithm for the quantum simulation of the ground state physics of a one-dimensional interacting quantum field using the continuous output of a cavity QED apparatus. This chapter is based on the work published in [Barrett et al., 2012], which was completed in collaboration with Sean Barrett, Klemens Hammerer, Tracy Northup and Tobias Osborne. In Chapter 6 we present a variational algorithm to simulate the dynamics and ground state properties of a disordered continuous quantum system, including a novel extension of the time-dependent variational principle applied to cMPS. The thesis concludes in Chapter 7.

Statement of originality

Part I is a review of previous work, with the exception of Chapter 4. Here I have included detailed derivations and clarification of methods used to obtain the results in [Haegeman, 2011, Haegeman et al., 2011a], which is novel. I elucidated these derivations largely for pedagogical reasons, with the hope that the review is enlightening and contributes to the general understanding of the topic, but also to ensure that readers can understand the background material required for Part II. Additionally, the derivations missing from [Haegeman, 2011, Haegeman et al., 2011a] do not, to the best of my knowledge, appear elsewhere and it is possible that the methods I use are different than those intended by the author.

All the material presented in Part II, that is Chapters 5 and 6, is my own original work, except where papers have been produced with co-authors, as indicated above. In Chapter 5 my particular contribution was the development and implementation of the classical simulation algorithm.

Part I

Chapter 2

Variational Methods

Many problems in fields such as mathematics, engineering, physics and chemistry are formulated in terms of integrating differential equations. Such problems can be difficult to solve directly due to their complex nature. However, it is often possible to replace the task of integrating a differential equation with the task of seeking an ansatz function that extremizes the value of some functional. Such problems are called variational problems. The methods that allow for the reduction of the problem of integrating a differential equation to the equivalent variational problem are called variational methods. The success of a variational method is highly dependent on the ability of the chosen class of ansatz functions, or states, to capture the system dynamics. There are many variational methods used in physics that provide powerful tools for approximating the state, physical quantities thereof and dynamics of a physical system. Examples include Fermat's principle in geometrical optics and the principle of stationary action in classical mechanics. This thesis uses variational methods to approximate the ground states and dynamics of continuous quantum systems. In this chapter we therefore introduce the concept of variational methods, focussing on applications in quantum mechanics.

The chapter is organised as follows. Since variational methods use variational classes of parameterised ansatz states, we first define such classes in section 2.1, along with notational conventions for the remainder of the chapter. In section 2.2 we briefly review the time-independent variational principle (TIVP), a method for computing approximations to ground and excited states of a time-independent Hamiltonian, before introducing the time-dependent variational principle (TDVP) in section 2.3. The TDVP is a method for approximating ground and excited states of a time-dependent Hamiltonian, as well as for studying dynamical properties of a system. We discuss the TDVP in full, considering the important conditions that ensure norm preservation and distinguishing between real and imaginary time evolution. The material presented in this chapter is well known in mathematical physics and can be found in many textbooks and lecture notes. In particular we follow [Haegeman, 2011, Kramer and Saraceno, 1981, Osborne, 2012].

2.1 Definition of a variational class

Variational methods rely on ansatz functions to solve or approximate the corresponding variational problem. The variational methods used in this thesis use classes of ansatz states to approximate ground state and dynamical properties of continuous quantum systems. We now define such classes in the context of general quantum systems.

Consider a quantum system with corresponding Hilbert space $\mathcal{H}$. Performing efficient numerical calculations using general states within $\mathcal{H}$ is a difficult problem, owing to the space's exponential growth with the size of the system. By restricting to classes of states occupying a subspace of Hilbert space calculations can become tractable. A subspace of Hilbert space consisting of a set of ansatz states is called a variational (differentiable) manifold[1]. A general ansatz state, or variational state, is given by the parameterised state $|\Psi(z)\rangle$ where z denotes a finite or countably infinite set of complex parameters $z^j \in \mathbb{C}$. A variational manifold of states $\mathcal{V} \subset \mathcal{H}$ is thereby defined as

$$\mathcal{V} = \left\{ |\Psi(z)\rangle \mid z^j \in \mathbb{C}, j \in \mathbb{Z}^+ \right\}.$$

We assume that the dependence of $|\Psi(z)\rangle$ on all variational parameters z^j is complex analytic. It is also possible to deal with a continuous set of variational parameters by replacing ordinary derivatives with respect to the parameters z^j by functional derivatives. We note that the hermitian conjugate of a general variational state, given by $\langle\Psi(\overline{z})|$, has an anti-complex analytic property, that is the derivative of $\langle\Psi(\overline{z})|$ with respect to $\overline{z}$ is well defined. The set of complex conjugate parameters $\overline{z}$ constitute an independent set of variational parameters. Clearly, by restricting to subspaces of the full state space $\mathcal{H}$ in such a way numerical calculations become easier. However, constructing variational manifolds of ansatz states that can both be used to perform calculations efficiently and which bear some resemblance to the actual states is an extremely hard task. Reasonable ansatz states should provide efficiency in numerical calculations, with a polynomial scaling in the number of parameters with increasing system size, whilst remaining complete in the sense that the state could, in principle, capture the physics of the system. It often requires deep insights into the physics of a system to be able to devise reasonable variational states. We describe and employ such a cleverly formulated class of states in the context of continuous quantum systems in following chapters.

[1] Roughly speaking, a manifold is a topological space that is locally approximable by a linear space in which we can perform calculus. The particular properties of differentiable manifolds that we require are differentiability and the ability to calculate tangent vectors and tangent spaces at a point in the manifold. For a comprehensive review on differential geometry see [Rudolph and Schmidt, 2013], for example.

In the remainder of this chapter we adopt the following notation conventions. We do not explicitly mark z as a vector to avoid cluttered equations - it should be clear from the context that z is indeed a vector. We use barred indices $\bar{j}$ for the complex conjugate of variational parameters z^j, and write $\overline{z}^{\bar{j}}$. Finally, we use the shorthand notation $\partial_j = \partial/\partial z^j$ and, unless specified otherwise, use Einstein's summation convention.

2.2 The time-independent variational principle

In quantum mechanics a well known variational method is the Schrödinger time-independent variational principle (TIVP). This method allows for estimation of the ground state energy, that is the lowest eigenvalue, of a quantum system described by a Hamiltonian $\hat{H}$ without the need for directly solving the time-independent Schrödinger equation (TISE)

$$\hat{H}\Psi_n = E_n\Psi_n, \qquad n = 0, 1, \ldots \tag{2.1}$$

for stationary states Ψ_n with energies E_n. We have assumed, for simplicity, that the spectrum of $\hat{H}$ is discrete and non degenerate. The method asserts that for any state $|\Psi\rangle$ in the Hilbert space $\mathcal{H}$ of a system with Hamiltonian $\hat{H}$ one can obtain an energy expectation value that exceeds the ground state, as shown in the following theorem.

Theorem 1 *Consider a Hamiltonian $\hat{H}$ and an arbitrary square integrable function Ψ which we choose to be normalised to one, namely $\langle\Psi|\Psi\rangle = 1$. We have that*

$$\langle\Psi|\hat{H}|\Psi\rangle \geq E_0, \tag{2.2}$$

where E_0 is the lowest eigenvalue of $\hat{H}$.

Proof. Let $\{E_n, \Psi_n\}$ be the exact eigenenergies and eigenfunctions of $\hat{H}$ satisfying the TISE $\hat{H}\Psi_n = E_n\Psi_n$ for all n. Then, an arbitrary square integrable function Ψ can be expanded in terms of the complete basis set of $\{\Psi_n\}$ as $\Psi = \sum_n c_n\Psi_n$, where $\sum_n |c_n|^2 = 1$. The energy expectation $\langle\Psi|\hat{H}|\Psi\rangle$ can then be written as

$$\begin{aligned}\sum_{n,m} c_n^* c_m \langle\Psi_n|\hat{H}|\Psi_m\rangle &= \sum_{n,m} c_n^* c_m E_m \langle\Psi_n|\Psi_m\rangle \\ &= \sum_n |c_n|^2 E_n\end{aligned}$$

since $\{\Psi_n\}$ form an orthonormal set. Now, using that $\sum_n |c_n|^2 = 1$ we can write

$$\langle\Psi|\hat{H}|\Psi\rangle - E_0 = \sum_n |c_n|^2 E_n - \sum_n |c_n|^2 E_0.$$

Since we have that $E_0 < E_n \forall n \neq 0$ this leads us to conclude that

$$\langle \Psi | \hat{H} | \Psi \rangle - E_0 \geq 0.$$

■

Thus, minimisation of the energy expectation will lead to an approximate ground state energy greater than or equal to the exact ground state. Since minimisation over the entire Hilbert space is intractable, the variational principle method is to take a class of variational ansatz states $|\Psi(z)\rangle \in \mathcal{V}$ and minimise the (normalised) energy function

$$E(\overline{z}, z) = \frac{\langle \Psi(\overline{z}) | \hat{H} | \Psi(z) \rangle}{\langle \Psi(\overline{z}) | \Psi(z) \rangle}, \tag{2.3}$$

with respect to the adjustable parameters z. An optimal choice of variational parameters z_{op} is therefore characterised by the set of equations

$$\begin{aligned} \partial_i E\left(\overline{z}_{\text{op}}, z_{\text{op}}\right) = 0, \qquad & \partial_i^2 E\left(\overline{z}_{\text{op}}, z_{\text{op}}\right) \geq 0, \\ \partial_{\bar{i}} E\left(\overline{z}_{\text{op}}, z_{\text{op}}\right) = 0, \qquad & \partial_{\bar{i}}^2 E\left(\overline{z}_{\text{op}}, z_{\text{op}}\right) \geq 0. \end{aligned} \tag{2.4}$$

Since Theorem 1 applies to all arbitrary Ψ, including variational ansatz states, one can then conclude that the best approximation of the ground state of $\hat{H}$ is given by $|\Psi(z_{\text{op}})\rangle$. However, one must be careful when applying this result. The "best" approximation of a state is not well defined. There is no a priori guarantee that the ansatz state corresponding to the minima of the energy expectation value will have any resemblance to or produce the ground state exactly. Furthermore, an ansatz state may well give an energy close to the ground state energy but this does not imply that other physical quantities depending on the state will exhibit behaviour close to that of the true ground state. The success of the method is entirely dependent on the choice of the variational class and its ability to capture relevant physical effects present in the exact ground state. Verifying the accuracy of the obtained approximation relies on comparison to other known methods or experimental results.

The TIVP is not restricted to finding approximations of ground states of quantum Hamiltonians $\hat{H}$. It can also be used to estimate the low-lying excited states of a general quantum system. Given the ground state energy eigenfunction, or an approximation thereof, one can choose an ansatz state $|\Psi(z)\rangle$ which is orthogonal to this ground state energy eigenfunction to construct approximations of excited states. By taking the same basis set as above, i.e. $\{\Psi_n\}$ with $n = 0$ the ground state, we can expand the ansatz function in terms of the eigenfunctions $\Psi(z) = \sum_n c_n \Psi_n$. We note that, due to the orthogonality assumption $\langle \Psi(z) | \Psi_0 \rangle = 0$, we have $c_0 = 0$. We can then repeat the argument in Theorem (1) to show that

$$\langle \Psi(z) | H | \Psi(z) \rangle - E_1 \geq 0.$$

This method does, however, rely on $\Psi(z)$ being accurately orthogonal to Ψ_0. To modify $\Psi(z)$ in order to ensure orthogonality we can construct another trial function $\Psi_t = \Psi(z) - \langle\Psi(z)|\Psi_0\rangle\Psi_0$. Then $\langle\Psi_t|\Psi_0\rangle = \langle\Psi(z)|\Psi_0\rangle - \langle\Psi(z)|\Psi_0\rangle\langle\Psi_0|\Psi_0\rangle = 0$.

The Ritz method is such an approach for approximating eigenstates of a Hamiltonian $\hat{H}$. The Ritz ansatz function $\Psi(z)$ is a linear combination of N known basis functions Ψ_i, $i = 1, 2, \ldots N$ parameterised by unknown coefficients z^i

$$|\Psi(z)\rangle = z^i|\Psi_i\rangle.$$

The variational manifold is therefore an N-dimensional vector space spanned by the set $\{|\Psi_i\rangle, i = 1, 2, \ldots, N\}$. The energy function is then

$$E(\overline{z}, z) = \frac{\overline{z}^i H_{ij} z^j}{\overline{z}^i S_{ij} z^j}$$

where $H_{ij} = \langle\Psi_i|H|\Psi_j\rangle$ and we have assumed that the basis functions are not necessarily orthogonal, and so have defined the overlap matrix $S_{ij} = \langle\Psi_i|\Psi_j\rangle$. We can now apply either relation in equation (2.4). If we differentiate $E(\overline{z}, z)$ with respect to $\overline{z}^i$ and equate to zero we obtain the following

$$\frac{dE(\overline{z}, z)}{d\overline{z}_i} = \frac{\left(H_{ij} - E(\overline{z}, z)S_{ij}\right) z^j}{\overline{z}^i S_{ij} z^j} = 0$$

which leads to a set of N equations

$$\left(H_{ij} - E(\overline{z}, z)S_{ij}\right) z^j = 0$$

for $i = 1, 2, \ldots, N$. This is a homogenous set of linear equations with respect to the unknown variational parameters z^i with which we can determine $E(\overline{z}, z)$. The eigenvalues $E(\overline{z}, z)$ give variational estimates for the exact eigenvalues of $\hat{H}$, and the corresponding eigenvectors give estimates for the corresponding eigenstates of $\hat{H}$.

The variational principle is applicable to any variational manifold $\mathcal{V}$, but as previously mentioned the success of the method is dependent on the capability of $\mathcal{V}$ to capture the relevant physical effects present in the exact ground state, and also on the applicability of an efficient method to find the variational optimum. Given such a setting, that is a suitable manifold and efficient optimisation method, the variational method can be advantageous over other approaches. Examples of such alternative approaches highlighted in [Haegeman, 2011] include Monte-Carlo sampling, mean field theory (Hartree-Fock theory) [Hartree, 1928a, Hartree, 1928b, Slater, 1930], density functional theory [Hohenberg and Kohn, 1964, Kohn and Sham, 1965] and the density matrix renormalisation group (DMRG) [Östlund and Rommer, 1995, Rommer and Östlund, 1997, Verstraete et al., 2004].

2.3 The time-dependent variational principle

In the previous section we reviewed the time independent variational principle for finding approximations of the ground and excited states of a time-independent Hamiltonian $\hat{H}$ within a variational manifold $\mathcal{V}$. We now consider the time-dependent variational principle (TDVP) [Dirac, 1930, Langhoff et al., 1972]. The TDVP is a powerful method used to simulate dynamics according to a time-dependent Hamiltonian $\hat{H}$ of general quantum systems that are governed by the time-dependent Schrödinger equation (TDSE)

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle \tag{2.5}$$

which gives a linear first-order differential equation in $\mathcal{H}$. Suppose that we want to simulate a finite dimensional quantum system with Hilbert space $\mathcal{H} = \mathbb{C}^n$. The dimension n could be very large, essentially we can imagine it to be unbounded. If the state of the system at some time t is written as $|\Psi(t)\rangle$ it is simple enough to specify the solution to the TDSE, namely

$$\begin{aligned}|\Psi(t)\rangle &= \mathcal{T} e^{-\frac{i}{\hbar}\int_0^t dt' \hat{H}(t')}|\Psi(0)\rangle \\ &= \lim_{\epsilon\to 0} e^{-\frac{i}{\hbar}\int_{t-\epsilon}^t dt' \hat{H}(t')} e^{-\frac{i}{\hbar}\int_{t-2\epsilon}^{t-\epsilon} dt' \hat{H}(t')} \dots e^{-\frac{i}{\hbar}\int_0^{\epsilon} dt' \hat{H}(t')}|\Psi(0)\rangle\end{aligned}$$

for some initial state $|\Psi(0)\rangle$ and where $\mathcal{T}$ denotes the time ordering operator. However, if we want to actually evaluate this expression for large n this can be an excessively difficult task. One way to potentially simplify this problem is to specify the state in terms of a smaller number of parameters, $z(t) = (z_1(t), z_2(t), \dots)$, such that the state $|\Psi(t)\rangle \equiv |\Psi(z(t))\rangle$. The problem now becomes the following: the parameterisation may not capture the dynamics of the system perfectly. The parameterised states live in a submanifold of the Hilbert space, namely the variational manifold $\mathcal{V}$. We therefore have to consider how to integrate the Schrödinger equation whilst remaining within the variational manifold $\mathcal{V}$. This is the essence of the TDVP and in the following we describe three approaches to do this. We consider general variational manifolds $\mathcal{V}$, before applying the method to a specific manifold in subsequent chapters.

2.3.1 Principle of stationary action

The principle of stationary action is the basic variational principle of particle and continuum systems. The actual dynamical trajectories of a system are found by imagining all possible trajectories that the system could conceivably take, computing the action (which is a function of the trajectory), for each of these trajectories and selecting the one that makes the action

stationary. For a comprehensive introduction to the topic of calculus of variation as well as principle of stationary action we refer the reader to [Arnold et al., 1989]. At this point we present a condensed overview of the method.

The action S is defined as an integral along an actual or trial space-time trajectory $q(t)$ connecting two specified space-time events $A \equiv (t_A, q_A = q(t_A))$ and $B \equiv (t_B > t_A, q_B = q(t_B))$

$$S(q, \overline{q}) = \int_{t_A}^{t_B} L(q(t), \dot{q}(t), t) dt$$

where L is the Lagrangian. The principle of stationary action states that among all conceivable trajectories $q(t)$ that could connect the given points q_A and q_B in the given time $t_B - t_A$, the actual trajectories are those that make S stationary. Using standard calculus of variations techniques one can calculate the first-order variation in S corresponding to the small variation $\delta q(t)$ in the trial trajectory, namely δS. Setting this variation to zero one can thereby derive differential equations for the actual trajectory, called the Euler-Lagrange equations of motion [Arnold et al., 1989]

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = 0$$

where q_j is the jth component of q. The time-dependent Schrödinger equation can be derived by extremising an action functional $S(\Psi, \overline{\Psi}) = \int_{t_A}^{t_B} dt\, L(\Psi(t), \dot{\Psi}(t), t)$ with Lagrangian

$$L_{\mathcal{H}}(\Psi(t), \dot{\Psi}(t), t) = \frac{i}{2}\langle \Psi(t)|\dot{\Psi}(t)\rangle - \frac{i}{2}\langle \dot{\Psi}(t)|\Psi(t)\rangle - \langle \Psi(t)|H(t)|\Psi(t)\rangle. \tag{2.6}$$

Stationarity of the action under independent variations of $\langle \Psi(t)|$ and $|\Psi(t)\rangle$ in the full Hilbert space $\mathcal{H}$ yields the TDSE and its complex conjugate respectively. This is easy to see, since the partial derivatives of $L_{\mathcal{H}}$ are $\partial L/\partial \langle \dot{\Psi}(t)| = -i/2|\Psi(t)\rangle$ and $\partial L/\partial \langle \Psi(t)| = i/2|\dot{\Psi}(t)\rangle - H|\Psi(t)\rangle$ so that the Euler-Lagrange equation gives the TDSE $d/dt|\Psi(t)\rangle = -iH|\Psi(t)\rangle$.

However, we may wish to parameterise our state $|\Psi(t)\rangle \equiv |\Psi(z(t))\rangle$ and restrict ourselves to a subspace or manifold $\mathcal{V} \subset \mathcal{H}$. In this case, we can still use the calculus of variations to define a time evolution for $|\Psi(z(t))\rangle \in \mathcal{V}$. The Lagrangian is now written explicitly in terms of the variables $z(t)$ via an application of the chain rule

$$L_{\mathcal{V}}(z, \overline{z}) = \frac{i}{2}\left(\dot{z}^j \partial_j - \dot{\overline{z}}^{\overline{j}} \partial_{\overline{j}}\right)\langle \Psi(\overline{z})|\Psi(z)\rangle - \langle \Psi(\overline{z})|H|\Psi(z)\rangle \tag{2.7}$$

such that application of the principle of stationary action to S via the variational parameters z requires the use of the following Euler-Lagrange equations

$$\frac{d}{dt}\frac{\partial L_{\mathcal{V}}}{\partial \dot{z}^j} - \frac{\partial L_{\mathcal{V}}}{\partial z^j} = 0 \text{ and } \frac{d}{dt}\frac{\partial L_{\mathcal{V}}}{\partial \dot{\overline{z}}^j} - \frac{\partial L_{\mathcal{V}}}{\partial \overline{z}^j} = 0$$

which in turn give the following equations of motion in terms of z:

$$i\langle\partial_{\bar{i}}\Psi(\overline{z})|\partial_j\Psi(z)\rangle\dot{z}^j = \langle\partial_{\bar{i}}\Psi(\overline{z})|H|\Psi(z)\rangle \tag{2.8}$$

$$-i\dot{\overline{z}}^{\bar{j}}\langle\partial_{\bar{j}}\Psi(\overline{z})|\partial_i\Psi(z)\rangle = \langle\Psi(\overline{z})|H|\partial_i\Psi(z)\rangle \tag{2.9}$$

The hermitian matrix $G_{\bar{i}j}(\overline{z},z)$ is defined as

$$G_{\bar{i}j}(\overline{z},z) = \langle\partial_{\bar{i}}\Psi(\overline{z})|\partial_j\Psi(z)\rangle \tag{2.10}$$

and is the Gram matrix or overlap matrix containing the scalar product between any two tangent vectors of $\mathcal{V}$. The tangent vectors $|\partial_j\Psi(z)\rangle$ are linearly independent since they are assumed to form a basis of the tangent plane $\mathbb{T}_z\mathcal{V}$. We can therefore in turn assume invertibility of $G_{\bar{i}j}(\overline{z},z)$. We define the inverse of $G_{\bar{i}j}(\overline{z},z)$ as $G_{\bar{i}j}(\overline{z},z)^{-1} = G^{j\bar{i}}(\overline{z},z)$ such that $G^{j\bar{i}}(\overline{z},z)G_{\bar{i}k}(\overline{z},z) = \delta^j_k$. We can then rewrite the Euler-Lagrange equations as

$$i\dot{z}^j = G^{j\bar{i}}(\overline{z},z)\langle\partial_{\bar{i}}\Psi(\overline{z})|H|\Psi(z)\rangle \tag{2.11}$$

$$-i\dot{\overline{z}}^{\bar{j}} = G^{\bar{j}i}(\overline{z},z)\langle\Psi(\overline{z})|H|\partial_i\Psi(z)\rangle. \tag{2.12}$$

The TDVP thus approximates state evolution governed by the Schrödinger equation in the full Hilbert space $\mathcal{H}$ by state evolution restricted to the variational class $\mathcal{V}$ which is governed by a set of non-linear first order differential equations. An advantage of this approach is that the number of variational parameters can be much smaller than the dimension of $\mathcal{H}$, and so the differential equations are more easily dealt with, for example using numerical methods.

2.3.2 Gross Pitaevskii equation

The procedure described above is familiar in quantum field theory in the derivation of the mean-field equations of motion. A classic example that we now present is the derivation of the time-dependent Gross-Pitaevskii equation. This derivation is of particular interest since we encounter equations of this type in Chapter 6.

We consider a Hamiltonian $\hat{H}$ modelling a dilute gas of bosons in one-dimension in second quantisation (see appendix A)

$$\hat{H} = \int_{-\infty}^{\infty} dx\hat{\psi}^\dagger(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_{\text{ext}}(x)\right)\hat{\psi}(x) + \frac{g}{2}\int_{-\infty}^{\infty} dx\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x)$$

where $\hat{\psi}(x)$ and $\hat{\psi}^\dagger(x)$ are the bosonic field annihilation and creation operators, g the interaction strength and $V_{\text{ext}}(x)$ is some external potential. The corresponding Hilbert space is Fock space $\mathcal{F}$ with one-particle space given by $L^2(\mathbb{R})$.

We take as our variational class $\mathcal{V}$ the set of field coherent states. A field coherent state is obtained via a continuum limit of coherent states as follows. Consider a one-dimensional lattice $\mathcal{L}$ with N sites, each labelled by an integer $j = 1,2,\dots N$. The physical length of the system is $\ell = N\epsilon$ where ϵ is the lattice spacing. At each site j we can create and annihilate particles by acting with the creation and annihilation operators $\hat{a}_j$ and $\hat{a}_j^\dagger$ for a single harmonic oscillator that obey the canonical commutation relations

$$\left[\hat{a}_j^\dagger, \hat{a}_i\right] = \delta_{ji}. \tag{2.13}$$

With this in mind, we can view the system as a collection of N quantum harmonic oscillators arranged on the line $\mathcal{L}$. A coherent state $|\boldsymbol{\alpha}\rangle$ of the complete system is defined to be the state generated by operating with the unitary displacement operator $D(\boldsymbol{\alpha}) = \exp\left[\sum_{j=1}^N (\alpha_j \hat{a}_j^\dagger - \overline{\alpha}_j \hat{a}_j)\right]$ on the vacuum state:

$$|\boldsymbol{\alpha}\rangle = D(\boldsymbol{\alpha})|0\rangle^{\otimes N}, \tag{2.14}$$

where $\boldsymbol{\alpha} \in \mathbb{C}^N$. One important property is that the coherent state at site j is an eigenstate of the annihilation operator $\hat{a}_j$, satisfying

$$\hat{a}_j|\alpha_j\rangle = \alpha_j|\alpha_j\rangle, \qquad \alpha_j \in \mathbb{C}. \tag{2.15}$$

Furthermore, the overlap between a coherent state and a position eigenstate $|x\rangle$ is given by [Mandel and Wolf, 1995]

$$|\langle\alpha|x\rangle|^2 = \frac{1}{\sqrt{2\pi\gamma}} e^{-(x-\mu)^2/\gamma}, \tag{2.16}$$

where μ and γ are the mean position value and variance respectively. The field coherent state, which we shall denote by $|\phi\rangle$, is obtained via a continuum limit of the coherent states. As in section 4.2 of Chapter 4, we define rescaled annihilation and creation operators $\hat{\psi}_j = \frac{\hat{a}_j}{\sqrt{\epsilon}}$ that in the limit $\epsilon \to 0$ will become field operators $\hat{\psi}(x)$. We then define the quantum field displacement operator as

$$D\left(\hat{\psi}(x), \phi(x)\right) = e^{\int_{-\ell/2}^{\ell/2} dx \phi(x)\hat{\psi}^\dagger(x) - \overline{\phi}(x)\hat{\psi}(x)}$$

where $\phi(x) \in \mathbb{C}$. Analogously to (2.14), the field displacement operator can be used to define the field coherent state via

$$|\phi(x,t)\rangle = D\left(\hat{\psi}(x), \phi(x)\right)|\Omega\rangle \tag{2.17}$$

with $|\Omega\rangle$ the field vacuum state. Analogous to (2.15), a field coherent state satisfies

$$\hat{\psi}(x)|\phi(x,t)\rangle = \phi(x)|\phi(x,t)\rangle. \tag{2.18}$$

Our variational class is therefore given by

$$\mathcal{V} = \left\{ |\phi(x,t)\rangle \,\middle|\, |\phi(x,t)\rangle = D\left(\psi\hat{(}x), \phi(x)\right)|\Omega\rangle, \phi(x) : \mathbb{R}^2 \to \mathbb{C} \right\}.$$

Recall from equation (2.7) that the Lagrangian for the TDSE is given by

$$\begin{aligned} L\left(\overline{\phi}(x,t), \phi(x,t), x, t, \right) = \frac{i}{2}\langle\phi(x,t)|\partial_t\phi(x,t)\rangle - \frac{i}{2}\langle\partial_t\phi(x,t)|\phi(x,t)\rangle \\ - \langle\phi(x,t)|\hat{H}(t)|\phi(x,t)\rangle, \end{aligned} \tag{2.19}$$

from which we will obtain the Gross-Pitaevskii equation using the Euler-Lagrange equations. The first two terms of equation (2.19) can be written

$$\begin{aligned} \frac{i}{2}\langle\phi(x,t)|\partial_t\phi(x,t)\rangle &= \frac{i}{2}\int dx\,\overline{\phi}(x,t)\partial_t\phi(x,t) \\ \frac{i}{2}\langle\partial_t\phi(x,t)|\phi(x,t)\rangle &= \frac{i}{2}\int dx\,\partial_t\overline{\phi}(x,t)\phi(x,t) \end{aligned}$$

using properties of the field coherent states, such as (2.17) and (2.18), and the relation $\frac{d}{dt}e^A = \int_0^1 e^{sA}\frac{d}{dt}Ae^{(1-s)A}ds$ for exponential operators. To evaluate the last term we use linearity of the expectation value $\langle\phi(x,t)|\hat{H}|\phi(x,t)\rangle$ and calculate the interaction, kinetic and potential parts of the Hamiltonian $\hat{H}$ separately. For the interaction term we use the eigenvalue equation (2.18) and write

$$\begin{aligned} &\langle\phi(x,t)|\int_{-\infty}^{\infty} dx\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x)|\phi(x,t)\rangle \\ &= \int_{-\infty}^{\infty} dx\langle\phi(x,t)|\overline{\phi}(x,t)\overline{\phi}(x,t)\phi(x,t)\phi(x,t)|\phi(x,t)\rangle = \int_{-\infty}^{\infty} dx|\phi(x,t)|^4. \end{aligned}$$

The potential term is similarly evaluated. We have

$$\begin{aligned} \langle\phi(x,t)|\int_{-\infty}^{\infty} dx\hat{\psi}^\dagger(x)V_{\text{ext}}(x)\hat{\psi}(x)|\phi(x,t)\rangle &= \int_{-\infty}^{\infty} dx\langle\phi(x,t)|\overline{\phi}(x,t)V_{\text{ext}}(x)\phi(x,t)|\phi(x,t)\rangle \\ &= \int_{-\infty}^{\infty} dx\,V_{\text{ext}}(x)|\phi(x,t)|^2. \end{aligned}$$

For the kinetic part of the Hamiltonian we also use the eigenvalue equation (2.18), which we can differentiate with respect to x and therefore obtain

$$\begin{aligned} \langle\phi(x,t)|\int_{-\infty}^{\infty} dx\hat{\psi}^\dagger(x)\frac{d}{dx^2}\hat{\psi}(x)|\phi(x,t)\rangle &\equiv -\langle\phi(x,t)|\int_{-\infty}^{\infty} dx\frac{d\hat{\psi}^\dagger(x)}{dx}\frac{d\hat{\psi}(x)}{dx}|\phi(x,t)\rangle \\ &= -\int_{-\infty}^{\infty} dx\frac{d\overline{\phi}(x,t)}{dx}\frac{d\phi(x,t)}{dx} \end{aligned}$$

The Lagrangian therefore can be written

$$L\left(\overline{\phi}(x,t),\phi(x,t),x,t\right)=\int dx\left(\frac{i}{2}\overline{\phi}(x,t)\partial_t\phi(x,t)-\frac{i}{2}\partial_t\overline{\phi}(x,t)\phi(x,t)\right.$$
$$\left.+\frac{\hbar^2}{2m}\frac{d\overline{\phi}(x,t)}{dx}\frac{d\phi(x,t)}{dx}+V_{\text{ext}}(x)|\phi(x,t)|^2+\frac{g}{2}|\phi(x,t)|^4\right)$$

To apply the TDVP we need to extremise $S=\int dt\int dx\mathcal{L}$ where the Lagrangian density $\mathcal{L}$ is given by

$$\mathcal{L}=\frac{i}{2}\overline{\phi}(x,t)\partial_t\phi(x,t)-\frac{i}{2}\partial_t\overline{\phi}(x,t)\phi(x,t)+\frac{\hbar^2}{2m}\frac{d\overline{\phi}(x,t)}{dx}\frac{d\phi(x,t)}{dx}$$
$$+V_{\text{ext}}(x)|\phi(x,t)|^2+\frac{g}{2}|\phi(x,t)|^4.$$

The corresponding Euler-Lagrange equations are

$$-\frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\left[\partial_t\overline{\phi}\right]}-\frac{d}{dx}\frac{\partial\mathcal{L}}{\partial\left[\partial_x\overline{\phi}\right]}+\frac{\partial\mathcal{L}}{\partial\overline{\phi}}=0$$

and lead us to the (time-dependent) Gross Pitaevskii equation

$$i\hbar\frac{\partial}{\partial t}\phi(x,t)=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V_{\text{ext}}(x)+g|\phi(x,t)|^2\right)\phi(x,t). \tag{2.20}$$

2.3.3 Geometric construction

The equations of motion (2.11) and (2.12) derived by means of the principle of stationary action can also be obtained from a geometric construction. We present this in order to provide a clear and graphical description of the approximation resulting from the TDVP.

The parameterisation of the state $|\Psi\rangle$ will not necessarily capture the time evolution according to the TDSE exactly. If it were to, the state would of course satisfy the TDSE, and we could write

$$\frac{d}{dt}|\Psi(z(t))\rangle=\dot{z}^j(t)|\partial_j\Psi(z(t))\rangle=-i\hat{H}(t)|\Psi(z(t))\rangle. \tag{2.21}$$

However, the right hand side of this equation is some general vector in the total Hilbert space $\mathcal{H}$ whereas the central side is a vector in the tangent space $\mathbb{T}_{z(t)}\mathcal{V}$ to the variational manifold $\mathcal{V}$ at the point $|\Psi(z(t)\rangle$. This tangent space is defined as

$$\mathbb{T}_{z(t)}\mathcal{V}=\text{span}\left\{|\partial_j\Psi(z))\rangle,\forall j\right\},$$

where a general tangent vector $|\Phi(z(t),c))\rangle\in\mathbb{T}_{z(t)}\mathcal{V}$ is given by

$$|\Phi(z,c))\rangle=c^j|\partial_j\Psi(z))\rangle$$

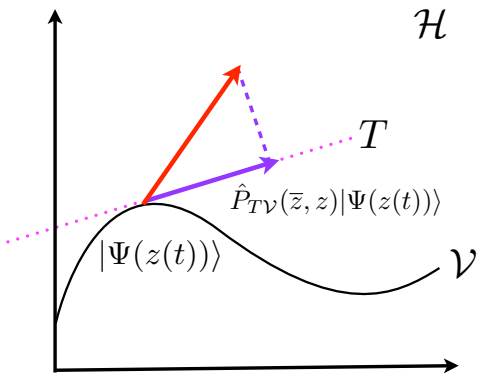

Figure 2.1: An illustration of the TDVP. The variational class $\mathcal{V}$ is shown with tangent plane (pink dashes) at the point $|\Psi(z(t))\rangle$. The exact dynamics leaves the variational class and is depicted by the evolution vector $\hat{H}|\Psi(z(t))\rangle$ (red arrow), whilst the evolution according to the TDVP follows the projected vector $\hat{P}_{T\mathcal{V}}(\overline{z},z)|\Psi(z(t))\rangle$ (purple arrow).

with $c=\left(c^1,c^2,\ldots\right)$, $c^j\in\mathbb{C}$. Since the tangent plane $\mathbb{T}_{z(t)}\mathcal{V}$ itself is embedded in the Hilbert space, the best approximation of the right hand side of equation (2.21) that lies within $\mathbb{T}_{z(t)}\mathcal{V}$ is found by performing an orthogonal projection onto it. We can project it onto any of the vectors $|\partial_j\Psi(z(t))\rangle$ and ignore any components of the right hand side that are orthogonal to the tangent plane. We can define a projector $\hat{P}_{\mathbb{T}\mathcal{V}}(\overline{z},z)$ as

$$\hat{P}_{\mathbb{T}\mathcal{V}}(\overline{z},z)=|\partial_j\Psi(z(t))\rangle G^{j,\overline{i}}(\overline{z},z)\langle\partial_{\overline{i}}\Psi(z(t))|$$

where the inverse of the Gram matrix of tangent vectors as given by (2.10) appears in order that $\hat{P}^2_{\mathbb{T}\mathcal{V}}(\overline{z},z)=\hat{P}_{\mathbb{T}\mathcal{V}}(\overline{z},z)$. Using this definition we can write that

$$\dot{z}^j(t)=-iG^{j\overline{i}}(\overline{z},z)\langle\partial_{\overline{i}}\Psi(z(t))|H|\Psi(z(t))\rangle \tag{2.22}$$

which is the same as the equation of motion (2.11) determined by the stationary action approximation. In a similar way we obtain the corresponding equation of motion for $\dot{\overline{z}}^{\overline{j}}(t)$, as in equation (2.27). In Fig. 2.1 we illustrate the TDVP procedure of projecting the exact evolution of a state onto the tangent plane of the variational class. The error between the exact evolution given by the Schrödinger equation and the evolution according to the TDVP, obtained by projecting onto the tangent plane $\hat{P}_{\mathbb{T}\mathcal{V}}(\overline{z},z)$, incurred in each step of the TDVP can, in principle, be quantified and subsequently used to assess the accuracy of the approximated evolution, see [Haegeman, 2011].

2.3.4 Intuitive construction

Our third approach for obtaining an approximate solution to the TDSE whilst remaining within the variational manifold $\mathcal{V}$ is arguably the most intuitive one. We have already emphasised that if the time evolution of the quantum system could be exactly simulated within $\mathcal{V}$, our parameterised state $|\Psi(z(t)\rangle$ would need to satisfy the TDSE equation as given in equation (2.21). The intuitive approach now is based on using the standard norm defined in $\mathcal{H}$ and approximate the actual evolution $-i\hat{H}(t)|\Psi(z(t))\rangle$ by the tangent vector $\frac{d}{dt}|\Psi(z(t))\rangle$ where the optimal solution is given by

$$\dot{z}_{\text{op}}(t) = \arg\min_{\dot{z}(t)} \left| \frac{d}{dt}|\Psi(z(t))\rangle + i\hat{H}(t)|\Psi(z(t))\rangle \right|^2, \tag{2.23}$$

that is simply minimise the difference between the rate of change $\frac{d}{dt}|\Psi(z(t))\rangle$ in our parameterised state to the actual evolution rate. By determining this optimum set of parameters we obtain the coefficients $c(t) \equiv \dot{z}_{\text{op}}(t)$ of the tangent vector $|\Phi(z,c)\rangle$ that will in turn enable us to calculate the time evolved state. To find $\dot{z}_{\text{op}}(t)$ we take the right hand side of equation (2.23) as our objective function

$$f(\dot{z}(t)) = \left| \dot{z}^j(t)|\partial_j\Psi(z(t))\rangle + i\hat{H}|\Psi(z(t))\rangle \right|^2 \tag{2.24}$$

and minimise with respect to $\dot{z}(t)$. We first expand this norm and obtain

$$\begin{aligned} f(\dot{z}(t)) = {} & \dot{\bar{z}}^{\bar{j}}(t)\dot{z}^k(t)\langle\partial_{\bar{j}}\Psi(z)|\partial_k\Psi(z)\rangle + i\dot{\bar{z}}^{\bar{j}}(t)\langle\partial_{\bar{j}}\Psi(z)|\hat{H}(t)|\Psi(z)\rangle \\ & - i\dot{z}^j(t)\langle\Psi(z)|\hat{H}(t)|\partial_j\Psi(z)\rangle + \langle\Psi(z)|\hat{H}^2(t)|\Psi(z)\rangle \end{aligned} \tag{2.25}$$

where the last term can be viewed as a constant, since it has no dependence on $\dot{z}(t)$. We now define the vector $L(\overline{z},z)$ component-wise as

$$L_{\bar{j}}(\overline{z},z) = \langle\partial_{\bar{j}}\Psi(z(t))|\hat{H}(t)|\Psi(z(t))\rangle \tag{2.26}$$

and recall from equation (2.10) that the Gram matrix $G(\overline{z},z)$ is defined as

$$G_{\bar{j}k}(\overline{z},z) = \langle\partial_{\bar{j}}\Psi(\overline{z})|\partial_k\Psi(z)\rangle. \tag{2.27}$$

We can then write our objective function f concisely as

$$f(\dot{z}(t)) = \dot{\bar{z}}^{\bar{j}}(t)\dot{z}^k(t)G_{\bar{j}k}(\overline{z},z) + i\dot{\bar{z}}^{\bar{j}}(t)L_{\bar{j}}(\overline{z},z) - i\dot{z}^j(t)L_j(\overline{z},z) + \text{const.}$$

To minimise f we simply differentiate with respect to $\dot{z}^j(t)$ and $\dot{\bar{z}}^{\bar{j}}(t)$ and set the results to zero. Differentiation with respect to $\dot{\bar{z}}^{\bar{j}}(t)$ shows that the minimum occurs when the following system of equations hold

$$\dot{z}^k(t)G_{\bar{j}k}(\overline{z},z) + iL_{\bar{j}}(\overline{z},z) = 0$$

As before, assuming that $G_{\bar{j}k}(\overline{z},z)$ is invertible we therefore have

$$\dot{z}^k(t) = -iG^{k\bar{j}}(\overline{z},z)L_{\bar{j}}(\overline{z},z). \tag{2.28}$$

Differentiating the objective function with respect to $\dot{z}^j(t)$ yields the corresponding equation of motion for $\dot{\overline{z}}^{\overline{k}}(t)$. As expected, we have obtained the same equations of motion as in the stationary action approximation (2.11) and (2.12) as well as the geometric construction (2.22). Generally, in subsequent applications of the TDVP in the remainder of this thesis we shall refer to equation (2.28) when approximating Schrödinger time evolution.

2.3.5 Norm Preserving dynamics

The previous subsections have introduced the general concept of the TDVP along with derivations of the equations of motion for the corresponding state parameterisation. However, so far the important property of norm preservation has not been considered. The Hamiltonian evolution in $\mathcal{H}$ is unitary and thus norm-preserving, but this is no longer guaranteed for the evolution governed by the Euler-Lagrange equations (2.22). In order to ensure norm preservation we apply the principle of stationary action to the modified Lagrangian

$$\tilde{L}_{\mathcal{H}}(\Psi(t),\overline{\Psi}(t),t) = \frac{L_{\mathcal{H}}(\Psi(t),\overline{\Psi}(t),t)}{\langle\Psi(t)|\Psi(t)\rangle}.$$

For a state parameterised via $z(t)$, this can be written as

$$\tilde{L}_{\mathcal{V}}(\Psi(z),\overline{\Psi}(z),z) = \frac{i}{2}\left(\dot{z}(t)\partial_j - \overline{z}(t)\partial_{\bar{j}}\right)\ln N(z(t),\overline{z}(t)) - H(z(t),\overline{z}(t))$$

where

$$N(z(t),\overline{z}(t)) = \langle\Psi(\overline{z}(t))|\Psi(z(t))\rangle, \qquad H(z(t),\overline{z}(t)) = \frac{\langle\Psi(\overline{z}(t))|\hat{H}|\Psi(z(t))\rangle}{\langle\Psi(\overline{z}(t))|\Psi(z(t))\rangle}$$

Proceeding in the same way as before, we can use this Lagrangian $\tilde{L}_{\mathcal{V}}$ to define a modified action $\tilde{S}_{\mathcal{V}}$ with which the modified Euler-Lagrange equations

$$i\tilde{G}_{\bar{i},j}(\overline{z}(t),z(t))\dot{z}^j(t) = \partial_{\bar{i}}H(z,\overline{z}), \tag{2.29}$$

$$-i\dot{\overline{z}}^{\bar{j}}(t)\tilde{G}_{\bar{j},i}(\overline{z}(t),z(t)) = \partial_i H(z,\overline{z}). \tag{2.30}$$

are obtained. Here we have introduced the modified Gram matrix

$$\tilde{G}_{\bar{i},j}(\overline{z}(t),z(t)) = \partial_{\bar{i}}\partial_j \ln N(\overline{z}(t),z(t)) = \frac{G_{\bar{i},j}(\overline{z},z)}{N(\overline{z}(t),z(t))} - \frac{\langle\partial_{\bar{i}}\Psi(\overline{z})|\Psi(z)\rangle\langle\Psi(\overline{z})|\partial_j\Psi(z)\rangle}{N(\overline{z}(t),z(t))^2} \tag{2.31}$$

and the gradients of the normalised expectation value

$$\partial_{\bar{i}} H(z,\overline{z}) = \frac{\langle \partial_{\bar{i}}\Psi(\overline{z})|\hat{H}|\Psi(z)\rangle}{N(\overline{z}(t),z(t))} - \frac{\langle \partial_{\bar{i}}\Psi(\overline{z})|\Psi(z)\rangle\langle\Psi(\overline{z})|\hat{H}|\Psi(z)\rangle}{N(\overline{z}(t),z(t))^2} \tag{2.32}$$

$$\partial_{i} H(z,\overline{z}) = \frac{\langle \Psi(\overline{z})|\hat{H}|\partial_{i}\Psi(z)\rangle}{N(\overline{z}(t),z(t))} - \frac{\langle \Psi(\overline{z})|\partial_{i}\Psi(z)\rangle\langle\Psi(\overline{z})|\hat{H}|\Psi(z)\rangle}{N(\overline{z}(t),z(t))^2}. \tag{2.33}$$

It is interesting to note the difference between the modified quantities (2.31), (2.32) and (2.33) that ensure norm preservation of the state evolution and the original ones in (2.27) and (2.26). Under an infinitesimal variation, the norm of a state $|\Psi\rangle$ changes if we move in the direction of the $|\Psi\rangle$. Therefore, to obtain norm-conservation we simply subtract from every tangent vector $|\partial_{\bar{i}}\Psi\rangle$ its component along $|\Psi\rangle$. This is precisely what the second terms in the above equations do. By defining the projector

$$\hat{P}_0(\overline{z},z) = \hat{\mathbb{I}} - \frac{|\Psi(z)\rangle\langle\Psi(\overline{z})|}{\langle\Psi(\overline{z})|\Psi(z)\rangle}$$

we can write the modified Gram matrix and gradients concisely as

$$\tilde{G}_{\bar{i},j}(\overline{z},z) = \frac{\langle \partial_{\bar{i}}\Psi(\overline{z})|\hat{P}_0(\overline{z},z)|\partial_j\Psi(z)\rangle}{N(\overline{z},z)} \tag{2.34}$$

and

$$\partial_{\bar{i}} H(z,\overline{z}) = \frac{\langle \partial_{\bar{i}}\Psi(\overline{z})|\hat{P}_0(\overline{z},z)\hat{H}|\Psi(z)\rangle}{N(\overline{z},z)} \tag{2.35}$$

$$\partial_{i} H(z,\overline{z}) = \frac{\langle \Psi(\overline{z})|\hat{H}\hat{P}_0(\overline{z},z)|\partial_i\Psi(z)\rangle}{N(\overline{z},z)} \tag{2.36}$$

Written in this form, these equations have a nice interpretation as encoding projection onto the space orthogonal to $|\Psi\rangle$.

In previous calculations we assumed at this point that the gram matrix $G_{\bar{i},j}(\overline{z},z)$ was invertible, in order to obtain an explicit equation of motion for $\dot{z}(t)$. For $\tilde{G}_{\bar{i},j}(\overline{z},z)$ we cannot necessarily make the same assumption- the presence of the second term in equation (2.31) means that $\tilde{G}_{\bar{i},j}(\overline{z},z)$ may not have full rank. In fact, as we will see shortly, $\tilde{G}_{\bar{i},j}(\overline{z},z)$ does indeed have a zero eigenvalue. To assume invertibility of the modified gram matrix we would have to ensure that the second term is zero, that is require $\langle \partial_{\bar{i}}\Psi(\overline{z})|\Psi(z)\rangle = 0$. Then, $\tilde{G}_{\bar{i},j}(\overline{z},z) = N(\overline{z},z)^{-1}G_{\bar{i},j}(\overline{z},z)$ so that $\tilde{G}_{\bar{i},j}(\overline{z},z)$ has the same rank as $G_{\bar{i},j}(\overline{z},z)$ and is thus invertible. In addition, we would have that $\partial_{\bar{i}}H(\overline{z},z) = N(\overline{z},z)^{-1}\langle\partial_{\bar{i}}\Psi(\overline{z})|\hat{H}|\Psi(z)\rangle$. The Euler-Lagrange equations following from $S_{\mathcal{V}}$ or $\tilde{S}_{\mathcal{V}}$ would then be identical.

Suppose now that $\langle \partial_{\bar{i}}\Psi(\overline{z})|\Psi(z)\rangle \neq 0$ so that we must consider the full expression for $\tilde{G}_{\bar{i},j}(\overline{z},z)$. The manifold $\mathcal{V}$ therefore allows for norm and phase variation of states and, since $|\Psi(z)\rangle \in \mathbb{T}_z\mathcal{V}$, we are able to define a contravariant vector $\Psi^i(z)$ such that

$|\Psi(z)\rangle = \Psi^i(z)|\partial_i\Psi(z)\rangle$. By definition of $\hat{P}_0(\overline{z},z)$ we notice that $\hat{P}_0(\overline{z},z)\Psi^i(z)|\partial_i\Psi(z)\rangle = \hat{P}_0(\overline{z},z)|\Psi(z)\rangle = 0$. Therefore we learn that $\tilde{G}_{\overline{j},i}(\overline{z},z)$ has a zero eigenvalue with corresponding eigenvector $\Psi^i(z)$, since

$$\tilde{G}_{\overline{j},i}(\overline{z},z)\Psi^i(z) = \frac{\langle\partial_{\overline{j}}\Psi(z)|\hat{P}_0(\overline{z},z)\Psi^i(z)|\partial_i\Psi(z)\rangle}{N(\overline{z},z)} = 0 = \overline{\Psi}^{\overline{j}}(z)\tilde{G}_{\overline{j},i}(\overline{z},z)$$

Since $\tilde{G}_{\overline{j},i}(\overline{z},z)$ is not invertible we therefore seek to define a pseudo-inverse of $\tilde{G}_{\overline{j},i}(\overline{z},z)$ in order to obtain an explicit equation of motion for $\dot{z}(t)$. We define a covariant vector $\Psi_{\overline{i}}(\overline{z},z)$ by multiplying the original gram matrix $G_{\overline{i},j}(\overline{z},z)$ by the contravariant vector $\Psi^j(z)$, that is $\Psi_{\overline{i}}(\overline{z},z) = G_{\overline{i},j}(\overline{z},z)\Psi^j(z) = \langle\partial_{\overline{i}}\Psi(\overline{z})|\partial_j\Psi(z)\rangle\Psi^j(z) = \langle\partial_{\overline{i}}\Psi(\overline{z})|\Psi(z)\rangle$. We then have that $\overline{\Psi_i}(\overline{z},z)\Psi^i(z) = \langle\Psi(\overline{z})|\Psi(z)\rangle = N(\overline{z},z)$. With these definitions, we can write

$$\tilde{G}_{\overline{i},j}(\overline{z},z) = \frac{G_{\overline{i},j}(\overline{z},z)}{N(\overline{z},z)} - \frac{\Psi_{\overline{i}}(\overline{z},z)\overline{\Psi}_j(\overline{z},z)}{N(\overline{z},z)^2}$$

We then define the pseudo-inverse as

$$\tilde{G}^{i,\overline{j}}(\overline{z},z) = N(\overline{z},z)G^{i,\overline{j}}(\overline{z},z) - \Psi^i(z)\overline{\Psi}^{\overline{j}}(\overline{z})$$

such that

$$\tilde{G}^{i,\overline{j}}(\overline{z},z)\tilde{G}_{\overline{j},k}(\overline{z},z) = \delta^i_k - \frac{\Psi^i(z)\overline{\Psi}_k(\overline{z},z)}{N(\overline{z},z)}, \tag{2.37}$$

$$\tilde{G}_{\overline{i},j}(\overline{z},z)\tilde{G}^{j,\overline{k}}(\overline{z},z) = \delta^{\overline{k}}_{\overline{i}} - \frac{\Psi_{\overline{i}}(\overline{z},z)\overline{\Psi}^{\overline{k}}(z)}{N(\overline{z},z)}. \tag{2.38}$$

We now apply this pseudo-inverse to the modified Euler-Lagrange equation (2.29). Since we can rewrite $\partial_{\overline{i}}H(\overline{z},z)$ as

$$\begin{aligned}\partial_{\overline{i}}H(\overline{z},z) &= N(\overline{z},z)^{-1}\left(\delta^{\overline{k}}_{\overline{i}} - N(\overline{z},z)^{-1}\Psi_{\overline{i}}(\overline{z},z)\overline{\Psi}^{\overline{k}}(z)\right)\langle\partial_{\overline{k}}\Psi(\overline{z})|\hat{H}|\Psi(z)\rangle \\ &= N(\overline{z},z)^{-1}\tilde{G}_{\overline{i},j}(\overline{z},z)\tilde{G}^{j,\overline{k}}(\overline{z},z)\langle\partial_{\overline{k}}\Psi(\overline{z})|\hat{H}|\Psi(z)\rangle\end{aligned}$$

we have that

$$\begin{aligned}&i\tilde{G}^{l,\overline{i}}(\overline{z},z)\tilde{G}_{\overline{i},j}(\overline{z}(t),z(t))\dot{z}^j(t) = N(\overline{z},z)^{-1}\tilde{G}^{l,\overline{i}}(\overline{z},z)\tilde{G}_{\overline{i},j}(\overline{z},z)\tilde{G}^{j,\overline{k}}(\overline{z},z)\langle\partial_{\overline{k}}\Psi(\overline{z})|\hat{H}|\Psi(z)\rangle \\ &\overset{(2.37)}{\Leftrightarrow} i\left(\delta^l_j - \frac{\Psi^l(z)\overline{\Psi}_j(z)}{N(\overline{z},z)}\right)\dot{z}^j(t) = N(\overline{z},z)^{-1}\left(\delta^l_j - \frac{\Psi^l(z)\overline{\Psi}_j(z)}{N(\overline{z},z)}\right)\tilde{G}^{j,\overline{k}}(\overline{z},z)\langle\partial_{\overline{k}}\Psi(\overline{z})|\hat{H}|\Psi(z)\rangle.\end{aligned}$$

A similar expression is found when considering equation (2.30). The particular form of this equation will give only $\dim(\tilde{G}) - 1$ equations to determine $z(t)$, where the zero eigenspace solution can be chosen freely. Therefore to obtain $\dim(\tilde{G})$ equations we fix

$\overline{\Psi}_i \dot{z}^i(t) = \langle\Psi(\overline{z})|\partial_i\Psi(z)\rangle\dot{z}^i(t) = 0$ and $\dot{\overline{z}}^{\overline{i}}(t)\Psi_{\overline{i}} = \dot{\overline{z}}^{\overline{i}}(t)\langle\partial_{\overline{i}}\Psi(\overline{z})|\Psi(z)\rangle = 0$. These are the required conditions for norm conservation since then

$$\frac{d}{dt}\langle\Psi(\overline{z})|\Psi(z)\rangle = \langle\Psi(\overline{z})|\partial_i\Psi(z)\rangle\dot{z}^i(t) + \dot{\overline{z}}^{\overline{i}}(t)\langle\partial_{\overline{i}}\Psi(\overline{z})|\Psi(z)\rangle = 0.$$

With this condition satisfied, we can therefore write the modified, norm-preserving Euler-Lagrange equations as

$$i\dot{z}^j(t) = \tilde{G}^{j,\overline{i}}(\overline{z}(t), z(t))\partial_{\overline{i}}H(z,\overline{z}), \tag{2.39}$$

$$-i\dot{\overline{z}}^{\overline{j}}(t) = \tilde{G}^{\overline{j},i}(\overline{z}(t), z(t))\partial_i H(z,\overline{z}). \tag{2.40}$$

2.3.6 Imaginary time evolution

All approaches described in this section so far result in equations of motion for real time evolution. The same equations can be used to simulate imaginary time evolution by setting $t = -i\tau$, which also provides a way of obtaining ground states. Before we present the altered equations according to imaginary time evolution and how we use these to simulate the state evolution, we briefly remind the reader of the general idea of imaginary time evolution. Assume for now that we have access to the full Hilbert space $\mathcal{H}$. Imaginary time evolution then provides an extremely stable way of finding the ground state of a system. Suppose that we start with some arbitrary initial state $|\Psi(0)\rangle$. Evolution in imaginary time leads to

$$|\Psi(\tau)\rangle = N(\tau)e^{-\tau\hat{H}}|\Psi(0)\rangle = N(\tau)\sum_n e^{-\lambda_n\tau}|\phi_n\rangle\langle\phi_n|\Psi(0)\rangle. \tag{2.41}$$

where $|\phi_n\rangle$ and λ_n are the eigenstates and eigenvalues of the Hamiltonian $\hat{H}$ respectively and $N(\tau)$ is a normalisation factor necessary for convergence. Therefore, as long as the ground state is not degenerate and the time is longer than the inverse gap between ground and excited state, the state $|\Psi(\tau)\rangle$ will converge exponentially fast to the ground state (given that the initial state was not orthogonal to the ground state). That the convergence speed crucially depends on the gap size is also to be expected, since it becomes more difficult to discriminate excited states with small energy from the ground state.

We now return to the equations of motion derived in the previous sections. The TDVP produces a non-linear set of coupled differential equations and thus requires a numerical integration scheme with a discretised time step dt. This discretisation introduces errors into the simulated evolution, but can be controlled [Haegeman, 2011]. For imaginary time evolution, application of the simple first-order Euler method is sufficient. Although the Euler method can introduce large second-order truncation errors, this is not problematic

when performing imaginary time evolution due to the stability and self-correcting properties described above. The rate of change of the energy expectation value for imaginary time evolution is given by

$$\frac{d}{d\tau}\left(\frac{\langle\Psi(\overline{z})|\hat{H}|\Psi(z)\rangle}{\langle\Psi(\overline{z})|\Psi(z)\rangle}\right) = -2\partial_i H(\overline{z},z)\tilde{G}^{i\overline{j}}(\overline{z},z)\partial_{\overline{j}}H(\overline{z},z) \leq 0 \tag{2.42}$$

and thus decreases monotonically until a minimum is reached. If the energy expectation value on the variational manifold $\mathcal{V}$ has many local minima, there is no guarantee that the equations of motion will converge towards the approximation of the exact ground state, namely the global minimum. However, if the variational manifold is able to capture the full imaginary time evolution in the total Hilbert space $\mathcal{H}$ one can safely assume that convergence to the global minimum will be achieved.

When implementing imaginary time evolution, we perform the following simple procedure to integrate forward in imaginary time from τ to $\tau+\epsilon$. Given an initial parameterisation $z(\tau)$ of the state $|\Psi(z)\rangle$ we compute the adapted gram matrix $G_{\overline{j}k}(\overline{z},z)$ as defined in equation (2.27), along with its inverse $G^{k,\overline{j}}(\overline{z},z)$, followed by the modified matrix $L_{\overline{j}}(\overline{z},z)$ as defined in equation (2.26). Insertion into the equation of motion (2.28) for imaginary time then allows us to determine $\dot{z}(\tau)$. Given the variational parameters along with their time derivatives at time τ, we then use the forward finite difference formula to approximate the time-evolved parameters $z(\tau+\epsilon)$ via

$$z(\tau+\epsilon) \approx z(\tau) + \epsilon\frac{dz(\tau)}{d\tau} = z(\tau) + \epsilon\underline{\underline{G}}^{-1}\underline{L}.$$

Iteration of this process allows one to integrate further ahead in time, where the value of z is overwritten after every step.

We note that imaginary time evolution can also be used to find approximations of excited states of a quantum system. The method then relies on choosing an ansatz state orthogonal to the approximate ground state and all lower excited states, much like the method described in section 2.2 for the time-independent variational principle.

Chapter 3

Quantum Optics Preliminaries

In Chapter 5 we describe an algorithm for simulating the ground state physics of a one-dimensional interacting quantum field using the output of a cavity quantum electrodynamic (cavity QED) apparatus. The apparatus consists of a driven cavity emitting a stationary output beam, on which measurements are performed in order to obtain various correlation functions. This chapter therefore introduces some fundamental concepts in the field of quantum optics and cavity quantum electrodynamics that are necessary in order to understand the presented simulation algorithm.

This chapter is organised as follows. The type of cavity QED apparatus we consider in Chapter 5 is that of an atom trapped in a cavity. To understand the dynamics of such a system, it is paramount to review the basic mechanisms of the interaction between the electromagnetic field and atoms, which will be the aim of the first three sections. In section 3.1 we recall the quantisation of the classical electromagnetic field. We then consider the interaction between an atom and quantised light in section 3.2, assuming suitable approximations such as treating the atom as a two-level system. In section 3.3 we then derive the so called Jaynes-Cummings Hamiltonian [Jaynes and Cummings, 1963] that describes the interaction between a two-level atom and one mode of the electromagnetic field. We do this explicitly, since the Jaynes-Cummings Hamiltonian will serve as a particular example in our future proposal. There are several extensions of the Jaynes-Cummings model, including the addition of an external driving field that leads to atom excitation and the inevitable effect of cavity decay, and we treat these processes in the same section. Thereafter in section 3.4 we present an overview of coupled mode theory and the input-output formalism for cavities, which is most important since the output field of a cavity-QED device is central to the scheme proposed in Chapter 5. Finally in section 3.5 we introduce the concept of Glauber correlation functions, the measurement of which is directly connected to determining the energy density of the quantum field we wish to simulate in Chapter 5.

The theory presented in this chapter is well known in quantum optics and can be found in most textbooks on this topic. We include it to make the thesis more self contained and to

highlight the particular concepts needed for the understanding of later chapters. We closely follow [Steck, 2011, Walls and Milburn, 1995].

3.1 Quantisation of the electromagnetic field

Our starting point is Maxwell's equations of classical electromagnetism in free-space. We postpone their more general formulation in the presence of sources to the study of the interaction between an atom and the quantised field, and are content with their source-free formulation which is given by

$$\mathrm{div}\vec{E}=0, \qquad \mathrm{div}\vec{B}=0, \qquad \mathrm{curl}\vec{E}=-\frac{\partial \vec{B}}{\partial t}, \qquad \mathrm{curl}\vec{B}=\frac{1}{c^2}\frac{\partial \vec{E}}{\partial t}.$$

where $\vec{E}=\vec{E}(t,\vec{r})$ is the electric field, $\vec{B}=\vec{B}(t,\vec{r})$ the magnetic field and c the speed of light. This form of Maxwell's equations ensures the existence of a vector and scalar potential $\vec{A}=\vec{A}(t,\vec{r})$ and $\phi=\phi(t,\vec{r})$ for the electric and magnetic field. Maxwell's equations are invariant under certain transformations (gauge transformations) of these potentials. A transformation particularly suited for our purposes is the Coulomb gauge where $\mathrm{div}\vec{A}=0$, which, in the absence of charges, implies $\phi=0$. In this gauge the fields are then given by [1]

$$\vec{E}=-\frac{\partial \vec{A}}{\partial t}, \qquad \vec{B}=\nabla\times\vec{A}. \tag{3.1}$$

In order to quantize the electromagnetic field we use the corresponding classical Hamilton function, in which the canonical variables will be substituted by their corresponding operators. The Hamilton function can be obtained from the Lagrangian for the electromagnetic field by a Legendre transformation. The Lagrangian is given by

$$L=\int d^3r\mathcal{L}=\frac{\epsilon_0}{2}\int d^3r\left[\left(\frac{\partial \vec{A}}{\partial t}\right)^2-c^2\left(\nabla\times\vec{A}\right)^2\right]. \tag{3.2}$$

That this is indeed the correct Lagrangian can be seen from employing the Euler-Lagrange equation which leads to

$$\frac{\delta\mathcal{L}}{\delta\vec{A}}-\frac{\partial}{\partial t}\left(\frac{\delta\mathcal{L}}{\delta\partial_t\vec{A}}\right)=0 \qquad \Rightarrow \qquad -\epsilon_0c^2(\nabla\times(\nabla\times\vec{A}))-\epsilon_0\frac{\partial^2\vec{A}}{\partial t^2}=0.$$

Using that $\nabla\times(\nabla\times\vec{A})=\nabla(\nabla\cdot\vec{A})-\nabla^2\vec{A}$ and recalling that we apply the Coulomb gauge, this is equivalent to the wave equation for the vector potential $\vec{A}$

$$\nabla^2\vec{A}-\frac{1}{c^2}\frac{\partial^2\vec{A}}{\partial t^2}=0. \tag{3.3}$$

[1] This source-free formulation of Maxwell's equations is symmetric in $\vec{E}$ and $\vec{B}$, so that the assignments of $\vec{E}$ and $\vec{B}$ in terms of $\vec{A}$ seems interchangeable. That this is in fact the correct choice becomes clearer when considering Maxwell's equations in the general setting, see section 3.2.

Finally, together with the chosen gauge and the connections between $\vec{A}$ and the electric and magnetic field, it is straightforward to show that this equation is equivalent to Maxwell's equations in free-space and without sources [Jackson, 1999]. The Hamilton function is now obtained using (3.2) by first identifying $\vec{A}$ as the "position" coordinate (since $L \equiv T - V$ we have that the "kinetic" term is $T = (\frac{\partial \vec{A}}{\partial t})^2$), such that the conjugate momentum is given by

$$\vec{\Pi} = \frac{\delta \mathcal{L}}{\delta(\partial_t \vec{A})} = \epsilon_0 \partial_t \vec{A} = -\epsilon_0 \vec{E},$$

then using the definition of H as the Legendre transform of the Lagrangian, i.e.

$$H = \int d r^3 (\vec{\Pi} \cdot \partial_t \vec{A}) - L = \int d r^3 \left[\frac{\Pi^2}{2\epsilon_0} + \frac{\epsilon_0}{2} c^2 (\nabla \times \vec{A})^2 \right]. \tag{3.4}$$

In terms of the fields this Hamiltonian is given by

$$H = \frac{\epsilon_0}{2} \int d r^3 [\vec{E}^2 + c^2 B^2], \tag{3.5}$$

which, since we are still in the classical setting, is the total energy of the electromagnetic field [Jackson, 1999]. This is the Hamilton function that we quantise.

We proceed with the quantisation by considering a single mode of the electromagnetic field, the general case will be presented afterwards. First we find a form of classical $\vec{A}$ that satisfies the wave equation (3.3) and in turn $\vec{E}$ and $\vec{B}$ that satisfies Maxwell's equations. The form of (3.3) allows the separation of variables of $\vec{A}$ into a time-dependent part $\alpha(t)$ and a position-dependent part $\vec{f}(\vec{r})$. This vector-valued function $\vec{f}(\vec{r})$ is the mode function, which contains all the spatial dependence. After separation of variables we can take an implicit Fourier transform of $\alpha(t)$, i.e.

$$\alpha(t) = \int d\omega \, \mathrm{e}^{-i\omega t} \alpha(\omega)$$

and, using the separated equation together with the separation constant, we find

$$\frac{\partial^2 \alpha(t)}{\partial t^2} = -\omega^2 \alpha(t) \Rightarrow \alpha(t) = \alpha(0) \mathrm{e}^{-i\omega t}.$$

We therefore have

$$\vec{A}(\vec{r}, t) = \alpha(t) \vec{f}(\vec{r}) + c.c. = \alpha(0) \mathrm{e}^{-i\omega t} \vec{f}(\vec{r}) + c.c. \tag{3.6}$$

Furthermore, we assume the mode function to be normalised, i.e. $\int d r^3 |\vec{f}(\vec{r})|^2 = 1$, where the spatial integral runs over the volume of the cavity considered – the quantisation volume. According to the wave equation (3.3) and $\vec{A}$ given in (3.6), the mode function satisfies the Helmholtz equation

$$(\nabla^2 + (\omega/c)^2) \vec{f}(\vec{r}) = 0. \tag{3.7}$$

We can now simplify the Hamilton function (3.4) in the single mode case by evaluating the contribution of $\nabla \times \vec{A}$ using

$$\int d r^3 (\nabla \times \vec{A})^2 = \int d r^3 \vec{A} \cdot (\nabla \times (\nabla \times \vec{A})) = - \int d r^3 \vec{A} \cdot (\nabla^2 \vec{A}) = (\omega/c)^2 \int d r^3 \vec{A}^2,$$

where in the first step we applied the divergence theorem to integrate by parts and used the fact that the surface term vanishes, in the second step we employed the identity $(\nabla \times (\nabla \times \vec{A})) = \nabla(\nabla \cdot \vec{A}) - \nabla^2 \vec{A}$ in combination with the Coulomb gauge and in the last step we used the Helmholtz equation (3.7). The Hamilton function therefore becomes

$$H = \int d r^3 \left[\frac{\vec{\Pi}^2}{2\epsilon_0} + \frac{\epsilon_0}{2} \omega^2 \vec{A}^2 \right].$$

The form of this Hamilton function is already in close relation to that of a harmonic oscillator with frequency ω and "mass" ϵ_0, where, as before, $\vec{\Pi} = -\epsilon_0 \vec{E}$ plays the role of momentum and $\vec{A}$ the role of position. The main difference with the harmonic oscillator Hamilton function is the spatial integral. However, the spatial dependence is solely carried by the normalised mode function $f(\vec{r})$ and furthermore we have the relation

$$\vec{E} = -\partial_t \vec{A} = i\omega\alpha(t)\vec{f}(\vec{r}) + c.c$$

such that we can evaluate the integral

$$H = \frac{\epsilon_0}{2} \int d r^3 \left[\vec{E}^2 + \omega^2 \vec{A}^2 \right] = \frac{\epsilon_0}{2} \int d r^3 \left[4\omega^2 |\alpha(t)|^2 |\vec{f}(\vec{r})|^2 \right] = \frac{\epsilon_0}{2} \left[4\omega^2 |\alpha(t)|^2 \right].$$

Now, defining the momentum $p = p(t)$ to be the time-dependent part of $\vec{\Pi}$ and the position $q = q(t)$ the time-dependent part of $\vec{A}$ via

$$p = -\omega\epsilon_0 [\alpha(t) + c.c.], \qquad q = -[i\alpha(t) + c.c.], \tag{3.8}$$

we can rewrite the Hamilton function as

$$H = \frac{p^2}{2\epsilon_0} + \frac{1}{2}\epsilon_0 \omega^2 q^2.$$

This clearly has the form of a Hamilton function for a classical harmonic oscillator with "mass" ϵ_0. This is a form well suited for quantisation and in the next step we introduce the operators that facilitate this process. By using (3.8) and the usual relations for the position and momentum operator with respect to the creation and annihilation operators $\hat{a}$ and $\hat{a}^\dagger$ in quantum mechanics, namely

$$\hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}^\dagger - \hat{a}), \qquad \hat{q} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a}),$$

we can identify $\alpha(t)$ as

$$\alpha(t) \to i\sqrt{\frac{\hbar}{2\omega\epsilon_0}}\hat{a}e^{-i\omega t}$$

and, using (3.6) and (3.1), our quantised fields (in the Heisenberg picture) are thus given by[2]

$$\vec{A}(\vec{r},t) = i\sqrt{\frac{\hbar}{2\omega\epsilon_0}}\vec{f}(\vec{r})\hat{a}e^{-i\omega t} + h.c. \tag{3.9}$$

$$\vec{E}(\vec{r},t) = -\sqrt{\frac{\hbar\omega}{2\epsilon_0}}\vec{f}(\vec{r})\hat{a}e^{-i\omega t} + h.c. \tag{3.10}$$

$$\vec{B}(\vec{r},t) = i\sqrt{\frac{\hbar}{2\omega\epsilon_0}}[\nabla\times\vec{f}(\vec{r})]\hat{a}e^{-i\omega t} + h.c., \tag{3.11}$$

Furthermore, using the canonical commutation relation of the creation and annihilation operators $\hat{a}$ and $\hat{a}^\dagger$, i.e. $\left[\hat{a},\hat{a}^\dagger\right] = \mathbb{I}$, we obtain the following form of the Hamiltonian

$$\hat{H}_{\text{field}} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right). \tag{3.12}$$

Thus, we have shown that a single field mode behaves both classically and quantum mechanically as a harmonic oscillator. This (single mode) quantisation of the classical field theory preserves the Hamilton structure, and is referred to as second quantisation of (a single mode of) the electromagnetic field.

After presenting the single mode quantisation, we now briefly state the results in the general multi-mode case. Different orthogonal modes of the electric field are either given by different frequencies or different directions resulting in different spatial mode profiles. These differences are contained in the wave vector $\vec{k}$ whose magnitude $|\vec{k}|$ is proportional to the frequency ω. In addition for every $\vec{k}$ we have two possible polarizations $p \in \{1,2\}$. Therefore in the multi-mode case we have the orthonormal mode functions $\vec{f}_{\vec{k},p}(\vec{r})$ satisfying

$$\int d\,r^3\,\vec{f}_{\vec{k},p}(\vec{r})\cdot\vec{f}^*_{\vec{k}',p'}(\vec{r}) = \delta^3_{\vec{k},\vec{k}'}\delta_{p,p'}.$$

Since the modes are completely independent, the above analysis can be carried out separately for each mode, enabling us to write the field operators (again in the Heisenberg picture) as a

[2]Notational remark: quantised expressions are written with hats, to distinguish them from their classical counterparts. However, to avoid cumbersome notation we refrain from using a hat for quantised vector quantities.

sum over the field modes:

$$\vec{A}(\vec{r},t)=\sum_{\vec{k},p} i\sqrt{\frac{\hbar}{2\omega_{\vec{k}}\epsilon_0}}\vec{f}_{\vec{k},p}(\vec{r})\hat{a}_{\vec{k},p}e^{-i\omega_{\vec{k}}t}+h.c. \tag{3.13}$$

$$\vec{E}(\vec{r},t)=-\sum_{\vec{k},p}\sqrt{\frac{\hbar\omega_{\vec{k}}}{2\epsilon_0}}\vec{f}_{\vec{k},p}(\vec{r})\hat{a}_{\vec{k},p}e^{-i\omega_{\vec{k}}t}+h.c. \tag{3.14}$$

$$\vec{B}(\vec{r},t)=\sum_{\vec{k},p} i\sqrt{\frac{\hbar}{2\omega_{\vec{k}}\epsilon_0}}[\nabla\times\vec{f}_{\vec{k},p}(\vec{r})]\hat{a}_{\vec{k},p}e^{-i\omega_{\vec{k}}t}+h.c.. \tag{3.15}$$

Furthermore, in this case we have that $\left[\hat{a}_{\vec{k},p},\hat{a}^{\dagger}_{\vec{k}',p'}\right]=\delta^3_{\vec{k},\vec{k}'}\delta_{p,p'}$, such that the Hamiltonian becomes

$$\hat{H}=\sum_{\vec{k},p}\hbar\omega_{\vec{k}}\left(\hat{a}^{\dagger}_{\vec{k},p}\hat{a}_{\vec{k},p}+\frac{1}{2}\right), \qquad \text{where } \omega_{\vec{k}}=c|\vec{k}|. \tag{3.16}$$

We can also determine the form of the mode function $\vec{f}_{\vec{k},p}(\vec{r})$, which requires the specification of the volume the electromagnetic field is contained in. Here we choose the case of a fictitious array of boxes with periodic boundary conditions for the vector potential $\vec{A}(\vec{r},t)$, each having a volume $V=L^3$, which fill free space. This approach is best suited for the limit of free space with $V\to\infty$, although the same result can also be obtained for a box whose volume is taken to infinity. It can be shown, for example by considering the wave equation, that the mode functions then have the form

$$\vec{f}_{\vec{k},p}(\vec{r})=\frac{1}{\sqrt{V}}\vec{\epsilon}_{\vec{k},p}e^{i\vec{k}\cdot\vec{r}} \tag{3.17}$$

where $\vec{\epsilon}_{\vec{k},p}$ is the polarization vector.

3.2 Interaction between a two-level atom and quantised light

In this section we describe the interaction between an atom and the quantised electromagnetic field. As before we will first consider the classical Hamilton function, this time for the complete interacting system. Since the Hamilton function for the non-interacting case is simply a sum of the individual Hamilton functions for the atom and the field we can then identify the difference between the functions for the interacting and non-interacting case, thus singling out the part of the Hamilton describing the interaction.

Since an atom consists of charged particles, namely electrons and protons (in the simplest case of a hydrogen atom exactly one of each), we now have to consider Maxwell's equations

in the presence of charges, which are given by

$$\begin{aligned}
\mathrm{div}\,\vec{E} &= \frac{\rho}{\epsilon_0} && \text{(Gauss' Law)}\\
\mathrm{div}\,\vec{B} &= 0 && \text{(Gauss' Law for magnetism)}\\
\mathrm{curl}\,\vec{E} &= -\frac{\partial \vec{B}}{\partial t} && \text{(Faraday's Law)}\\
\mathrm{curl}\,\vec{B} &= \mu_0 \vec{J} + \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t} && \text{(Ampére-Maxwell's Law)}
\end{aligned}$$

where $\rho = \rho(\vec{r}, t)$ is the charge density, $\vec{J} = \vec{J}(\vec{r}, t)$ the current density, ϵ_0 the electric constant and μ_0 the magnetic constant. We again introduce the vector potential $\vec{A}(\vec{r}, t)$ and scalar potential $\phi(\vec{r}, t)$ defined such that

$$\vec{E} = -\nabla\phi - \frac{\partial \vec{A}}{\partial t}, \qquad \vec{B} = \nabla \times \vec{A}, \tag{3.18}$$

where we choose the Coulomb gauge $\mathrm{div}\vec{A} = 0$ as before. In this more general setting $\mathrm{div}\vec{B} = 0$ is always satisfied, clarifying the form of $\vec{E}$ and $\vec{B}$ as first presented in (3.1).

We are interested in the dynamics of a charged particle when interacting with the electromagnetic field. In contrast to the previous section our starting point is now the Newton equation of motion for a point particle with charge q and mass m interacting with the electromagnetic field, which describes the particle dynamics and from which we seek the Hamilton function. This equation of motion takes the form

$$\vec{F} = m\ddot{\vec{r}} = q\left(\vec{E} + \dot{\vec{r}} \times \vec{B}\right) \tag{3.19}$$

where here and in the following we have taken $c = 1$. The force on the right hand side is known as the *Lorentz force*. Alternatively we can rewrite the Lorentz force in terms of the potentials $\vec{A}$ and ϕ

$$\vec{F} = -q\left(\nabla\phi + \frac{d\vec{A}}{dt} - \nabla(\dot{\vec{r}} \cdot \vec{A})\right) \tag{3.20}$$

where we have used the vector identity $\nabla(\dot{\vec{r}} \cdot \vec{A}) = \dot{\vec{r}} \times (\nabla \times \vec{A}) + (\dot{\vec{r}} \cdot \nabla)\vec{A}$ and the so-called convective derivative $d\vec{A}/dt = \partial_t \vec{A} + (\dot{\vec{r}} \cdot \nabla)\vec{A}$. We again introduce a Lagrangian in order to obtain the Hamilton function via a Legendre transformation. In this potential representation it is clear to see that the Lorentz force can be derived from the Lagrangian

$$L = \frac{1}{2} m \dot{\vec{r}}^2 + q\dot{\vec{r}} \cdot \vec{A} - q\phi. \tag{3.21}$$

via the Euler-Lagrange equation, i.e.

$$\frac{\partial L}{\partial \vec{r}} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\vec{r}}} = 0 \qquad \Rightarrow \qquad q\nabla(\dot{\vec{r}} \cdot \vec{A}) - q\nabla\phi - m\ddot{\vec{r}} - q\frac{d\vec{A}}{dt} = 0,$$

since employing Newton's law $F = m\ddot{\vec{r}}$ we recover (3.20). The Hamilton function is obtained using (3.21) by first noting that the canonical momentum is given by

$$\vec{p} = \frac{\partial L}{\partial \dot{\vec{r}}} = m\dot{\vec{r}} + q\vec{A} \tag{3.22}$$

such that the Legendre transformation gives

$$H = \vec{p}\dot{\vec{r}} - L = \frac{1}{2m}\left(\vec{p} - q\vec{A}\right)^2 + q\phi. \tag{3.23}$$

For more than one particle the kinetic term is given by a sum over the individual contributions $\frac{1}{2m_j}\left(\vec{p}_j - q_j\vec{A}_j\right)^2$ of each particle j. This Hamilton function is well suited for quantisation, since we can directly replace the classical coordinate momentum and position functions $\vec{p}$ and $\vec{r}$ by their operator counterparts. It is worth noting that in order to obtain the full Hamiltonian for the interacting system one would have to include the field Hamiltonian, as given by (3.16). For now we neglect this contribution, since our primary focus is the interaction term of the Hamiltonian.

The interaction of the atom and the field is now incorporated in the first term on the RHS of (3.23). We can expand this kinetic term to obtain

$$\frac{1}{2m}\left(\vec{p} - q\vec{A}\right)^2 = \frac{1}{2m}\vec{p}^2 - \frac{q}{m}\vec{p}\vec{A} + \frac{q^2}{2m}\vec{A}^2. \tag{3.24}$$

In general $\vec{p}$ and $\vec{A}(\vec{r}, t)$ do not commute. However, due to the form of $\vec{p} = -i\hbar\nabla$ in position representation it is clear that they do, because of the Coulomb gauge $\nabla \cdot \vec{A}(\vec{r}, t) = 0$. Comparison to the kinetic term of a non-interacting system $\frac{1}{2m}\vec{p}^2$ therefore shows that the interaction part of the Hamiltonian is given by

$$-\frac{q}{m}\vec{p}\vec{A} + \frac{q^2}{2m}\vec{A}^2. \tag{3.25}$$

For purposes which will become clear, we now employ a standard approximation in context known as the dipole- or long-wavelength approximation. The physical idea behind this approximation is that the atomic size is usually orders of magnitude smaller than the electromagnetic wavelength, which implies that $\vec{A}$ (as well as $\vec{E}$) hardly changes over the size of the atom and therefore one assumes that it is independent of $\vec{r}$ on this scale. Instead we now assume that $\vec{A}$ depends on some fixed location specified by $\vec{R}$. Furthermore we neglect the contribution quadratic in $\vec{A}$, that is we assume the field is sufficiently weak. Finally, we also express the Hamiltonian in terms of the electric field $\vec{E}(\vec{R}, t)$ instead of the potential $\vec{A}(\vec{R}, t)$, in order to obtain a final expression with a more obvious physical interpretation. This is achieved by applying a certain unitary transformation, the so-called Power-Zienau

transformation. We omit details of this calculation and instead refer the reader to [Steck, 2011]. The Hamiltonian obtained is given by

$$\hat{H} = \frac{1}{2m}\vec{p}^2 + q\phi - \vec{\mu}_D\vec{E} \tag{3.26}$$

with $\vec{E} = \vec{E}(\vec{R}, t)$ and $\vec{\mu}_D = q\vec{r}$ the dipole operator. The interaction part is therefore now given by the electric-dipole Hamiltonian

$$\hat{H}_{\text{int}} = -\vec{\mu}_D\vec{E}. \tag{3.27}$$

In the next step we fix a representation of the full Hamiltonian $\hat{H}$ in which the atomic term $\hat{H}_{\text{atom}} = \frac{1}{2m}\vec{p}^2 + q\phi$ diagonalises. We choose the occupation number representation with eigenstates of $\hat{H}_{\text{atom}}$ denoted by $|j\rangle$ and corresponding eigenvalues $\hbar\omega_j$. The atom's Hamiltonian is then given by

$$\hat{H}_{\text{atom}} = \sum_{i,j} |i\rangle\langle i|\hat{H}_{\text{atom}}|j\rangle\langle j| = \sum_j \hbar\omega_j |j\rangle\langle j|.$$

We will treat the atom as a two-level atom. This is clearly an approximation to a true atom, which has infinitely many levels. We justify this approximation by considering near-resonant interactions, so that the transitions to other levels are negligible. We label the ground and excited levels as $|1\rangle$ and $|2\rangle$ respectively and therefore have

$$\hat{H}_{\text{atom}} = \hbar\omega_1|1\rangle\langle 1| + \hbar\omega_2|2\rangle\langle 2| = \hbar\omega_1\hat{\sigma}\hat{\sigma}^\dagger + \hbar\omega_2\hat{\sigma}^\dagger\hat{\sigma}, \tag{3.28}$$

where we have introduced the usual notation $\hat{\sigma}^\dagger = |2\rangle\langle 1|$ and $\hat{\sigma} = |1\rangle\langle 2|$ for the atomic raising and lowering operators. Accordingly, in the occupation number representation and under the two-level approximation, the interaction Hamiltonian is given by

$$\hat{H}_{\text{int}} = -\Big(|1\rangle\langle 1|q\vec{r}|1\rangle\langle 1| + |1\rangle\langle 1|q\vec{r}|2\rangle\langle 2| + |2\rangle\langle 2|q\vec{r}|1\rangle\langle 1| + |2\rangle\langle 2|q\vec{r}|2\rangle\langle 2|\Big)\vec{E}(\vec{R}, t)$$

with the dipole operator $\vec{\mu}_D$ in occupation number representation defined by the terms in brackets. Assuming that the states $|1\rangle$ and $|2\rangle$ have well defined parity, the diagonal elements of the dipole operator vanish such that it reduces to

$$\sum_{i\neq j} |i\rangle\langle i|\vec{\mu}_D|j\rangle\langle j| = |1\rangle\langle 1|q\vec{r}|2\rangle\langle 2| + |2\rangle\langle 2|q\vec{r}|1\rangle\langle 1| = \mu_{12}|1\rangle\langle 2| + \mu_{12}^*|2\rangle\langle 1| = \mu_{12}\hat{\sigma} + \mu_{12}^*\hat{\sigma}^\dagger. \tag{3.29}$$

For the Hamiltonian in (3.26) we therefore have

$$\hat{H} = \hbar\omega_1\hat{\sigma}\hat{\sigma}^\dagger + \hbar\omega_2\hat{\sigma}^\dagger\hat{\sigma} - \left(\mu_{12}\hat{\sigma} + \mu_{12}^*\hat{\sigma}^\dagger\right)\vec{E}(\vec{R}, t). \tag{3.30}$$

3.3 The Jaynes-Cummings model

We now consider the simplest fully quantum model for the atom-field interaction: a two-level atom and a single mode of the electromagnetic field. Recall from (3.28) and (3.12) that the *uncoupled* Hamiltonian for a two level atom and a single mode of the optical field is

$$\hat{H}_{\text{atom}} + \hat{H}_{\text{field}} = \hbar\omega_2 \hat{\sigma}^\dagger \hat{\sigma} + \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right),$$

where ω_2 is the atomic transition frequency, ω is the frequency of the single field mode that we consider and since we are only interested in the energy difference of the two levels considered, without loss of generality we have set the ground state energy to zero. Recalling (3.30), the dipole form of the field-atom interaction Hamiltonian is

$$\hat{H}_{\text{int}} = -(\mu_{12}\hat{\sigma} + \mu_{12}^* \hat{\sigma}^\dagger)\vec{E}(\vec{R}, t).$$

We will continue the analysis in the Schrödinger picture. The electric field mode of the cavity was derived in (3.10) and in the Schrödinger picture is given by

$$\vec{E}(\vec{R}) = -\sqrt{\frac{\hbar\omega}{2\epsilon_0}} \left(\vec{f}(\vec{R})\hat{a} + \vec{f}^*(\vec{R})\hat{a}^\dagger \right), \tag{3.31}$$

Thus, the interaction Hamiltonian in the Schrödinger picture can be written

$$\hat{H}_{\text{int}} = \left(\mu_{12}\hat{\sigma} + \mu_{12}^* \hat{\sigma}^\dagger \right) \cdot \left(\sqrt{\frac{\hbar\omega}{2\epsilon_0}} \vec{f}(\vec{R})\hat{a} + \sqrt{\frac{\hbar\omega}{2\epsilon_0}} \vec{f}^*(\vec{R})\hat{a}^\dagger \right). \tag{3.32}$$

Then, defining the atom-field coupling energy

$$\hbar g(\vec{R}) = \vec{\mu}_{12} \sqrt{\frac{\hbar\omega}{2\epsilon_0}} \vec{f}(\vec{R}),$$

where $g(\vec{R})$ is called the cavity QED coupling constant and where we omit the fixed location $\vec{R}$ in the following, the interaction Hamiltonian becomes

$$\hat{H}_{\text{int}} = \hbar \left(\hat{\sigma} + \hat{\sigma}^+ \right) \left(g\hat{a} + g^* \hat{a}^\dagger \right).$$

We now assume that at any given location $\vec{R}$ we may choose the phase of the atomic dipole such that g is real and positive. Then we can write that

$$\hat{H}_{\text{int}} = \hbar g \left(\hat{\sigma} + \hat{\sigma}^+ \right) \left(\hat{a} + \hat{a}^\dagger \right). \tag{3.33}$$

We now emphasise that this Hamiltonian is given in the Schrödinger picture. In order to further simplify it we now change from the Schrödinger picture to the interaction picture

and apply the so called *rotating wave approximation*. The interaction picture can be viewed as the intermediate picture between the Schrödinger picture, where the time-dependence is carried by the states, and the Heisenberg picture, where the time-dependence is carried by the observables. Given a state $|\psi_s(t)\rangle$ and Hamiltonian $\hat{H}_s(t) = \hat{H}_0 + \hat{H}_1(t)$ in the Schrödinger picture, we obtain the state $|\psi_i(t)\rangle$ in the interaction picture by

$$|\psi_i(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}|\psi_s(t)\rangle \tag{3.34}$$

and, by considering the corresponding Schrödinger equation, the Hamiltonian in the interaction picture $\hat{H}_i(t)$ is given by

$$\hat{H}_i(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{H}_1(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}. \tag{3.35}$$

We now proceed by defining $\hat{H}_0 := \hat{H}_{\text{atom}} + \hat{H}_{\text{field}}$ and $\hat{H}_1 := \hat{H}_{\text{int}}$ and obtain for the Hamiltonian $\hat{H}_i$ in the interaction picture

$$e^{\frac{i}{\hbar}t\hat{H}_0}\hat{H}_1 e^{-\frac{i}{\hbar}t\hat{H}_0} = e^{\frac{i}{\hbar}t\hat{H}_0}\hbar g\left(\hat{\sigma}+\hat{\sigma}^\dagger\right)\left(\hat{a}+\hat{a}^\dagger\right)e^{-\frac{i}{\hbar}t\hat{H}_0}. \tag{3.36}$$

The atomic parts of $\hat{H}_0$ commute with the field parts, furthermore we use the relations

$$\begin{aligned} e^{it\omega_2\hat{\sigma}^\dagger\hat{\sigma}}\hat{\sigma}e^{-it\omega_2\hat{\sigma}^\dagger\hat{\sigma}} &= e^{-it\omega_2}\hat{\sigma}, \qquad & e^{it\omega_2\hat{\sigma}^\dagger\hat{\sigma}}\hat{\sigma}^\dagger e^{-it\omega_2\hat{\sigma}^\dagger\hat{\sigma}} &= e^{it\omega_2}\hat{\sigma}^\dagger \\ e^{it\omega(\hat{a}^\dagger\hat{a}+\frac{1}{2})}\hat{a}e^{-it\omega(\hat{a}^\dagger\hat{a}+\frac{1}{2})} &= e^{-it\omega}\hat{a}, \qquad & e^{it\omega(\hat{a}^\dagger\hat{a}+\frac{1}{2})}\hat{a}^\dagger e^{-it\omega(\hat{a}^\dagger\hat{a}+\frac{1}{2})} &= e^{it\omega}\hat{a}^\dagger, \end{aligned} \tag{3.37}$$

which are straightforward to verify using the series expansion of the exponential operators and the anti-commutation relation $\left\{\hat{\sigma},\hat{\sigma}^\dagger\right\} = \mathbb{I}$, for example

$$\begin{aligned} e^{it\omega_2\hat{\sigma}^\dagger\hat{\sigma}}\hat{\sigma}e^{-it\omega_2\hat{\sigma}^\dagger\hat{\sigma}} &= \left[\mathbb{I}+\sum_{n=1}^{\infty}\frac{1}{n!}(it\omega_2)^n(\hat{\sigma}^\dagger\hat{\sigma})^n\right]\hat{\sigma}\left[\mathbb{I}+\sum_{m=1}^{\infty}\frac{1}{m!}(-it\omega_2)^m(\hat{\sigma}^\dagger\hat{\sigma})^m\right] \\ &= \left[\mathbb{I}+\left(\sum_{n=1}^{\infty}\frac{1}{n!}(it\omega_2)^n\right)\hat{\sigma}^\dagger\hat{\sigma}\right]\hat{\sigma}\left[\mathbb{I}+\left(\sum_{m=1}^{\infty}\frac{1}{m!}(-it\omega_2)^m\right)\hat{\sigma}^\dagger\hat{\sigma}\right] \\ &= \left[\mathbb{I}+(e^{it\omega_2}-1)\hat{\sigma}^\dagger\hat{\sigma}\right]\hat{\sigma}\left[\mathbb{I}+(e^{-it\omega_2}-1)\hat{\sigma}^\dagger\hat{\sigma}\right] \\ &= \hat{\sigma}+(e^{-it\omega_2}-1)\hat{\sigma} = e^{-it\omega_2}\hat{\sigma}, \end{aligned} \tag{3.38}$$

such that the Hamiltonian can be written as

$$\hat{H}_i(t) = \hbar g\left(\hat{\sigma}\hat{a}e^{-it(\omega_2+\omega)}+\hat{\sigma}^\dagger\hat{a}^\dagger e^{it(\omega_2+\omega)}+\hat{\sigma}^\dagger\hat{a}e^{it(\omega_2-\omega)}+\hat{\sigma}\hat{a}^\dagger e^{-it(\omega_2-\omega)}\right).$$

Finally, under the assumption that $\omega_2+\omega \gg |\omega_2-\omega|$, we apply the rotating wave approximation[3], that is we neglect all fast oscillating terms since their contributions will cancel

[3] As noted in [Steck, 2011], the two-level approximation of the atom and the rotating wave approximation are at the same level of accuracy, that is if one approximation is applied, it is nonsensical to not assume the other.

when averaged over a sufficiently large time interval. We obtain

$$\hat{H}_i(t) = \hbar g \left(\hat{\sigma}^\dagger \hat{a} e^{it(\omega_2 - \omega)} + \hat{\sigma} \hat{a}^\dagger e^{-it(\omega_2 - \omega)} \right), \tag{3.39}$$

that is, terms corresponding to photon annihilation with atomic excitation, and atomic lowering with photon creation are retained. Transforming back into the Schrödinger picture, the full Hamiltonian in the two-level and rotating wave approximation is therefore given by

$$\hat{H} = \hbar \omega_2 \hat{\sigma}^\dagger \hat{\sigma} + \hbar \omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) + \hbar g \left(\hat{\sigma}^\dagger \hat{a} + \hat{\sigma} \hat{a}^\dagger \right). \tag{3.40}$$

This Hamiltonian defines the **Jaynes-Cummings model** [Jaynes and Cummings, 1963]. It models an atom interacting with a single, nearly resonant cavity mode within the rotating wave approximation, ignoring any dissipation process such as spontaneous emission or any input or output from the cavity.

3.3.1 Driving field

There are some refinements of the cavity model presented so far that make it more realistic and less idealised. One important modification for our purposes in Chapter 5 is the addition of a driving term to the Hamiltonian (3.40). An external source of energy is typically needed for interesting atom-field interactions, since damping will force the system towards the vacuum steady state. It is therefore common to pump the cavity with an external classical field, providing photons in a steady state that excite the atom in the cavity. Laser light can be described very well classically, so to model the interaction between the laser and the atom we do not need a fully quantum mechanical treatment. The derivation for the interaction between an atom and classical light is analogous to that of the interaction between an atom and quantised light as presented in section 3.2. We can therefore use the former results and substitute for the classical quantity. We start by considering (3.30), that is

$$\hat{H} \quad = \quad \hbar \omega_2 \hat{\sigma}^\dagger \hat{\sigma} - (\mu_{12} \hat{\sigma} + \mu_{12}^* \hat{\sigma}^\dagger) \vec{E}(\vec{R}, t), \tag{3.41}$$

where μ_{12} is given by (3.29) and, as above, we set $\omega_1 = 0$. We continue by restricting the following analysis to classical monochromatic light, e.g. laser light, that is

$$\vec{E}(\vec{R}, t) = \mathrm{Re}\left[\vec{E}_0(\vec{R}) e^{i \vec{k}_L \vec{R} - i \omega_L t} \right], \tag{3.42}$$

where $\vec{E}_0(\vec{R})$ denotes the amplitude, $\vec{k}_L$ the wave vector and ω_L the laser frequency. In addition we consider the case that $\vec{k}_L$ and $\vec{R}$ are orthogonal. This restriction is generally not

necessary, but is applicable for our setup in Chapter 5. We now write the Hamiltonian (3.30) in a more convenient form

$$\begin{aligned}\hat{H} &= \hat{H}_0 - \hbar(\omega_L - \omega_2)\hat{\sigma}^\dagger\hat{\sigma} - \mu_{12}(\hat{\sigma} + \hat{\sigma}^\dagger)\vec{E}(\vec{R}, t) \\ &= \hat{H}_0 - \hbar\Delta\hat{\sigma}^\dagger\hat{\sigma} - \mu_{12}(\hat{\sigma} + \hat{\sigma}^\dagger)\vec{E}(\vec{R}, t),\end{aligned} \tag{3.43}$$

with $\hat{H}_0 = \hbar\omega_L\hat{\sigma}^\dagger\hat{\sigma}$ and the so-called detuning $\Delta := \omega_L - \omega_2$, which measures how far off-resonance the laser light is from the atomic transition frequency. As in section 3.2 we now transform to the interaction picture using (3.35) and obtain

$$\hat{H}_i = e^{it\omega_L\hat{\sigma}^\dagger\hat{\sigma}}\left\{-\hbar\Delta\hat{\sigma}^\dagger\hat{\sigma} - \mu_{12}(\hat{\sigma} + \hat{\sigma}^\dagger)\frac{\vec{E}_0(\vec{R})e^{-i\omega_L t} + \vec{E}_0^*(\vec{R})e^{i\omega_L t}}{2}\right\}e^{-it\omega_L\hat{\sigma}^\dagger\hat{\sigma}}.$$

Again we can further simplify this expression by using (3.37) which leads to

$$\hat{H}_i = -\hbar\Delta\hat{\sigma}^\dagger\hat{\sigma} - \mu_{12}\hat{\sigma}\frac{1}{2}\left\{\vec{E}_0(\vec{R})e^{-2i\omega_L t} + \vec{E}_0^*(\vec{R})\right\} - \mu_{12}\hat{\sigma}^\dagger\frac{1}{2}\left\{\vec{E}_0(\vec{R}) + \vec{E}_0^*(\vec{R})e^{2i\omega_L t}\right\}.$$

Finally, we again apply the rotating wave approximation, neglecting the fast oscillating terms (which in this case are all the time-dependent terms). Defining the Rabi frequency $\Omega(\vec{R}) := -\frac{\vec{\mu}_{12}\vec{E}_0^*(\vec{R})}{2\hbar} \in \mathbb{R}$, which characterises the strength of the atom-field coupling, and omitting its dependence on the fixed location $\vec{R}$ we obtain the Hamiltonian $\hat{H}_i$ in the rotating wave approximation

$$\hat{H}_i \quad = \quad -\hbar\Delta\hat{\sigma}^\dagger\hat{\sigma} + \hbar\Omega\left[\hat{\sigma} + \hat{\sigma}^\dagger\right]. \tag{3.44}$$

Therefore, to describe a cavity system where the atomic transitions are driven by a laser, we add this driving term to the cavity Hamiltonian, in our case (3.40).

3.3.2 Cavity Losses

Another refinement of the Jaynes-Cummings model is to include the effect of cavity decay, where photons exit the cavity through one of its mirrors. Cavity decay is a necessary ingredient of the setup proposed in Chapter 5 and therefore essential to our model's description. We omit derivations and are content with stating the results; for a comprehensive introduction to the treatment of dissipative systems see, for example, [Garbaczewski and Olkiewicz, 2002, Alicki and Lendi, 2007] and also the seminal paper [Lindblad, 1976] on generators of dynamical semigroups.

For a closed quantum system, for example a system that does not interact with its environment, the time-evolution of a state $\hat{\rho}$ is generally given by the von Neumann equation

$$\partial_t\hat{\rho} = -\frac{i}{\hbar}\left[\hat{H}, \hat{\rho}\right]. \tag{3.45}$$

We could decide to treat the cavity system and environment together as a closed system and use the above equation to describe its time-evolution. However determining the dynamics of the combined system in this way becomes intractable very quickly. Also, for our purposes we are interested in the time-evolution of the state of the cavity system only. We therefore consider the time-evolution of the former and treat the cavity loss as dissipation into the environment. It can be shown [Gardiner and Zoller, 2000, Steck, 2011], that we can account for this process by the addition of a Lindblad term to the above equation in order to obtain the master equation

$$\partial_t \hat{\rho} = -\frac{i}{\hbar}\left[\hat{H}, \hat{\rho}\right] + \kappa\left(\hat{a}\hat{\rho}\hat{a}^\dagger - \frac{1}{2}\hat{a}^\dagger\hat{a}\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{a}^\dagger\hat{a}\right), \tag{3.46}$$

where the Hamiltonian $\hat{H}$ is the atom-cavity system Hamiltonian, which in the case of a two-level atom interacting with one cavity mode is given above in (3.40), and κ is the decay rate of the cavity energy (it is also common to use the convention where κ is the field decay rate, which would be smaller by a factor of 2). The inclusion of this damping rate can have a strong effect on the cavity dynamics. Therefore, if we wish to use the Jaynes-Cummings model to approximate true dynamics, the atom-cavity system must be in the regime of *strong coupling*, where the cavity coupling constant $g \gg \kappa, \gamma$. This means that the dissipation is relatively slow, and the dynamics are Hamiltonian for short times.

We note that cavity decay is only one possible source of losses in a cavity-QED system and other sources, for example spontaneous emission, can be included in a similar way. We do not explore these further, since cavity decay is the more relevant, essential ingredient of the scheme proposed in Chapter 5, and instead refer to [Steck, 2011].

3.4 The input-output formulation of optical cavities

3.4.1 Coupled mode theory

Coupled mode theory describes the coupling between modes of neighbouring, interacting cavities. Applications of coupled mode theory essential to future chapters of this thesis are the quantum theory of cavity decay and the input-output formalism of cavities introduced in the next section, both of which are employed in Chapter 5. We will not detail the basics of coupled mode theory, but rather motivate its study and introduce the equations which are important for our purposes, in particular the interaction part of the Hamiltonian describing a single-mode cavity linked to a continuum of modes outside the cavity.

We consider two cavities, labelled cavity one and two, that correspond to the cavity system that we model and a cavity containing the output field respectively. We take the limit as cavity two becomes large, so that we obtain a free-space output field. The single mode approximation for cavity two will thus break down, and we therefore consider the coupling of the single mode cavity (cavity one) to many modes of cavity two. Cavity two will initially be in the ground state, and will approximately remain so in order that the radiated energy will never re-enter the cavity. The interaction between cavity one and cavity two is thus given by

$$\hat{H}_{\text{int}} = \hbar(\hat{a} + \hat{a}^\dagger)\sum_q g_q \left(\hat{a}_q^\dagger + \hat{a}_q\right), \tag{3.47}$$

where $\hat{a}$ is the annihilation operator of the single field mode of cavity one, $\hat{a}_q$ are the annihilation operators for cavity two, namely the output field modes, and g_q is the cavity-cavity coupling. This form is in close analogy to (3.33) and is obtained in a similar way. As before we can transform to the interaction picture and neglect fast oscillating terms to obtain

$$\hat{H}_{\text{int}} = \hbar\sum_q g_q \left(\hat{a}\hat{a}_q^\dagger + \hat{a}^\dagger\hat{a}_q\right). \tag{3.48}$$

We then take a continuum limit of the interaction Hamiltonian to eliminate cavity two and obtain irreversible decay from cavity one into a continuum. We pass the sum of the modes q over to an integral over the external-mode frequencies ω', and replace the cavity-cavity coupling

$$\sum_q \to \int_0^\infty d\omega', \qquad g_q \to \sqrt{\frac{\kappa(\omega')}{2\pi}}.$$

We also have $\hat{a}_q \to \hat{a}(\omega')$ where the external cavity, or bath, operators $\hat{a}(\omega')$ satisfy $[\hat{a}(\omega'), \hat{a}^\dagger(\omega'')] = \delta(\omega' - \omega'')$, which is the continuum version of $[\hat{a}_q, \hat{a}_{q'}^\dagger] = \delta_{qq'}$. Making these replacements in the interaction Hamiltonian yields

$$\hat{H}_{\text{int}} = \hbar\int_0^\infty \sqrt{\frac{\kappa(\omega')}{2\pi}}\left(\hat{a}\hat{a}^\dagger(\omega') + \hat{a}^\dagger\hat{a}(\omega')\right)d\omega' \tag{3.49}$$

where we explicitly indicate the dependence of the cavity decay rate on the frequency ω'. As stated above, this interaction assumes the rotating wave approximation in omitting terms like $\hat{a}\hat{a}(\omega')$ and $\hat{a}^\dagger\hat{a}^\dagger(\omega')$. We can extend the lower limit of integration from 0 to $-\infty$ since only bath frequencies ω' near the cavity resonance ω should be important.

In addition to the interaction Hamiltonian we also have the corresponding Hamiltonians describing free evolution of the cavity and the external bath modes respectively. The free evolution Hamiltonian for the cavity is simply

$$\hat{H}_{\text{sys}} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

and by making the same replacements as above we obtain for the external bath modes

$$\hat{H}_{\text{bath}} = \hbar \int_0^\infty d\omega' \omega' \hat{a}^\dagger(\omega')\hat{a}(\omega') \approx \hbar \int_{-\infty}^\infty d\omega' \omega' \hat{a}^\dagger(\omega')\hat{a}(\omega').$$

In the following we use this formulation to connect the input and output field of a cavity.

3.4.2 The input-output formalism

The input-output formalism [Collett and Gardiner, 1984] is an extension of the coupled mode theory formalism. The main purpose of the formalism is that it allows us to keep explicit track of the input and output fields of the cavity system via Heisenberg-picture operators. Instead of assigning a passive role to the external field and treating it as a heat bath, for example in order to describe the photon statistics inside a cavity, the input-output formalism treats the external cavity field explicitly in order to determine the effect of the intracavity dynamics on the quantum statistics of the output field. In addition we also consider the field input to the cavity explicitly. The following treatment is based on the more detailed discussions in [Gardiner and Collett, 1985, Steck, 2011].

Consider a single cavity mode interacting with an external multi-mode field, where we assume that the cavity has one partially transmitting mirror that couples the intracavity mode to the external field. As motivated in the previous section, the Hamiltonian describing the interaction between the cavity and the external field is given by $\hat{H} = \hat{H}_{\text{sys}} + \hat{H}_{\text{int}} + \hat{H}_{\text{ext}}$, with

$$\hat{H}_{\text{sys}} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \tag{3.50}$$

$$\hat{H}_{\text{ext}} = \hbar \int_{-\infty}^\infty d\omega' \omega' \hat{a}^\dagger(\omega')\hat{a}(\omega') \tag{3.51}$$

$$\hat{H}_{\text{int}} = \frac{\hbar}{\sqrt{2\pi}} \int_{-\infty}^\infty d\omega' \sqrt{\kappa(\omega')} \left[\hat{a}\hat{a}^\dagger(\omega') + \hat{a}^\dagger \hat{a}(\omega') \right] \tag{3.52}$$

where $\hat{a}(\omega')$ are boson annihilation operators for the bath satisfying $\left[\hat{a}(\omega'), \hat{a}^\dagger(\omega'')\right] = \delta(\omega' - \omega'')$. Here we have specified the system Hamiltonian to tailor the discussion to our setting of interest. Generally $\hat{H}_{\text{sys}}$ and the types of operators it includes do not have to be specified at this point. The same analysis can be applied for general system operators, see [Steck, 2011]. For the following analysis we change the notation for the bath modes $\hat{a}(\omega') \to \hat{b}(\omega')$ to ensure that no confusion between bath and cavity operators occurs. From (3.50) we can derive the Heisenberg equations of motion for $\hat{b}(\omega')$ and $\hat{a}$ (or more generally

any arbitrary system operator), namely

$$\begin{aligned}\partial_t \hat{b}(\omega') &= -\frac{i}{\hbar}\left[\hat{b}(\omega'), \hat{H}\right] = -\frac{i}{\hbar}\left[\hat{b}(\omega'), \hat{H}_{\text{int}}\right] - \frac{i}{\hbar}\left[\hat{b}(\omega'), \hat{H}_{\text{ext}}\right] \\ &= -i\sqrt{\frac{\kappa(\omega')}{2\pi}}a - i\omega'\hat{b}(\omega') \qquad (3.53)\\ \partial_t \hat{a} &= -\frac{i}{\hbar}\left[\hat{a}, \hat{H}\right] = -\frac{i}{\hbar}\left[\hat{a}, \hat{H}_{\text{sys}}\right] - \frac{i}{\hbar}\left[\hat{a}, \hat{H}_{\text{int}}\right] \\ &= -i\omega\hat{a} - \frac{i}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\omega' \sqrt{\kappa(\omega')}\hat{b}(\omega') \qquad (3.54)\end{aligned}$$

where we have used $\left[\hat{a}, \hat{a}^\dagger\right] = \mathbb{I}$ and $\left[\hat{a}, \hat{a}^\dagger\hat{a}\right] = \hat{a}$. We can solve the equation of motion for $\hat{b}(\omega')$ by first transforming to a rotating frame $\hat{b}(\omega') \to \hat{b}(\omega')e^{i\omega' t}$ such that

$$\begin{aligned}\partial_t\left(\hat{b}(\omega')e^{i\omega' t}\right) &= \partial_t\left(\hat{b}(\omega')\right)e^{i\omega' t} + i\omega'\hat{b}(\omega')e^{i\omega' t} \\ &= -i\sqrt{\frac{\kappa(\omega')}{2\pi}}\hat{a}\,e^{i\omega' t}, \qquad (3.55)\end{aligned}$$

where in the last step we have used (3.53). In the following analysis we distinguish between the case of an input or an output field, which corresponds to integrating the above equation from some time in the past to the present time or from some future time to the present time. Afterwards we will combine the results to obtain a relation between these input and output fields, which is the objective of this section and formalism. We first treat the input field.

Input fields

Integrating (3.55) from some past time t_0 to t we obtain

$$\hat{b}(\omega')e^{i\omega' t} - \hat{b}_0(\omega')e^{i\omega' t_0} = -i\sqrt{\frac{\kappa(\omega')}{2\pi}}\int_{t_0}^{t}\hat{a}(t')e^{i\omega' t'}dt'$$

where $\hat{b}_0(\omega')$ is the initial value of $\hat{b}(\omega')$ at $t = t_0$ satisfying the same commutation relations as $\hat{b}(\omega')$. We rewrite this equation to obtain an expression for $\hat{b}(\omega')$

$$\hat{b}(\omega') = \hat{b}_0(\omega')e^{-i\omega'(t-t_0)} - i\sqrt{\frac{\kappa(\omega')}{2\pi}}\int_{t_0}^{t}\hat{a}(t')e^{-i\omega'(t-t')}dt' \qquad (3.56)$$

and substitute this into the equation of motion (3.54) for $\hat{a}(t)$. We find that

$$\begin{aligned}\partial_t\hat{a} = &-i\omega\hat{a} - i\int_{-\infty}^{\infty}d\omega'\sqrt{\frac{\kappa(\omega')}{2\pi}}\hat{b}_0(\omega')e^{-i\omega'(t-t_0)} \\ &-\int_{-\infty}^{\infty}d\omega'\frac{\kappa(\omega')}{2\pi}\int_{t_0}^{t}dt'\hat{a}(t')e^{-i\omega'(t-t')}. \qquad (3.57)\end{aligned}$$

We now introduce the Markov approximation where we ignore the frequency dependence of the coupling constant, namely $\kappa(\omega') \approx \kappa$(constant). Although this is in principle untrue, it is

a good approximation over the frequency range of interest - the resonance linewidth in the case of the optical cavity. We then define an input field operator by

$$\hat{a}_{\text{in}}(t) := \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega' \hat{b}_0(\omega') e^{-i\omega'(t-t_0)} \tag{3.58}$$

such that the integral in the second term of (3.57) can be written $\sqrt{\kappa}\hat{a}_{\text{in}}(t)$. To evaluate the third term of the same equation we first use the identity $\int_{-\infty}^{\infty} dx e^{-ix(t-t')} = 2\pi\delta(t-t')$ such that

$$\frac{\kappa}{2\pi} \int_{-\infty}^{\infty} d\omega' \int_{t_0}^{t} dt' \hat{a}(t') e^{-i\omega'(t-t')} = \kappa \int_{t_0}^{t} dt' \hat{a}(t') \delta(t-t').$$

We then use that $\int_{t_0}^{t} dt' \hat{a}(t')\delta(t-t') = \frac{\hat{a}(t)}{2}$, an equality that holds since t appears as the limit of integration, i.e. the delta distribution is "split" and only half the contribution is retained. Combining these definitions and identities we finally write the Heisenberg equation for $\hat{a}(t)$ as

$$\partial_t \hat{a}(t) = -i\omega\hat{a}(t) - \sqrt{\kappa}\hat{a}_{\text{in}}(t) - \kappa\frac{\hat{a}(t)}{2}. \tag{3.59}$$

This equation is called the quantum Langevin equation, since it takes the similar form to the Langevin equation in statistical physics. The second term represents quantum noise, as well as an input to the system. The last term represents damping, and in this case where the system operators are harmonic oscillator operators, the damping is Markovian, that is it depends only on the system operators evaluated at time t and not at any previous time.

Output fields

It is also possible to define a corresponding output field. We proceed as before, but instead we integrate (3.55) from t to a future time t_1 instead of from a past time t_0 to t. We obtain

$$\hat{b}_1(\omega')e^{i\omega' t_1} - \hat{b}(\omega')e^{i\omega' t} = -i\sqrt{\frac{\kappa(\omega')}{2\pi}} \int_{t}^{t_1} \hat{a}(t) e^{i\omega' t'} dt'$$

where $\hat{b}_1(\omega')$ is the value of $\hat{b}(\omega')$ at $t = t_1$ satisfying the same commutation relations as $\hat{b}(\omega')$. We can again rewrite this equation

$$\hat{b}(\omega') = \hat{b}_1(\omega')e^{-i\omega'(t-t_1)} + i\sqrt{\frac{\kappa(\omega')}{2\pi}} \int_{t}^{t_1} \hat{a}(t) e^{-i\omega'(t-t')} dt', \tag{3.60}$$

and substitute this expression into the equation of motion for $\hat{a}(t)$ (3.54). We find that

$$\begin{aligned} \partial_t \hat{a}(t) = -i\omega\hat{a} - i\int_{-\infty}^{\infty} d\omega' \sqrt{\frac{\kappa(\omega')}{2\pi}} \hat{b}_1(\omega') e^{-i\omega'(t-t_1)} \\ + \int_{-\infty}^{\infty} d\omega' \frac{\kappa(\omega')}{2\pi} \int_{t}^{t_1} \hat{a}(t) e^{-i\omega'(t-t')} dt'. \end{aligned} \tag{3.61}$$

After application of the Markov approximation we can then define

$$\hat{a}_{\text{out}}(t) := \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega' \hat{b}_1(\omega') e^{-i\omega'(t-t_1)}$$

such that following the same procedure as before we arrive at the time reversed Langevin equation

$$\partial_t \hat{a}(t) = -i\omega \hat{a}(t) - \sqrt{\kappa}\hat{a}_{\text{out}}(t) + \frac{\kappa}{2}\hat{a}(t). \tag{3.62}$$

Here the output operator $\hat{a}_{\text{out}}(t)$ represents the coupling of the system to future bath modes, and so we interpret this to be the system output. Since the influence of $\hat{a}_{\text{out}}(t)$ is in the future, this equation represents the backwards evolution of the system, hence the negativity of the damping term in (3.59).

Input-output relation

In a final step we can now relate the input and output fields to one another by integrating both (3.56) and (3.60) over all frequencies (in the Markov approximation) and equating the obtained expressions. From (3.56) we have

$$\int_{-\infty}^{\infty} d\omega' \hat{b}(\omega') = -i\sqrt{2\pi}\hat{a}_{\text{in}}(t) - i\sqrt{\frac{\kappa\pi}{2}}\hat{a}(t).$$

Similarly we can integrate (3.60) over all frequencies to obtain

$$\int_{-\infty}^{\infty} d\omega' \hat{b}(\omega') = -i\sqrt{2\pi}\hat{a}_{\text{out}}(t) + i\sqrt{\frac{\pi\kappa}{2}}\hat{a}(t).$$

Equating the right hand sides of both these expressions for $\int_{-\infty}^{\infty} d\omega' \hat{b}(\omega')$ leads to the important relation

$$\hat{a}_{\text{out}}(t) - \hat{a}_{\text{in}}(t) = \sqrt{\kappa}\hat{a}(t) \tag{3.63}$$

for the input, output and system fields, which can also be used to transform between the forward and time reversed Langevin equations. This condition can be viewed as a boundary condition, relating the input, output and internal modes. The general strategy for the input-output formalism is to specify the input field $\hat{a}_{\text{in}}(t)$ for a system, use the Langevin equation (3.59) to determine the influence of the input on the system operator $\hat{a}(t)$ and then use the input-output relation (3.63) to determine the output field $\hat{a}_{\text{out}}(t)$.

3.5 Field-Correlation Functions

In this section we briefly review detection of the quantised electric field as introduced by Glauber[4] [Glauber, 1963]. This formalism is paramount to our proposal in Chapter 5 where we indirectly determine the expected energy density of a quantum field by measuring different characteristic properties, such as the intensity, of a cavity output field. We begin by considering an ideal photon counter, or detector, that works on an absorbtion mechanism sensitive to the positive frequency electric field $\vec{E}^{+}(\vec{r},t)$ at the space-time point $(\vec{r},t)$. We closely follow the treatment presented in [Walls and Milburn, 1995]. Recall from (3.14) the quantised electric field

$$\vec{E}(\vec{r},t) = -\sum_{\vec{k},p}\sqrt{\frac{\hbar\omega_{\vec{k}}}{2\epsilon_0}}\vec{f}_{\vec{k},p}(\vec{r})\hat{a}_{\vec{k},p}e^{-i\omega_{\vec{k}}t} + h.c.$$

It can be shown (see for example [Dirac, 1947]) that the positive frequency part of the field $\vec{E}^{+}(\vec{r},t)$ belongs to the annihilation term and the negative frequency $\vec{E}^{-}(\vec{r},t)$ part to the creation term. We can therefore isolate the annihilation component of the field and write

$$\vec{E}^{+}(\vec{r},t) = -\sum_{\vec{k},p}\sqrt{\frac{\hbar\omega_{\vec{k}}}{2\epsilon_0}}\vec{f}_{\vec{k},p}(\vec{r})\hat{a}_{\vec{k},p}e^{-i\omega_{\vec{k}}t}. \tag{3.64}$$

The detection of a photon can be viewed as a transition in the state of the field, $|i\rangle \rightarrow |f\rangle$, where $|i\rangle$ is the initial state of the field before the detection event, and $|f\rangle$ is the final state after the detection, where one photon in mode $(\vec{k},p)$ is removed from the field at time t. The transition probability of the detector absorbing a photon at position $\vec{r}$ and time t is proportional to

$$T_{if} = |\langle f|\vec{E}^{+}(\vec{r},t)|i\rangle|^2.$$

To obtain the probability of detecting a photon we must sum the transition probabilities over all states of the field that can be reached from the initial state by an absorption process. We can extend this sum to include the complete set of final states, since the states that cannot be reached are orthogonal to $\vec{E}^{+}(\vec{r},t)|i\rangle$ and thus will not contribute to the sum. The probability of detecting a photon, or average field intensity is

$$I(\vec{r},t) = \sum_f T_{if} = \sum_f \langle i|\vec{E}^{-}(\vec{r},t)|f\rangle\langle f|\vec{E}^{+}(\vec{r},t)|i\rangle \tag{3.65}$$

$$= \langle i|\vec{E}^{-}(\vec{r},t)\vec{E}^{+}(\vec{r},t)|i\rangle. \tag{3.66}$$

[4]Note that a similar treatment applies to the quantised magnetic field.

This result assumes that the field is initially in a pure state $|i\rangle$. The result is easily generalised to a statistical mixture state by averaging over all possible initial states with probability P_i so that the photodetection probability

$$I(\vec{r},t)=\sum_i P_i\langle i|\vec{E}^-(\vec{r},t)\vec{E}^+(\vec{r},t)|i\rangle=\mathrm{Tr}\left[\hat{\rho}\,\vec{E}^-(\vec{r},t)\vec{E}^+(\vec{r},t)\right] \tag{3.67}$$

where $\hat{\rho}$ is the density operator $\hat{\rho}=\sum_i P_i|i\rangle\langle i|$. If the field is initially in the vacuum state, i.e. $\hat{\rho}=|0\rangle\langle 0|$, then the intensity is $I(\vec{r},t)=\langle 0|\vec{E}^-(\vec{r},t)\vec{E}^+(\vec{r},t)|0\rangle=0$. It is the particular ordering of the field operators, called normal ordering, with the annihilation operators to the right of all creation operators, that appropriately gives zero intensity for the vacuum. The reversed ordering would correspond to detection of photons from the vacuum, which is physically nonsensical.

The expression for the photodetection probability (3.67) motivates the definition of a first order field correlation function $G^{(1)}(\vec{r}_1,t_1,\vec{r}_2,t_2)$, named after R. Glauber [Glauber, 1963], given by

$$G^{(1)}(\vec{r}_1,t_1,\vec{r}_2,t_2):=\mathrm{Tr}\left[\hat{\rho}\,\vec{E}^-(\vec{r}_1,t_1)\vec{E}^+(\vec{r}_2,t_2)\right]. \tag{3.68}$$

For our proposal in Chapter 5 it is only important that we can measure the simulated system's average energy via such correlation functions and we will not discuss the importance of the Glauber functions in the context of coherence in quantum optics. For a comprehensive treatment we refer to [Mandel and Wolf, 1995].

In a next step we can also describe two-photon experiments, where two detectors located at positions $\vec{r},\vec{r}'$ detect photons at times t and t' respectively. These are necessary to describe experiments involving intensity correlations such as the Hanbury-Brown and Twiss experiment [Hanbury Brown and Twiss, 1956, Walls and Milburn, 1995]. As before we proceed to define the second-order correlation function. We consider two detectors at different locations, where the joint probability amplitude to detect one photon at $(\vec{r},t)$ and another at $(\vec{r}',t')$ is proportional to $T'_{if}=|\langle f|\vec{E}^+(\vec{r},t)\vec{E}^+(\vec{r}',t')|i\rangle|^2$. To compute the detection probability, or average field intensity, we again consider mixed initial states and sum these probabilities over all final states of the field, resulting in

$$I(\vec{r},\vec{r}',t,t')=\mathrm{Tr}\left[\hat{\rho}\,\vec{E}^-(\vec{r}',t')\vec{E}^-(\vec{r},t)\vec{E}^+(\vec{r},t)\vec{E}^+(\vec{r}',t')\right]. \tag{3.69}$$

This joint detection probability motivates the definition of the second-order correlation function

$$G^{(2)}(\vec{r}_1,t_1,\vec{r}'_1,t'_1,\vec{r}_2,t_2,\vec{r}'_2,t'_2):=\mathrm{Tr}\left[\hat{\rho}\,\vec{E}^-(\vec{r}_1,t_1)\vec{E}^-(\vec{r}'_1,t'_1)\vec{E}^+(\vec{r}'_2,t'_2)\vec{E}^+(\vec{r}_2,t_2)\right]. \tag{3.70}$$

Note that these joint expectation values are still normally ordered, causing the value to vanish unless there are at least two photons available for detection.

The quantities defined so far are sufficient for the understanding of the detection scheme measuring the average energy density of a boson field discussed as an example in Chapter 5. Extensions of this scheme could involve the measurement of higher order correlation functions. The definition of such functions, although straightforward, is not necessary for this thesis and we therefore conclude our exploration.

Chapter 4

Continuous Matrix Product States

The success of a variational method is highly dependent on the choice of variational class and its ability to capture system dynamics. In Chapter 2 we discussed the difficulty of designing reasonable variational classes. Such classes should provide the capability to perform calculations efficiently whilst bearing some resemblance to the actual states of a given system. A promising candidate for the study of continuous quantum systems satisfying the requirements for a successful variational class is the family of continuous matrix product states (cMPS). These states describe one-dimensional quantum field theories and were first introduced by F. Verstraete and J. I. Cirac in 2010 [Verstraete and Cirac, 2010]. It has been shown that cMPS are capable of the classical simulation of both nonrelativistic and relativistic quantum fields [Haegeman et al., 2010, Osborne et al., 2010, Verstraete and Cirac, 2010], and that the class is complete, since in principle any pure state in Fock space admits a cMPS representation [Brockt et al., 2012]. In addition, the generalisation of the cMPS to higher dimensions has been considered [Jennings et al., 2012].

Applications of variational methods in subsequent chapters of this thesis utilise the class of cMPS as a variational class. In this chapter we therefore present a thorough review of cMPS, including details of their construction, regularity properties, representation redundancy and how to calculate physical quantities of interest such as energy expectation values. The chapter is organised as follows. In section 4.1 we define the class of cMPS along with a description of their corresponding tangent vectors. To obtain a better understanding of the structure of these states we review their construction as a continuum limit of MPS in section 4.2. We also present the connection between cMPS and the stationary output of a cavity QED apparatus, an identification necessary for the proposal in Chapter 5. Sections 4.3 and 4.5 describe some important properties and restrictions a cMPS must satisfy. Calculating expectation values of physical quantities using cMPS is reviewed in section 4.4. Finally, since applications in this thesis consider translationally invariant systems in the thermodynamic limit, we present the cMPS formalism in such a setting in section 4.6. Due to the short history of cMPS there is a lack of literature providing overviews and details of properties and

applications of such states. What does exist is limited to the account given in [Haegeman, 2011, Haegeman et al., 2011a], which we follow and often elucidate with the hope that our presentation is enlightening and contributes to the general understanding of the topic.

4.1 Definition of continuous matrix product states

Consider a one-dimensional system of N species of bosons and/or fermions on a line of length ℓ that are created and annihilated by the field operators $\hat{\psi}_\alpha^\dagger$ and $\hat{\psi}_\alpha$, $\alpha = 1, \ldots, N$. When both species α and β represent fermionic particles the field operators obey the anticommutation relations

$$\left\{\hat{\psi}_\alpha(x), \hat{\psi}_\beta^\dagger(y)\right\} = \delta_{\alpha\beta}\ \delta(x-y), \qquad \left\{\hat{\psi}_\alpha(x), \hat{\psi}_\beta(y)\right\} = 0$$

where $-\ell/2 \leq x, y \leq \ell/2$ are space coordinates. If one of the two or both particle species are bosonic the field operators obey the following canonical commutation relations

$$\left[\hat{\psi}_\alpha(x), \hat{\psi}_\beta^\dagger(y)\right] = \delta_{\alpha\beta}\ \delta(x-y), \qquad \left[\hat{\psi}_\alpha(x), \hat{\psi}_\beta(y)\right] = 0.$$

Since this thesis deals only with bosonic systems and applications thereof, we restrict to this case from now on. Generally, the cMPS formulation and all further calculations hold also for fermions and mixtures of fermions and bosons, see [Haegeman, 2011, Haegeman et al., 2011a]. The Hilbert space for such a system is given by the Fock space $\mathcal{F}$, see appendix (A.2).

A continuous matrix product state $|\Psi\rangle$ is a variational quantum field state in Fock space $\mathcal{F}$. To define the state it is first necessary to introduce a D-dimensional auxiliary system. This auxiliary system provides the variational element to the cMPS, since the variational parameters that specify the state compose a set of operators that act on the auxiliary space. The quantum field system and auxiliary system interact according to an operator $U_{\ell/2,-\ell/2}$, which we define below, and the cMPS is obtained by subsequent tracing over the auxiliary system, that is

$$|\Psi\rangle = \mathrm{tr}_{\mathrm{aux}}\left[B U_{\ell/2,-\ell/2}\right]|\Omega\rangle, \tag{4.1}$$

where $|\Omega\rangle$ is the vacuum state of the quantum field that is annihilated by $\hat{\psi}_\alpha(x)$, i.e. $\hat{\psi}_\alpha(x)|\Omega\rangle = 0$ and B is a $D \times D$ matrix acting on the auxiliary space encoding boundary conditions. The interaction operator $U_{\ell/2,-\ell/2}$ acts on both the quantum field system and auxiliary system. In general it is a non-unitary operator and is given by

$$U_{\ell/2,-\ell/2} = \mathcal{P}\exp\left(\int_{-\ell/2}^{\ell/2} \hat{H}_{\mathrm{cMPS}}(x)\,dx\right). \tag{4.2}$$

Here $\mathcal{P}\exp$ is the notation for the path ordered exponential (ordering arguments increasingly from right to left), and the Hamiltonian $\hat{H}_{\text{cMPS}}(x)$ is given by

$$\hat{H}_{\text{cMPS}}(x) = Q(x)\otimes\mathbb{I} + \sum_{\alpha=1}^{N} R_\alpha(x)\otimes\hat{\psi}^\dagger_\alpha(x) \tag{4.3}$$

with $Q(x), R_\alpha(x)$ position dependent matrices of dimension $D\times D$ that act in the auxiliary space. We note that $\hat{H}_{\text{cMPS}}(x)$ is generally non-hermitian, which is why (4.2) is generally non-unitary. However, when acting on the field vacuum $|\Omega\rangle$ (as in (4.1)) it can be shown that (4.3) is equivalent to the hermitian Hamiltonian (4.12), see section 4.2. We therefore have that (4.2) is also equivalent to a unitary operator when acting on $|\Omega\rangle$, see for example [Brockt et al., 2012, Haegeman, 2011].

The matrix elements of $Q(x)$ and $\{R_\alpha(x)\}$, $\alpha = 1,\ldots,N$ form the set of variational parameters. These parameters can be both position- and time-dependent. Since these matrices are D-dimensional there are at most $(N+1)D^2$ parameters where the choice of D can be arbitrary, but finite for computational purposes. The cMPS is therefore a variational ansatz state and we highlight this by adopting the notation

$$|\Psi\rangle = |\Psi(Q,\{R_\alpha\})\rangle = \text{tr}_{\text{aux}}\left[BU_{\ell/2,-\ell/2}\right]|\Omega\rangle. \tag{4.4}$$

For a system with periodic boundary conditions, for example a system of bosons on a ring, we have $B=\mathbb{I}$. A system with open boundary conditions can be obtained by replacing the tr_{aux} with a left and right multiplication of the auxiliary system with a row and column vector respectively. That is, we choose $B=|\omega_R\rangle\langle\omega_L|$ and write

$$|\Psi(Q,\{R_\alpha\})\rangle = \langle\omega_L|U_{\ell/2,-\ell/2}|\omega_R\rangle|\Omega\rangle. \tag{4.5}$$

We typically consider states with open boundary conditions. We note that B is not included in the set of variational parameters as it can often be completely fixed to a constant matrix and does not enter in physical expectation values in the thermodynamic limit.

As was shown in [Osborne et al., 2010], an equivalent representation (equivalent in the sense that they give rise to identical expectation values of normal and position ordered expressions of field operators) of the cMPS $|\Psi(Q,\{R_\alpha\})\rangle$ as defined in (4.5) is given by

$$|\Psi(Q,\{R_\alpha\})\rangle\langle\Psi(\overline{Q},\{\overline{R_\alpha}\})| \propto \text{tr}_{\text{aux}}\left[U_{\ell/2,-\ell/2}\left(\rho\otimes\Omega\right)U^\dagger_{\ell/2,-\ell/2}\right] \tag{4.6}$$

with $\Omega=|\Omega\rangle\langle\Omega|$ the field vacuum and ρ an arbitrary initial state of the auxiliary system. ρ plays the role of a boundary condition at $-\ell/2$, and is therefore linked to the boundary matrix B in (4.1). This representation gives some intuition of the structure of the hitherto abstract

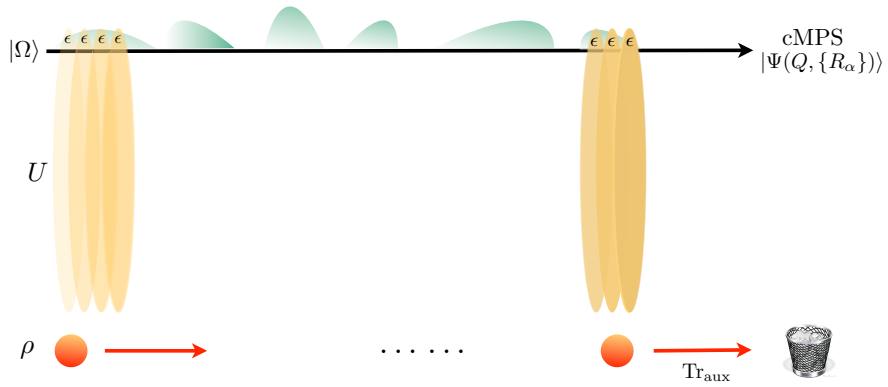

Figure 4.1: An illustration of the cMPS concept. The field is initialised in the vacuum state $|\Omega\rangle$ and infinitesimally thin strips are sequentially interacted via U with the auxiliary system initialised in some state ρ. At the end of the process the auxiliary system is discarded, and we obtain a cMPS.

definition of the cMPS, and enables us to visualise how such a state is prepared. A quantum field is initialised in the vacuum state Ω and to it a D-dimensional auxiliary system in an initialised state ρ is adjoined. The two systems interact according to the dynamics $U_{\ell/2,-\ell/2}$. The auxiliary system is then discarded by tracing it out to obtain the evolved quantum state. We illustrate this process in Fig. 4.1.

Having introduced the continuous matrix product state we can now define the variational manifold of cMPS $\mathcal{V}_{\mathrm{cMPS}} \subset \mathcal{F}$. We have

$$\mathcal{V}_{\mathrm{cMPS}} = \left\{ |\Psi(Q,\{R_\alpha\})\rangle | Q(x) : \mathbb{R} \mapsto \mathbb{C}^{D\times D}; \{R_\alpha(x)\} : \mathbb{R} \mapsto \mathbb{C}^{D\times D}, \forall \alpha = 1,\ldots,N \right\}.$$

We do not at this stage attempt to further specify the parameter space of the variational manifold $\mathcal{V}_{\mathrm{cMPS}}$, and have not considered any restrictions or particular properties (other than the dimension) of the matrices $Q(x)$ and $R_\alpha(x)$. However, limitations do exist. In future applications of cMPS we must ensure that characteristic physical quantities are well defined. One example is the expectation value of the kinetic energy which, in position representation, involves spatial derivatives. Ensuring that this quantity is sufficiently regular imposes constraints on the matrices $Q(x)$ and $R_\alpha(x)$. This will be discussed in subsection 4.3. Also, there is a parameter redundancy in the cMPS representation and so we are able to apply gauge fixing conditions that impose specific canonical forms on $Q(x)$ and $R_\alpha(x)$. This will be discussed in subsection 4.5.

We now also define the tangent plane $\mathbb{T}_{(Q,\{R_\alpha\})}\mathcal{V}_{\mathrm{cMPS}}$ at a certain point $|\Psi(Q,\{R_\alpha\})\rangle$ in the variational manifold $\mathcal{V}_{\mathrm{cMPS}}$. A general tangent vector, which we will denote by $|\Phi(q,\{r_\alpha\};Q,\{R_\alpha\})\rangle$, is a linear combination of all $(N+1)D^2$ derivatives of the state with

respect to each variational parameter, that is each matrix element of $Q(x)$ and $R_\alpha(x)$, given by

$$|\Phi(q,\{r_\alpha\};Q,\{R_\alpha\})\rangle = \sum_{j,k=1}^{D^2} q_{jk}\partial[Q]_{jk}|\Psi(Q,\{R_\alpha\})\rangle + \sum_{j,k=D^2+1}^{2D^2}\sum_{\alpha=1}^{N}(r_\alpha)_{jk}\,\partial\,[R_\alpha]_{jk}\,|\Psi(Q,\{R_\alpha\})\rangle$$

where $\partial[Q]_{jk} = \partial/\partial[Q]_{jk}$, $\partial\,[R_\alpha]_{jk} = \partial/\partial\,[R_\alpha]_{jk}$ and $[Q]_{jk}$ and $[R_\alpha]_{jk}$ denote the jk-th entry of the matrices $Q(x)$ and $R_\alpha(x)$ respectively. We have that

$$\begin{aligned}|\Phi(q,\{r_\alpha\};Q,\{R_\alpha\})\rangle &= \sum_{j,k=1}^{D^2} q_{jk}\langle\omega_L|\int_{-\ell/2}^{\ell/2} U_{\ell/2,x}\left(|j\rangle\langle k|\otimes\mathbb{I}\right)U_{x,-\ell/2}dx|\omega_R\rangle|\Omega\rangle \\ &\quad+\sum_{j,k=D^2+1}^{2D^2}\sum_{\alpha=1}^{N}[r_\alpha]_{jk}\,\langle\omega_L|\int_{-\ell/2}^{\ell/2} U_{\ell/2,x}\left(|j\rangle\langle k|\otimes\hat{\psi}_\alpha^\dagger(x)\right)U_{x,-\ell/2}dx|\omega_R\rangle|\Omega\rangle \\ &= \int_{-\ell/2}^{\ell/2}\langle\omega_L|U_{\ell/2,x}\left(q(x)\otimes\mathbb{I}+\sum_{\alpha=1}^{N}r_\alpha(x)\otimes\hat{\psi}_\alpha^\dagger(x)\right)U_{x,-\ell/2}|\omega_R\rangle|\Omega\rangle dx.\end{aligned} \tag{4.7}$$

where we define $q(x)$ and $r_\alpha(x)$ as the matrices whose jk-th entries are precisely the weightings q_{jk} and $(r_\alpha)_{jk}$ of the linear combination of the $(N+1)D^2$ derivatives (for an explicit construction of the tangent vectors, see appendix (B.1)). Note that by choosing $q(x)=\mathbb{I}$ and $r_\alpha(x)=\underline{0}$ for all α we obtain $|\Phi(q,\{r_\alpha\};Q,\{R_\alpha\})\rangle = L|\Psi(Q,\{R_\alpha\})\rangle$, which means that the state $|\Psi(Q,\{R_\alpha\})\rangle$ itself lies in the tangent plane at the point $|\Psi(Q,\{R_\alpha\})\rangle$ in the variational manifold. This means that the tangent space allows for norm and phase variation of states, the consequences of which were discussed in section 2.3.5 of Chapter 2.

4.2 Constructions and Identifications

Although the cMPS formalism was originally established as a continuum limit of matrix product states (MPS), as presented below, other constructions and identifications exist. For example, a cMPS can be identified as the stationary output of a cavity QED apparatus. Since this connection is central to the proposed scheme in Chapter 5, we present it in detail below. Other constructions, such as the generation of cMPS through the paradigm of continuous measurement or the link between cMPS and exactly solvable models, are not presented here and we instead refer the reader to [Osborne et al., 2010, Maruyama and Katsura, 2010].

cMPS from the continuum limit of MPS

The cMPS formalism was originally formulated in [Verstraete and Cirac, 2010] as the continuum limit of a subclass of MPS. We present this construction here. Although this thesis is not concerned with MPS, it is important to explore the connection between MPS and cMPS since most inherent properties of cMPS can be most easily understood and derived from the correspondence with MPS. We merely define MPS below, then set about taking the continuum limit to show the equivalence to cMPS. For more information regarding MPS, including their formulation, properties and extensive applications, see [Perez-Garcia et al., 2007].

A matrix product state can be defined on a one dimensional lattice $\mathcal{L}$ with N sites, each labelled by an integer $j \in \{1,\dots,N\}$, and periodic boundary conditions such that site $N+1 \equiv 1$. The physical length of the system is $\ell = N\epsilon$ where ϵ is the lattice spacing. Each site j contains a d_j-dimensional quantum system. Therefore, the local Hilbert space is $\mathbb{C}^{d_j}$, and is spanned by a basis $\{|i_j\rangle | i_j = 0,\dots,d_j-1\}$. The complete Hilbert space is given by $\mathbb{H} = \bigotimes_{j=1}^{N} \mathbb{C}_j^d$ with $\dim\mathbb{H} = \Pi_{j=1}^{N} d_j$ and is spanned by the product basis $\{|i_1 i_2 \dots i_N\rangle = |i_1\rangle \otimes |i_2\rangle \otimes \dots \otimes |i_N\rangle | \forall i_j = 0,\dots,d_j-1, \forall j = 1,\dots,N\}$. A matrix product state $|\Psi(A)\rangle$ is defined as

$$|\Psi(A)\rangle = \sum_{i_1=0}^{d_1-1} \sum_{i_2=0}^{d_2-1} \dots \sum_{i_N=0}^{d_N-1} \mathrm{tr}\left[A_{i_1}(1) A_{i_2}(2) \dots A_{i_N}(N)\right] |i_1 i_2 \dots i_N\rangle \tag{4.8}$$

where, for each $i_j = 0,\dots,d_j-1$, $A_{i_j}(j)$ is a $D_j \times D_{j+1}$ matrix corresponding to site $j \in \{1,\dots,N\}$ with $D_1 = D_{N+1}$. An arbitrary state $|\Psi\rangle \in \mathbb{H}$ is a linear combination of the general basis state $|i_1 i_2 \dots i_N\rangle$, the coefficients of the individual basis states being a product of the matrices $A_{i_j}(j)$, hence the name matrix product state.

We now show how continuous matrix product states can be understood as the limit of a subclass of matrix product states. For simplicity, we consider a translationally invariant system of bosons, although the construction also works for both fermionic and mixed systems. We define our family of translationally invariant matrix product states of $N = \ell/\epsilon$ modes on the lattice L described above, where on every site j of the lattice we can create and annihilate particles by acting with the creation and annihilation operators $\hat{a}_j$ and $\hat{a}_j^\dagger$ that obey the canonical commutation relations $\left[\hat{a}_i^\dagger, \hat{a}_j\right] = \delta_{ij}$. We assume that the local Hilbert space for each site is $\mathbb{C}^d$, that is the quantum systems at each site are of the same dimension. The local Hilbert space is therefore spanned by the basis $\left\{ \left(\hat{a}_j^\dagger\right)^{i_j} |0\rangle \mid i_j = 0,1,\dots,d-1 \right\}$ where we use the convention that $\left(\hat{a}_j^\dagger\right)^0 = \mathbb{I}$. We define rescaled creation and annihilation operators

$\hat{\psi}_j = \frac{\hat{a}_j}{\sqrt{\epsilon}}$ that in the limit $\epsilon \to 0$ will become field operators $\hat{\psi}^\dagger(x)$. Our MPS therefore can be written as

$$|\Psi(A)\rangle = \sum_{i_1,\ldots,i_N=0}^{d-1} \mathrm{tr}\left[A_{i_1}A_{i_2}\ldots A_{i_N}\right]\left(\hat{\psi}_1^\dagger\right)^{i_1}\ldots\left(\hat{\psi}_N^\dagger\right)^{i_N}|\Omega\rangle \tag{4.9}$$

with $|\Omega\rangle \equiv |0\rangle$ the vacuum on which the operators $\hat{a}_j$ act. We then identify

$$A_0 = \mathbb{I} + \epsilon Q, \qquad A_{i_j} = \left(\sqrt{\epsilon}\right)^{i_j}\frac{R^{i_j}}{\left(i_j!\right)} \text{ for } i_j = 1,2,\ldots,d-1 \tag{4.10}$$

where Q and R are $D \times D$ matrices, as previously defined. This particular identification ensures that the limit $\epsilon \to 0$ of (4.9) is well defined. Additionally, the specific form of the matrices A_{i_j} have also been determined in order that certain physical requirements, such as ensuring that in the limit $\epsilon \to 0$ the same physics is obtained for a doubly occupied site as for two bosons on two neighbouring sites, are satisfied.

With these conventions, the continuum limit of this MPS is equivalent to the cMPS defined in (4.1). This can be shown via a Taylor expansion of the exponential operator $U_{-\ell/2,\ell/2}$ defined in (4.2), but is only mathematically rigorous when the entries of Q and R_α are finite and the operators $\hat{\psi}^\dagger(x)$ are bounded.

cMPS and cavity-QED

A continuous matrix product state can be identified as the stationary output of a cavity-QED apparatus. This identification was anticipated in [Verstraete and Cirac, 2010, Osborne et al., 2010, Schön et al., 2005] and is further elucidated below. It implies that the stationary quantum field states emerging from a cavity are of cMPS type. Furthermore, all quantum field states admit a cMPS description [Brockt et al., 2012].

Consider a cavity with several relevant modes described by annihilation/creation operators $\hat{a}_\alpha$, $\hat{a}_\beta^\dagger$ with $[\hat{a}_\alpha, \hat{a}_\beta^\dagger] = \delta_{\alpha\beta}$, that are coupled to some intracavity medium. The Hamiltonian describing the cavity modes, intracavity medium and their coupling is denoted by $\hat{H}_{\mathrm{sys}}$. Furthermore, each cavity mode is coupled to a continuum of field modes $\hat{a}_\alpha(\omega)$ with $[\hat{a}_\alpha(\omega), \hat{a}_\beta^\dagger(\overline{\omega})] = \delta(\omega - \overline{\omega})\delta_{\alpha\beta}$ outside the cavity through one of its end mirrors. (The generalisation to the case of double-sided cavities, for example, is immediate.) The total Hamiltonian for the cavity, the intracavity medium, and the outside field (see (3.52) in section 3.4.2) is

$$\hat{H}_{cQED}(t) = \hat{H}_{sys}\otimes\mathbb{I} + \sum_\alpha \int d\omega \sqrt{\frac{\kappa_\alpha(\omega)}{2\pi}}\left(\hat{a}_\alpha \otimes \hat{a}_\alpha^\dagger(\omega)e^{-i\omega t} + \mathrm{h.c.}\right).$$

This Hamiltonian is written in an interaction picture with respect to the free energy of the continuous fields, and it is taken in a frame rotating at the resonance frequencies of the cavities. In the interaction picture and rotating frame each integral extends over a band width of frequencies around the respective cavity frequencies. The Markov approximation, which assumes $\kappa_\alpha(\omega) = \text{const.}$, holds to an excellent degree over the frequency range of interest, (see section 3.4.2). Under these assumptions it is common to define time-dependent operators

$$\hat{E}^+_\alpha(t) = \int \frac{d\omega}{\sqrt{2\pi}} \hat{a}_\alpha(\omega) \exp(-i\omega t), \tag{4.11}$$

that fulfill $[\hat{E}^+_\alpha(t), \hat{E}^-_\beta(t')] = \delta(t-t')$. These operators correspond to the time-dependent parts of the electric field components of the cavity output, and are defined such that $\langle \hat{E}^-(t)\hat{E}^+(t)\rangle$ denotes the intensity, or flux of photons per second. The Hamiltonian then becomes

$$\hat{H}_{cQED}(t) = \hat{H}_{sys} \otimes \mathbb{I} + \sum_\alpha \sqrt{\kappa_\alpha} \left(\hat{a}_\alpha \otimes \hat{E}^-_\alpha(t) + \text{h.c.} \right). \tag{4.12}$$

This Hamiltonian can be rewritten in a more suitable form. A state $|\psi(t)\rangle$ can be obtained by applying the unitary time evolution operator generated by (4.12) on an initial state $|\psi_0\rangle$

$$|\psi(t)\rangle = \mathcal{T} \exp\left(-i \int_0^t ds \hat{H}_{cQED}(s) \right) |\psi_0\rangle$$

This time-ordered exponential can be rewritten as an infinitesimal product of exponentials

$$\mathcal{T} \exp\left(-i \int_0^t ds \hat{H}_{cQED}(s) \right) = \lim_{\epsilon \to 0} \exp\left(-i \int_{t-\epsilon}^t ds \hat{H}_{cQED}(s) \right) \ldots \exp\left(-i \int_0^\epsilon ds \hat{H}_{cQED}(s) \right)$$

and each exponential rewritten using the Baker-Campbell-Hausdorff formula, see [Hall, 2003] for example, that is

$$\begin{aligned} \exp\left(\int_{n\epsilon}^{(n+1)\epsilon} ds \left(A(s) + B(s)\right) \right) = \exp\left(\int_{n\epsilon}^{(n+1)\epsilon} ds A(s) \right) \exp\left(\int_{n\epsilon}^{(n+1)\epsilon} ds B(s) \right) \\ \times \exp\left(-\frac{1}{2} \int_{n\epsilon}^{(n+1)\epsilon} \int_{n\epsilon}^{(n+1)\epsilon} ds ds' \left[A(s), B(s')\right] \right) \times \ldots \end{aligned}$$

By identifying $A(s) = -i\hat{H}_{sys} \otimes \mathbb{I} - i \sum_\alpha \sqrt{\kappa_\alpha} \left(\hat{a}_\alpha \otimes \hat{E}^-_\alpha(t) \right)$ and $B(s) = -i \sum_\alpha \sqrt{\kappa_\alpha} \left(\hat{a}^\dagger_\alpha \otimes \hat{E}^+_\alpha(t) \right)$, neglecting higher order terms (since we take $\epsilon \to 0$) and assuming that the outside field modes are in the vacuum we find that the states generated by (4.12) are equivalent to those generated by an effective non-hermitian Hamiltonian

$$\hat{H}_{cQED}(t) = \hat{H}_{sys} \otimes \mathbb{I} - \sum_\alpha \frac{\kappa_\alpha}{2} \hat{a}^\dagger_\alpha \hat{a}_\alpha \otimes \mathbb{I} + \sum_\alpha \sqrt{\kappa_\alpha} \hat{a}_\alpha \otimes \hat{E}^-_\alpha(t).$$

When this Hamiltonian is compared to $\hat{H}_{\mathrm{cMPS}}(x)$ given in (4.3) the identification of the formalism of cMPS and cavity QED is immediate. By identifying $x = s\,t$, for an arbitrary scaling factor s, we have

$$\begin{aligned}\hat{H}_{cQED}(t) &= \hat{H}_{sys}\otimes\mathbb{I} - \sum_{\alpha}\frac{\kappa_\alpha}{2}\hat{a}_\alpha^\dagger\hat{a}_\alpha\otimes\mathbb{I} + \sum_{\alpha}\sqrt{\kappa_\alpha}\hat{a}_\alpha\otimes\hat{E}_\alpha^-(x/s)\\ &= Q\otimes\mathbb{I} + \sum_{\alpha=1}^{N} R_\alpha\otimes\hat{\psi}_\alpha^\dagger(x) = \hat{H}_{\mathrm{cMPS}}(x)\end{aligned}$$

with

$$\hat{\psi}^\dagger(x) = \frac{1}{\sqrt{s}}\hat{E}_\alpha^-(t), \qquad R_\alpha = \sqrt{\frac{\kappa_\alpha}{s}}\hat{a}_\alpha, \qquad Q = \frac{1}{s}\hat{H}_{sys} - \sum_{\alpha}\frac{R_\alpha^\dagger R_\alpha}{2}. \tag{4.13}$$

Note that the resulting cMPS is translationally invariant, since the parametrisation is position independent. In section 4.6 we will consider cMPS with this property in more detail. In any case, under the assumption that the field and the cavity system are in a state $|\Omega\rangle\otimes|\psi\rangle$ at some initial time t_0, we can see that the final state of the field outside the cavity at time t_1 is given by expression (4.6), allowing us to conclude that the state of the output modes of a cavity is always a continuous matrix product state. Formally these states are cMPS with an infinite-dimensional auxiliary system $D\to\infty$, evidently seen in the identification of R_α and Q in (4.13). However, due to energy constraints, the dimensions of the cavity system are effectively finite. The relevant dimension of the cavity Hilbert space then sets the dimension D of the auxiliary system in the cMPS formalism.

4.3 Regularity properties

Recall that at the beginning of this chapter we commented on the existence of certain constraints on the matrices $Q(x)$ and $R_\alpha(x)$ to ensure that characteristic physical quantities are well defined. One important property is that the expectation value of the kinetic energy term is sufficiently regular, that is sufficiently well behaved so as to produce a finite value. In second quantisation, see appendix A, the kinetic energy operator $\hat{T}$ is given by

$$\hat{T} = \int_{-\ell/2}^{\ell/2} dx\,\sum_{\alpha=1}^{N}\frac{1}{2m_\alpha}\frac{d\hat{\psi}_\alpha^\dagger(x)}{dx}\frac{d\hat{\psi}_\alpha(x)}{dx} \tag{4.14}$$

where the integrand gives the kinetic energy density at position x. We want to compute the kinetic energy expectation value $\langle\Psi(Q,\{R_\alpha\})|\hat{T}|\Psi(Q,\{R_\alpha\})\rangle$ and thus find constraints on $Q(x)$ and $R_\alpha(x)$ that ensure a finite value is always obtained. This means that we need to evaluate

$\frac{d\hat{\psi}_\alpha(x)}{dx}|\Psi(Q,\{R_\alpha\})\rangle$. First, we consider $\hat{\psi}_\alpha(x)|\Psi(Q,\{R_\alpha\})\rangle$

$$\begin{aligned}\hat{\psi}_\alpha(x)|\Psi(Q,\{R_\alpha\})\rangle &= \langle\omega_R|\hat{\psi}_\alpha(x)U_{\ell/2,-\ell/2}|\omega_L\rangle|\Omega\rangle \\ &= \langle\omega_R|\left[\hat{\psi}_\alpha(x),U_{\ell/2,-\ell/2}\right]|\omega_L\rangle|\Omega\rangle\end{aligned}$$

where in the second line we have used that $\hat{\psi}_\alpha(x)|\Omega\rangle = 0$ and inserted a commutator. Recall from (4.2) that $U_{\ell/2,-\ell/2} = \mathcal{P}e^{\int_{-\ell/2}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(t)dt}$. Therefore, to evaluate the above commutator we first remove the need of path ordering by partitioning the field into infinitesimally small sections that are correctly ordered, such that

$$\mathcal{P}e^{\int_{-\ell/2}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(t)dt} = \lim_{\epsilon\to 0}\left\{e^{\int_{\ell/2-\epsilon}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(t)dt}e^{\int_{\ell/2-2\epsilon}^{\ell/2-\epsilon}\hat{H}_{\mathrm{cMPS}}(t)dt}\dots e^{\int_{-\ell/2}^{-\ell/2+\epsilon}\hat{H}_{\mathrm{cMPS}}(t)dt}\right\}. \tag{4.15}$$

We then apply the commutation relation $[A,BC] = [A,B]C + B[A,C]$ to write

$$\begin{aligned}\left[\hat{\psi}_\alpha(x),\mathcal{P}e^{\int_{-\ell/2}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(t)dt}\right] &= \left[\hat{\psi}_\alpha(x),e^{\int_{\ell/2-\epsilon}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(t)dt}\right]\mathcal{P}e^{\int_{-\ell/2}^{\ell/2-\epsilon}\hat{H}_{\mathrm{cMPS}}(t)dt} \\ &+ e^{\int_{\ell/2-\epsilon}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(t)dt}\left[\hat{\psi}_\alpha(x),e^{\int_{\ell/2-2\epsilon}^{\ell/2-\epsilon}\hat{H}_{\mathrm{cMPS}}(t)dt}\right]\mathcal{P}e^{\int_{-\ell/2}^{\ell/2-2\epsilon}\hat{H}_{\mathrm{cMPS}}(t)dt} \\ &+ \dots + \mathcal{P}e^{\int_{-\ell/2+\epsilon}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(t)dt}\left[\hat{\psi}_\alpha(x),e^{\int_{-\ell/2}^{-\ell/2+\epsilon}\hat{H}_{\mathrm{cMPS}}(t)dt}\right] \\ &= \sum_i e^{\int_{\ell/2-i\epsilon}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(t)dt}\left[\hat{\psi}_\alpha(x),e^{\int_{\ell/2-(i+1)\epsilon}^{\ell/2-i\epsilon}\hat{H}_{\mathrm{cMPS}}(t)dt}\right]\mathcal{P}e^{\int_{-\ell/2}^{\ell/2-(i+1)\epsilon}\hat{H}_{\mathrm{cMPS}}(t)dt}\end{aligned}$$

We now further evaluate this expression by considering the commutator in the above RHS. We first approximate the integral in the exponential to first order, then further approximate the resulting exponential also to first order, leaving

$$\left[\hat{\psi}_\alpha(x),e^{\int_{\ell/2-(i+1)\epsilon}^{\ell/2-i\epsilon}\hat{H}_{\mathrm{cMPS}}(t)dt}\right] \approx \left[\hat{\psi}_\alpha(x),e^{\hat{H}_{\mathrm{cMPS}}(\ell/2-i\epsilon)}\right] \approx \left[\hat{\psi}_\alpha(x),\epsilon\hat{H}_{\mathrm{cMPS}}(\ell/2-i\epsilon)\right].$$

By taking the limit $\epsilon\to 0$ and a suitable substitution ($s=\ell/2-i\epsilon$) we can turn the sum into an integral. Furthermore, we can evaluate the commutator $\left[\hat{\psi}_\alpha(x),\hat{H}_{\mathrm{cMPS}}(s)\right] = R_\alpha(s)\otimes\delta(s-x)$ such that

$$\begin{aligned}\left[\hat{\psi}_\alpha(x),\mathcal{P}e^{\int_{-\ell/2}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(t)dt}\right] &= \int_{-\ell/2}^{\ell/2}ds\left(\mathcal{P}e^{\int_s^{\ell/2}\hat{H}_{\mathrm{cMPS}}(t)dt}\left[\hat{\psi}_\alpha(x),\hat{H}_{\mathrm{cMPS}}(s)\right]\mathcal{P}e^{\int_{-\ell/2}^{s}\hat{H}_{\mathrm{cMPS}}(t)dt}\right) \\ &= \mathcal{P}e^{\int_x^{\ell/2}\hat{H}_{\mathrm{cMPS}}(t)dt}R_\alpha(x)\mathcal{P}e^{\int_{-\ell/2}^{x}\hat{H}_{\mathrm{cMPS}}(t)dt}\end{aligned} \tag{4.16}$$

where again we have adopted the notation $R_\alpha(x)\equiv R_\alpha(x)\otimes\mathbb{I}$. We thus obtain

$$\hat{\psi}_\alpha(x)|\Psi(Q,\{R_\alpha\})\rangle = \langle\omega_R|U_{\ell/2,x}R_\alpha(x)U_{x,-\ell/2}|\omega_L\rangle|\Omega\rangle. \tag{4.17}$$

We can now use this result to calculate $\frac{d\hat{\psi}_\alpha(x)}{dx}|\Psi(Q,\{R_\alpha\})\rangle$. We are able to write that

$$\frac{d\hat{\psi}_\alpha(x)}{dx}|\Psi(Q,\{R_\alpha\})\rangle = \frac{d}{dx}\left(\hat{\psi}_\alpha(x)|\Psi(Q,\{R_\alpha\})\rangle\right)$$

since $\frac{d}{dx}|\Psi(Q,\{R_\alpha\})\rangle = \langle\omega_R|\frac{d}{dx}\left(U_{\ell/2,-\ell/2}\right)|\omega_L\rangle|\Omega\rangle = 0$ – the path ordered exponential $U_{\ell/2,-\ell/2}$ is not a function of x. Therefore, we apply the derivative to the product $\hat{\psi}_\alpha(x)|\Psi(Q,\{R_\alpha\})\rangle$ which, using (4.17), gives

$$\begin{aligned}\frac{d}{dx}\left(\hat{\psi}_\alpha(x)|\Psi(Q,\{R_\alpha\})\rangle\right) &= \langle\omega_R|\frac{dU_{(\ell/2,x)}}{dx}R_\alpha(x)U_{(x,-\ell/2)}|\omega_L\rangle|\Omega\rangle \\ &+ \langle\omega_R|U_{(\ell/2,x)}\frac{dR_\alpha(x)}{dx}U_{(x,-\ell/2)}|\omega_L\rangle|\Omega\rangle \\ &+ \langle\omega_R|U_{(\ell/2,x)}R_\alpha(x)\frac{dU_{(x,-\ell/2)}}{dx}|\omega_L\rangle|\Omega\rangle. \end{aligned} \tag{4.18}$$

The derivatives with respect to x of $U_{(\ell/2,x)}$ and $U_{(x,-\ell/2)}$ are non-zero. To show this we again use the representation of the path ordered exponential as given in (4.15) such that

$$\begin{aligned}\frac{d}{dx}\left(\mathcal{P}e^{\int_x^{\ell/2}\hat{H}_{\text{cMPS}}(s)ds}\right) &= \lim_{\epsilon\to 0}\left\{e^{\int_{\ell/2-\epsilon}^{\ell/2}\hat{H}_{\text{cMPS}}(s)ds}\ldots e^{\int_{x+\epsilon}^{x+2\epsilon}\hat{H}_{\text{cMPS}}(s)ds}\frac{d}{dx}\left(e^{\int_x^{x+\epsilon}\hat{H}_{\text{cMPS}}(s)ds}\right)\right\} \\ &= -\lim_{\epsilon\to 0}\left\{e^{\int_{\ell/2-\epsilon}^{\ell/2}\hat{H}_{\text{cMPS}}(s)ds}\ldots e^{\int_{x+\epsilon}^{x+2\epsilon}\hat{H}_{\text{cMPS}}(s)ds}\hat{H}_{\text{cMPS}}(x)e^{\int_x^{x+\epsilon}\hat{H}_{\text{cMPS}}(s)ds}\right\}\end{aligned}$$

Now, since in the limit $\epsilon\to 0$ we can write $e^{\int_x^{x+\epsilon}\hat{H}_{\text{cMPS}}(s)ds}\approx e^{\epsilon\hat{H}_{\text{cMPS}}(x)}$ we find that $\hat{H}_{\text{cMPS}}(x)$ and $e^{\int_x^{x+\epsilon}\hat{H}_{\text{cMPS}}(s)ds}$ commute. Therefore

$$\frac{d}{dx}\left(\mathcal{P}e^{\int_x^{\ell/2}\hat{H}_{\text{cMPS}}(s)ds}\right) = -\mathcal{P}e^{\int_x^{\ell/2}\hat{H}_{\text{cMPS}}(s)ds}\hat{H}_{\text{cMPS}}(x). \tag{4.19}$$

Similarly, it is straightforward to show that

$$\frac{d}{dx}\left(\mathcal{P}e^{\int_{-\ell/2}^{x}\hat{H}_{\text{cMPS}}(s)ds}\right) = \hat{H}_{\text{cMPS}}(x)\mathcal{P}e^{\int_{-\ell/2}^{x}\hat{H}_{\text{cMPS}}(s)}. \tag{4.20}$$

Substitution of these identities into (4.18) leads to

$$\begin{aligned}\frac{d\hat{\psi}_\alpha(x)}{dx}|\Psi(Q,\{R_\alpha\})\rangle &= \langle\omega_R|U_{(\ell/2,x)}\left(-[Q(x),R_\alpha(x)]+\frac{dR_\alpha(x)}{dx}\right)U_{(x,-\ell/2)}|\omega_L\rangle|\Omega\rangle \\ &+ \langle\omega_R|U_{(\ell/2,x)}\left(\left[\sum_{\beta=1}^{N}R_\alpha(x)R_\beta(x)-R_\beta(x)R_\alpha(x)\right]\otimes\hat{\psi}^\dagger_\beta(x)\right)U_{(x,-\ell/2)}|\omega_L\rangle|\Omega\rangle\end{aligned} \tag{4.21}$$

The second term of the RHS contains a divergent contribution, since the $\hat{\psi}^\dagger_\beta(x)|\Omega\rangle$ means that particles of any bosonic species $\beta = 1,\ldots,N$ are being created at fixed position x. Therefore this second term is not normalisable unless we impose the condition that

$$\left[R_\alpha(x),R_\beta(x)\right] = 0 \qquad \forall x\in[-\ell/2,\ell/2]\,. \tag{4.22}$$

Thus the matrices $\{R_\alpha\}$ should satisfy the same commutation relations as the particle creation and annihilation operators to which they couple. When considering systems with a single species of bosons this regularity condition is automatically satisfied.

The differentiability constraint is sufficient to ensure a finite kinetic energy expectation is produced, which is arguably the most important physical requirement. In addition it is also possible to impose higher regularity constraints of n-th order derivatives and mixed derivatives. Physical considerations concerning particle statistics also leads to restrictions on the form of $Q(x)$ and $R_\alpha(x)$, but we do not explore this any further in this thesis and instead refer to [Haegeman, 2011, Haegeman et al., 2011a].

4.4 Calculating expectation values

In this section we calculate quantities of interest such as the norm of the cMPS, expectation values of operators and correlation functions. Since such quantities depend on the auxiliary system, we first consider the associated state and system dynamics in order to perform the desired calculations.

4.4.1 Density Matrices

In the case of open boundary conditions $B = |\omega_R\rangle\langle\omega_L|$ we define a density matrix $\rho(x) \in \mathbb{C}^D \otimes \overline{\mathbb{C}}^D$ corresponding to $|\omega_R\rangle$ as the state of the auxiliary system after $U_{x,-\ell/2}$ has been applied to the composite system $|\omega_R\rangle\langle\omega_R| \otimes |\Omega\rangle\langle\Omega|$, that is

$$\rho(x) = \mathrm{Tr}_{\mathcal{F}[-\ell/2,x])} \left(U_{x,-\ell/2} \left(|\omega_R\rangle\langle\omega_R| \otimes |\Omega\rangle\langle\Omega|_{[-\ell/2,x]} \right) U_{x,-\ell/2}^\dagger \right) \tag{4.23}$$

with the initial condition $\rho(-\ell/2) = |\omega_R\rangle\langle\omega_R|$. $\mathrm{Tr}_{\mathcal{F}[-\ell/2,x]}$ denotes the partial trace over the field from $-\ell/2$ to x and $|\Omega\rangle\langle\Omega|_{[-\ell/2,x]}$ is the field vacuum at $[-\ell/2, x]$. We think of $\rho(x)$ as the *right* density matrix of the auxiliary system. Starting from a pure state at $-\ell/2$ and working from left to right towards x the auxiliary system interacts with the field, which is initially in the vacuum state, via the operator $U_{x,-\ell/2}$, as illustrated in Fig. 4.1. The auxiliary system therefore influences the state of the quantum field, and for this reason it is of interest to study the auxiliary system dynamics. To do this we derive a master equation for the density operator $\rho(x)$. Using (4.23) we have that

$$\rho(x+\epsilon) = \mathrm{Tr}_{\mathcal{F}[x,x+\epsilon])} \left(U_{x+\epsilon,x} \left(\rho(x) \otimes |\Omega\rangle\langle\Omega|_{[x,x+\epsilon]} \right) U_{x+\epsilon,x}^\dagger \right). \tag{4.24}$$

By expanding $U_{x+\epsilon,x}$ as a Taylor series and using the definition of $\rho(x)$ in (4.23) (see appendix (B.2) for a detailed calculation) we find that

$$\rho(x+\epsilon) = \rho(x) + \epsilon \left(\rho(x)Q^\dagger(x) + Q(x)\rho(x) + \sum_{\alpha=1}^{N} R_\alpha(x)\rho(x)R_\alpha^\dagger(x) \right) + O(\epsilon\sqrt{\epsilon}).$$

We then use the forward finite difference formula to find that $\rho(x)$ satisfies

$$\frac{d\rho(x)}{dx} = \lim_{\epsilon\to 0}\frac{\rho(x+\epsilon)-\rho(x)}{\epsilon} = Q(x)\rho(x)+\rho(x)Q^\dagger(x)+\sum_{\alpha=1}^{N} R_\alpha(x)\rho(x)R_\alpha^\dagger(x). \tag{4.25}$$

The master equation is of Lindblad form, see e.g [Gardiner and Zoller, 2000], and describes the dynamics of the auxiliary system. We note that the evolution is trace preserving, since taking the trace of the master equation gives $\mathrm{tr}\left[d\rho(x)/dx\right] = d\,\mathrm{tr}\left[\rho(x)\right]/dx = 0$.

We can also define a *left* density matrix $\sigma(x) \in \mathbb{C}^D \otimes \overline{\mathbb{C}}^D$ with the initial condition $\sigma(\ell/2) = |\omega_L\rangle\langle\omega_L|$ that this time works from right to left. Because of this reverse direction, $\sigma(x)$ is defined to be the state of the auxiliary system after $U_{\ell/2,x}^\dagger$ has been applied to $|\omega_L\rangle\langle\omega_L|\otimes\mathbb{I}$, that is

$$\sigma(x) = \mathrm{Tr}_{\mathcal{F}[x,\ell/2])}\left(U_{\ell/2,x}^\dagger\left(|\omega_L\rangle\langle\omega_L|\otimes\mathbb{I}\right)U_{\ell/2,x}\left(\mathbb{I}\otimes|\Omega\rangle\langle\Omega|_{x,\ell/2}\right)\right). \tag{4.26}$$

We view this operator as acting backwards, or undoing the interaction of $U_{\ell/2,x}$ with the field vacuum, and as a result the structure of (4.26) is notably different to that of (4.23). Following similar calculations to that presented in appendix (B.2) we find that $\sigma(x)$ satisfies the following differential equation

$$\frac{d\sigma(x)}{dx} = \sigma(x)Q(x)+Q^\dagger(x)\sigma(x)+\sum_{\alpha=1}^{N} R_\alpha^\dagger(x)\sigma(x)R_\alpha(x). \tag{4.27}$$

It is now slightly more convenient to move to a different representation for the state of our auxiliary system. This representation, known as the Jamiolkowski isomorphism [Jamiolkowski, 1972, Arrighi and Patricot, 2004] in the quantum information literature, is simply an alternative notation to represent the Hilbert space of operators on a Hilbert space. Operators A (of dimension D, say) are identified with quantum state vectors $|A\rangle$ via

$$A = \sum_{j,k=1}^{D} a_{jk}|j\rangle\langle k| \qquad \mapsto \qquad |A\rangle = \sum_{j,k=1}^{D} a_{jk}|j\rangle|k\rangle. \tag{4.28}$$

Thus, we simply flatten given operators into vector form. From this definition we see that the operation of multiplication on the left or right of A by operator B becomes in this notation

$$BA \mapsto B\otimes\mathbb{I}|A\rangle, \qquad AB \mapsto \mathbb{I}\otimes B^T|A\rangle \tag{4.29}$$

such that the operation of multiplication on the left and right by matrices B and C respectively gives $BAC = B\otimes C^T|A\rangle$. In terms of this new notation the Lindblad equations (4.25) and

(4.27) that describe the dynamics of the auxiliary system become matrix equations:

$$\frac{d}{dx}|\rho(x)\rangle = \left[Q(x)\otimes\mathbb{I}+\mathbb{I}\otimes\overline{Q}(x)+\sum_{\alpha=1}^{N}R_\alpha(x)\otimes\overline{R}_\alpha(x)\right]|\rho(x)\rangle =: M(x)|\rho(x)\rangle \tag{4.30}$$

$$\frac{d}{dx}|\sigma(x)\rangle = \left[\mathbb{I}\otimes Q^T(x)+Q^\dagger(x)\otimes\mathbb{I}+\sum_{\alpha=1}^{N}R_\alpha^\dagger(x)\otimes R_\alpha^T(x)\right]|\sigma(x)\rangle = M^\dagger(x)|\sigma(x)\rangle. \tag{4.31}$$

The solutions of (4.30) and (4.31) are given by

$$|\rho(x)\rangle = \mathcal{P}e^{\int_{-\ell/2}^{x}M(s)ds}|\rho(-\ell/2)\rangle = \mathcal{P}e^{\int_{-\ell/2}^{x}M(s)ds}|\omega_R\rangle|\omega_R\rangle \tag{4.32}$$

$$\langle\sigma(x)| = \langle\sigma(\ell/2)|\mathcal{P}e^{\int_{x}^{\ell/2}M(s)ds} = \langle\omega_L|\langle\omega_L|\mathcal{P}e^{\int_{x}^{\ell/2}M(s)ds}. \tag{4.33}$$

We now give some important properties of the generator $M(x)$. It is known that the matrix is diagonalisable, such that the spectral decomposition can be written

$$M = S\left(\sum_{j=1}^{D}m_j|j\rangle\langle j|\right)S^{-1} = SDS^{-1} \tag{4.34}$$

where S is the matrix whose i-th column is the i-th right eigenvector of M (and correspondingly the i-th column of the matrix S^{-1} is the i-th left eigenvector of M). The eigenvalues m_j are assumed to be arranged in decreasing real part, such that $m_1 = 0$. The existence of this eigenvalue is ensured by the existence of a stationary state, i.e. $d|\rho(x)\rangle/dx = 0$. All other eigenvalues $m_j, j > 1$ have negative real part. For details and proofs of these and further properties, see [Baumgartner and Narnhofer, 2008].

4.4.2 Normalisation of state

We are now in a position to calculate the norm of the continuous matrix product state and expectation values of observables. First we consider the norm of the state. Using the relation $\langle x|y\rangle = \mathrm{Tr}\left[|y\rangle\langle x|\right]$ for any vectors $|x\rangle$ and $|y\rangle$ we have that

$$\begin{aligned}
&\langle\Psi(\overline{Q},\{\overline{R}_\alpha\})|\Psi(Q,\{R_\alpha\})\rangle = \mathrm{Tr}\left[|\Psi(Q,\{R_\alpha\})\rangle\langle\Psi(\overline{Q},\{\overline{R}_\alpha\})|\right]\\
&= \mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,-\ell/2}|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|U^\dagger_{\ell/2,-\ell/2}|\omega_L\rangle\right]\\
&= \mathrm{Tr}_{x,\ell/2}\left[\mathrm{Tr}_{-\ell/2,x}\left[\langle\omega_L|U_{\ell/2,x}U_{x,-\ell/2}|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|U^\dagger_{x,-\ell/2}U^\dagger_{\ell/2,x}|\omega_L\rangle\right]\right]\\
&= \mathrm{Tr}_{x,\ell/2}\left[\langle\omega_L|U_{\ell/2,x}\rho(x)\otimes|\Omega\rangle\langle\Omega|_{x,\ell/2}U^\dagger_{\ell/2,x}|\omega_L\rangle\right]
\end{aligned}$$

where $\mathrm{Tr}_{a,b}$ denotes the trace over the field from a to b and $|\Omega\rangle\langle\Omega|_{a,b}$ the field vacuum on $[a,b]$ only. We then explicitly include the trace over the auxiliary system, denoted by tr, by

moving the boundary vector $|\omega_L\rangle$ and perform the trace over the remaining field to obtain

$$\begin{aligned}\langle\Psi(\overline{Q},\{\overline{R}_\alpha\}|\Psi(Q,\{R_\alpha\}\rangle &= \mathrm{Tr}_{x,\ell/2}\left[\mathrm{tr}\left[|\omega_L\rangle\langle\omega_L|U_{\ell/2,x}\rho(x)\otimes|\Omega\rangle\langle\Omega|_{x,\ell/2}U^\dagger_{\ell/2,x}\right]\right]\\ &= \mathrm{tr}\left[\langle\Omega|_{x,\ell/2}U^\dagger_{\ell/2,x}\left(|\omega_L\rangle\langle\omega_L|\otimes\mathbb{I}\right)U_{\ell/2,x}|\Omega\rangle_{x,\ell/2}\rho(x)\right]\\ &= \mathrm{tr}\left[\sigma(x)\rho(x)\right] = \langle\sigma(x)|\rho(x)\rangle, \qquad \forall x\in[-\ell/2,\ell/2]\end{aligned}$$

with $|\rho(x)\rangle$ and $\langle\sigma(x|$ are as defined in (4.32) and (4.33) respectively. This norm is guaranteed to be positive since the Jamiolkowski representation preserves the positivity of the density matrices $\rho(x)$ and $\sigma(x)$ [Jamiolkowski, 1972].

4.4.3 Calculation of expectation values

We now consider calculating expectation values of observables. Let $\mathcal{O}$ be an observable on $\mathcal{F}$ that is some product of the field operators $\hat{\psi}_\alpha(x),\hat{\psi}^\dagger_\alpha(x)$ and their derivatives at locations $x_1,x_2,\ldots,x_n\in[-\ell/2,\ell/2]$ in the continuum. We calculate quantities of the form

$$\langle\Psi(\overline{Q},\{\overline{R_\alpha}\})|\mathcal{O}|\Psi(Q,\{R_\alpha\})\rangle = \mathrm{Tr}\left[(\mathbb{I}\otimes\mathcal{O})\langle\omega_L|U_{\ell/2,-\ell/2}|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|U^\dagger_{\ell/2,-\ell/2}|\omega_L\rangle\right]$$

where we assume that the observable is normally ordered, that is with all field annihilation operators on the right. We illustrate the method by defining a generic Hamiltonian for a single-species (α =1) bosonic system in second quantisation

$$\begin{aligned}\hat{H}=\hat{T}+\hat{V}+\hat{W} = &\int_{-\ell/2}^{\ell/2}dx\frac{1}{2m}\frac{d\hat{\psi}^\dagger(x)}{dx}\frac{d\hat{\psi}(x)}{dx}+\int_{-\ell/2}^{\ell/2}dx\,v(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\\ &+\frac{1}{2}\int_{-\ell/2}^{\ell/2}dx\int_{-\ell/2}^{\ell/2}dy\,w(x,y)\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)\hat{\psi}(y)\hat{\psi}(x)\end{aligned} \tag{4.35}$$

that describes particles with mass m interacting with an external potential $v(x)$ and with each other through a two-particle interaction $w(x,y)=w(y,x)$. We detail the calculation for the expected value of the interaction term $\hat{W}$; a pattern for evaluating other, similar expectation values can be quickly established.

Interaction

We consider the expectation of the interaction energy, i.e. $\mathcal{O}=\hat{W}$. We first focus on the expectation value of the combination of field operators that form the integrand and calculate

$$\begin{aligned}&\langle\Psi|\left(\hat{\psi}^\dagger(y)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(y)\right)|\Psi\rangle = \mathrm{Tr}\left[\left(\hat{\psi}(y)\hat{\psi}(x)|\Psi\rangle\right)\left(\hat{\psi}(y)\hat{\psi}(x)|\Psi\rangle\right)^\dagger\right]\\ &\quad=\mathrm{Tr}_{-\ell/2,\ell/2}\left[\langle\omega_L|\hat{\psi}(x)\hat{\psi}(y)U_{\ell/2,-\ell/2}|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|U^\dagger_{\ell/2,-\ell/2}\hat{\psi}^\dagger(y)\hat{\psi}^\dagger(x)|\omega_L\rangle\right]\end{aligned}$$

where we have omitted the arguments Q and R_α in the state $|\Psi(Q,\{R_\alpha\})\rangle$. To eliminate the field operators we employ the techniques used in section 4.3, in particular (4.16) and (4.17). Since the field operator $\hat{\psi}(y)$ annihilates the vacuum $|\Omega\rangle$, that is $\hat{\psi}(y)|\Omega\rangle = 0$, we are able to replace the products $\hat{\psi}(y)U_{\ell/2,-\ell/2}$ and $\left(\hat{\psi}(y)U_{\ell/2,-\ell/2}\right)^\dagger$ with commutators $\left[\hat{\psi}(y), U_{\ell/2,-\ell/2}\right]$ and $\left[\hat{\psi}(y), U_{\ell/2,-\ell/2}\right]^\dagger$. Using (4.16) we can then write

$$\begin{aligned}&\langle\Psi|\left(\hat{\psi}^\dagger(y)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(y)\right)|\Psi\rangle \\ &= \mathrm{Tr}_{-\ell/2,\ell/2}\left[\langle\omega_L|\hat{\psi}(x)U_{\ell/2,y}R(y)U_{y,-\ell/2}|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|U^\dagger_{y,-\ell/2}R^\dagger(y)U^\dagger_{\ell/2,y}\hat{\psi}^\dagger(x)|\omega_L\rangle\right].\end{aligned} \tag{4.36}$$

The remaining field operators can be eliminated by applying the same method as before. We replace the products $\hat{\psi}(x)U_{\ell/2,y}R(y)U_{y,-\ell/2}$ and $\left(\hat{\psi}(x)U_{\ell/2,y}R(y)U_{y,-\ell/2}\right)^\dagger$ with the commutators

$$\begin{aligned}\left[\hat{\psi}(x), U_{\ell/2,y}R(y)U_{y,-\ell/2}\right] &= \Theta(x-y)U_{\ell/2,x}R(x)U_{x,y}R(y)U_{y,-\ell/2} \\ &\quad+\Theta(y-x)U_{\ell/2,y}R(y)U_{y,x}R(x)U_{x,-\ell/2}\end{aligned} \tag{4.37}$$

$$\begin{aligned}\left[\hat{\psi}(x), U_{\ell/2,y}R(y)U_{y,-\ell/2}\right]^\dagger &= \Theta(x-y)U^\dagger_{y,-\ell/2}R^\dagger(y)U^\dagger_{x,y}R^\dagger(x)U^\dagger_{\ell/2,x} \\ &\quad+\Theta(y-x)U^\dagger_{x,-\ell/2}R^\dagger(x)U^\dagger_{y,x}R^\dagger(y)U^\dagger_{\ell/2,y}\end{aligned} \tag{4.38}$$

where Θ is the heaviside step function, defined via

$$\Theta(x-y) = \begin{cases} 1 & x < y, \\ 0 & x > y \end{cases}$$

with the convention that $\Theta(0) = 1/2$. We then proceed as follows. For $x > y$ we evaluate

$$\begin{aligned}\mathrm{Tr}_{-\ell/2,\ell/2}\left[\langle\omega_L|U_{\ell/2,x}R(x)U_{x,y}R(y)U_{y,-\ell/2}|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|\right. \\ \left.\times U^\dagger_{y,-\ell/2}R^\dagger(y)U^\dagger_{x,y}R^\dagger(x)U^\dagger_{\ell/2,x}|\omega_L\rangle\right].\end{aligned} \tag{4.39}$$

We first separate the trace over the field into two regions, $\mathrm{Tr}_{-\ell/2,\ell/2} = \mathrm{Tr}_{-\ell/2,y}\mathrm{Tr}_{y,\ell/2}$. Using the definition of the right density matrix $\rho(y)$, as introduced in (4.23), the above then simplifies to

$$\mathrm{Tr}_{y,\ell/2}\left[\langle\omega_L|U_{\ell/2,x}R(x)U_{x,y}\left(R(y)\rho(y)R^\dagger(y)\right)\otimes|\Omega\rangle\langle\Omega|_{y,\ell/2}U^\dagger_{x,y}R^\dagger(x)U^\dagger_{\ell/2,x}|\omega_L\rangle\right]. \tag{4.40}$$

Separating the trace once more into regions $\left[y,x\right]$ and $[x,\ell/2]$ we repeat the procedure above. We define $\tau(x)$ to be the state of the auxiliary system after $U_{x,y}$ has been applied to the composite system $R(y)\rho(y)R^\dagger(y)\otimes|\Omega\rangle\langle\Omega|_{y,x}$, namely

$$\tau(x) = \mathrm{Tr}_{y,x}\left[U_{x,y}\left(R(y)\rho(y)R^\dagger(y)\otimes|\Omega\rangle\langle\Omega|_{y,x}\right)U^\dagger_{x,y}\right]$$

with the initial condition $\tau(y) = R(y)\rho(y)R^\dagger(y)$. It can be shown that $\tau(x)$ satisfies the following differential equation

$$\frac{d\tau(x)}{dx} = Q(x)\tau(x) + \tau(x)Q^\dagger(x) + \sum_{\alpha=1}^{N} R_\alpha(x)\tau(x)R_\alpha^\dagger(x),$$

with solution $\tau(x) = \mathcal{P}e^{\int_y^x M(s)ds} R(y)\rho(y)R^\dagger(y)$ by using techniques analogous to that in appendix (B.2). Substituting this expression into (4.40) means we evaluate

$$\mathrm{Tr}_{x,\ell/2}\left[\langle\omega_L|U_{\ell/2,x}\left(R(x)\tau(x)R^\dagger(x)\right)\otimes|\Omega\rangle\langle\Omega|_{x,\ell/2}U_{\ell/2,x}^\dagger|\omega_L\rangle\right]. \tag{4.41}$$

Application of the formula $\mathrm{Tr}_{I,II}\left[A_{I,II}(B_I\otimes|C\rangle\langle C|_{II})\right] = \mathrm{tr}_I\left[\langle C|_I A_{I,II}|C\rangle_{II}B_I\right]$, where in this case I and II denotes the auxiliary and field systems respectively, $A_{I,II} = U_{\ell/2,x}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,x}$, $B_I = \left(R(x)\tau(x)R^\dagger(x)\right)$ and $|C\rangle_{II} = |\Omega\rangle$, gives

$$\begin{aligned}&\mathrm{Tr}_{x,\ell/2}\left[\mathrm{tr}\left[U_{\ell/2,x}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,x}\left(R(x)\tau(x)R^\dagger(x)\right)\otimes|\Omega\rangle\langle\Omega|_{x,\ell/2}\right]\right]\\ =&\mathrm{tr}\left[\langle\Omega|_{x,\ell/2}U_{\ell/2,x}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,x}|\Omega\rangle_{x,\ell/2}\left(R(x)\tau(x)R^\dagger(x)\right)\right]\end{aligned} \tag{4.42}$$

with tr denoting the trace over the auxiliary system only.

We now use the definition of the left density matrix $\sigma(x)$ given by (4.26) to simplify this expression further. We have that

$$\begin{aligned}\mathrm{tr}\left[\langle\Omega|_{x,\ell/2}U_{\ell/2,x}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,x}|\Omega\rangle_{x,\ell/2}\left(R(x)\tau(x)R^\dagger(x)\right)\right] &= \mathrm{tr}\left[\sigma(x)R(x)\tau(x)R^\dagger(x)\right]\\ &= \langle R^\dagger(x)\sigma(x)R(x)|\tau(x)\rangle\end{aligned}$$

where in the last line we have switched representations and flattened our matrices into vector form via the Jamiolkowski representation. To obtain our final form we now substitute for $\tau(x)$ and, to separate the density matrices from the variational matrices, write the vectors as products of matrices and vectors. We have that, for $x > y$,

$$\begin{aligned}\langle\Psi|\left(\hat\psi^\dagger(y)\hat\psi^\dagger(x)\hat\psi(x)\hat\psi(y)\right)|\Psi\rangle &= \langle R^\dagger(x)\sigma(x)R(x)|\mathcal{P}e^{\int_y^x M(s)ds}|R(y)\rho(y)R^\dagger(y)\rangle \qquad (4.43)\\ &= \langle\sigma(x)|\left(R(x)\otimes\overline{R}(x)\right)\mathcal{P}e^{\int_y^x M(s)ds}\left(R(y)\otimes\overline{R}(y)\right)|\rho(y)\rangle.\end{aligned}$$

Evaluating $y > x$ is analogous: We obtain

$$\langle\Psi|\left(\hat\psi^\dagger(y)\hat\psi^\dagger(x)\hat\psi(x)\hat\psi(y)\right)|\Psi\rangle = \langle\sigma(y)|\left(R(y)\otimes\overline{R}(y)\right)\mathcal{P}e^{\int_x^y M(s)ds}\left(R(x)\otimes\overline{R}(x)\right)|\rho(x)\rangle. \tag{4.44}$$

For the case $x = y$ the calculation above is less complicated. We proceed as before, first simplifying (4.36) by inserting the corresponding commutation relations (4.37) and

(4.38). Clearly, from the definition given in (4.2) we have that $U_{y,x} = U_{x,y} = \mathbb{I}$ for $x = y$. Along with the convention $\Theta(0) = 1/2$, this means that (4.37) and (4.38) can be written $\left[\hat{\psi}(x), U_{\ell/2,x} R(x) U_{x,-\ell/2}\right] = U_{\ell/2,x} R^2(x) U_{x,-\ell/2}$ and $\left[\hat{\psi}(x), U_{\ell/2,x} R(x) U_{x,-\ell/2}\right]^\dagger = U^\dagger_{x,-\ell/2} \left(R^\dagger(x)\right)^2 U^\dagger_{\ell/2,x}$, such that (4.40) becomes

$$\mathrm{Tr}_{y,\ell/2}\left[\langle\omega_L| U_{\ell/2,x}\left(R^2(x)\rho(x)\left(R^\dagger(x)\right)^2\right) \otimes |\Omega\rangle\langle\Omega|_{x,\ell/2} U^\dagger_{\ell/2,x} |\omega_L\rangle\right].$$

We now have an equation of the form (4.41) and so the need to define an auxiliary system density matrix τ is avoided. We therefore proceed as before, rewriting the field trace in terms of the auxiliary system trace as in (4.42), then using the definition of $\sigma(x)$ to obtain

$$\langle\Psi|\left(\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x)\right)|\Psi\rangle = \langle\sigma(x)|R^2(x)\rho(x)\left(R^\dagger(x)\right)^2\rangle = \langle\sigma(x)|\left(R(x)\otimes\overline{R}(x)\right)^2|\rho(x)\rangle. \tag{4.45}$$

Note that this result can be seen directly from (4.43) and (4.44), since taking $x = y$ removes the path-ordered exponential, which along with the symmetry of the expressions for $x > y$ and $y > x$ and the convention $\Theta(0) = 1/2$ gives precisely (4.45). Combining the evaluations we hence find that

$$\begin{aligned}\langle\Psi|\hat{\psi}^\dagger(y)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(y)|\Psi\rangle = \\ \Theta(x-y)\langle\sigma(x)|\left(R(x)\otimes\overline{R(x)}\right)\mathcal{P}e^{\int_y^x M(s)ds}\left(R(y)\otimes\overline{R(y)}\right)|\rho(y)\rangle \\ +\Theta(y-x)\langle\sigma(y)|\left(R(y)\otimes\overline{R(y)}\right)\mathcal{P}e^{\int_x^y M(s)ds}\left(R(x)\otimes\overline{R(x)}\right)|\rho(x)\rangle.\end{aligned}$$

Therefore, for every $y \in [-\ell/2, x)$ say, we can write the expectation value of the interaction energy as

$$\begin{aligned}\langle\Psi|\hat{W}|\Psi\rangle = \int_{-\ell/2}^{\ell/2} dx \int_{-\ell/2}^{x} dy\, w(x,y)\langle\sigma(x)|\left(R(x)\otimes\overline{R(x)}\right) \\ \times\mathcal{P}e^{\int_y^x M(s)ds}\left(R(y)\otimes\overline{R(y)}\right)|\rho(y)\rangle\end{aligned} \tag{4.46}$$

Kinetic and Chemical Potential

Using similar techniques and results from section 4.3 one can readily show that

$$\begin{aligned}\langle\Psi|\hat{T}|\Psi\rangle &= \frac{1}{2m}\int_{-\ell/2}^{\ell/2} dx\ \langle\sigma(x)|\left([Q(x),R(x)] + \frac{dR(x)}{dx}\right)\otimes\left(\left[\overline{Q(x)},\overline{R(x)}\right] + \frac{d\overline{R(x)}}{dx}\right)|\rho(x)\rangle \\ \langle\Psi|\hat{V}|\Psi\rangle &= \int_{-\ell/2}^{\ell/2} dx\ v(x)\langle\sigma(x)|R(x)\otimes\overline{R(x)}|\rho(x)\rangle.\end{aligned} \tag{4.47}$$

We can therefore use the linearity of the expectation value operator and combine the above results to calculate $\langle\Psi|\hat{H}|\Psi\rangle = \langle\Psi|\hat{V}|\Psi\rangle + \langle\Psi|\hat{W}|\Psi\rangle + \langle\Psi|\hat{T}|\Psi\rangle$.

4.4.4 Correlation functions

Here we show how to calculate one particle and density-density correlation functions. These functions can be used to verify that our cMPS captures characteristic features of the physical system of interest by showing expected, or sometimes even known, behaviour. The one-particle correlation function shows how likely a particle created at position x will be found at some other position y. The density-density correlation function provides information about the separation distance between two particles.

One particle correlation function

For the one particle correlation function we calculate, again omitting the arguments Q and R_α in the state $|\Psi(Q,\{R_\alpha\})\rangle$,

$$\begin{aligned}\langle\Psi|\hat{\psi}^\dagger(x)\hat{\psi}(y)|\Psi\rangle &= \mathrm{Tr}_{-\ell/2,\ell/2}\left[\left(\hat{\psi}(y)|\Psi\rangle\right)\left(\hat{\psi}(x)|\Psi\rangle\right)^\dagger\right]\\ &= \mathrm{Tr}_{-\ell/2,\ell/2}\left[\langle\omega_L|\hat{\psi}(y)U_{\ell/2,-\ell/2}|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|U^\dagger_{\ell/2,-\ell/2}\hat{\psi}^\dagger(x)|\omega_L\rangle\right].\end{aligned}$$

We follow a method similar to the above calculation of the expectation value of the interaction energy $\langle\Psi|\hat{W}|\Psi\rangle$. We again use that $\hat{\psi}(y)|\Omega\rangle = 0$ so that we can replace the products $\hat{\psi}(y)U_{\ell/2,-\ell/2}$ and $U^\dagger_{\ell/2,-\ell/2}\hat{\psi}^\dagger(x)$ with the commutators $\left[\hat{\psi}(y),U_{\ell/2,-\ell/2}\right]$ and $\left[U^\dagger_{\ell/2,-\ell/2},\hat{\psi}^\dagger(x)\right]$ respectively. Evaluating these commutators using (4.16) gives

$$\begin{aligned}&\langle\Psi|\hat{\psi}^\dagger(x)\hat{\psi}(y)|\Psi\rangle\\ &= \mathrm{Tr}_{-\ell/2,\ell/2}\left[\langle\omega_L|U_{\ell/2,y}R(y)U_{y,-\ell/2}|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|U^\dagger_{x,-\ell/2}R^\dagger(x)U^\dagger_{\ell/2,x}|\omega_L\rangle\right].\end{aligned}$$

To complete the calculation we now distinguish between the different cases $x<y$ and $y<x$ and separate the operators $U_{c,a}$ into products $U_{c,b}U_{b,a}$ for $a\le b\le c$ accordingly:

$$\begin{aligned}&\langle\Psi|\hat{\psi}^\dagger(x)\hat{\psi}(y)|\Psi\rangle\\ &= \Theta\left(x-y\right)\mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,x}U_{x,y}R(y)U_{y,-\ell/2}|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|U^\dagger_{y,-\ell/2}U^\dagger_{x,y}R^\dagger(x)U^\dagger_{\ell/2,x}|\omega_L\rangle\right]\\ &+ \Theta\left(y-x\right)\mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,y}R(y)U_{y,x}U_{x,-\ell/2}|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|U^\dagger_{x,-\ell/2}R^\dagger(x)U^\dagger_{y,x}U^\dagger_{\ell/2,y}|\omega_L\rangle\right].\end{aligned}$$

The method is then as follows. For $x>y$ we first separate the trace over the field into two regions $\mathrm{Tr}=\mathrm{Tr}_{-\ell/2,y}\mathrm{Tr}_{y,\ell/2}$ and use the definition of the right density matrix $\rho(y)$ to write

$$\begin{aligned}&\mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,x}U_{x,y}R(y)U_{y,-\ell/2}|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|U^\dagger_{y,-\ell/2}U^\dagger_{x,y}R^\dagger(x)U^\dagger_{\ell/2,x}|\omega_L\rangle\right]\\ &= \mathrm{Tr}_{y,\ell/2}\left[\langle\omega_L|U_{\ell/2,x}U_{x,y}\left(R(y)\rho(y)\right)\otimes|\Omega\rangle\langle\Omega|_{y,\ell/2}U^\dagger_{x,y}R^\dagger(x)U^\dagger_{\ell/2,x}|\omega_L\rangle\right].\end{aligned}\tag{4.48}$$

We then again separate the trace over the field into another two regions $\mathrm{Tr}_{y,\ell/2} = \mathrm{Tr}_{y,x}\mathrm{Tr}_{x,\ell/2}$ and define $\eta(x)$ to be the state of the auxiliary system after $U_{x,y}$ has been applied to the composite system $R(y)\rho(y)\otimes|\Omega\rangle\langle\Omega|_{y,x}$, namely

$$\eta(x) = \mathrm{Tr}_{y,x}\left[U_{x,y}R(y)\rho(y)\otimes|\Omega\rangle\langle\Omega|_{y,x}U_{x,y}^{\dagger}\right]$$

with the initial condition $\eta(y) = R(y)\rho(y)$. It can be shown using techniques analogous to those presented in appendix B.2 that $\eta(x)$ satisfies the differential equation

$$\frac{d\eta(x)}{dx} = Q(x)\eta(x) + \eta(x)Q^{\dagger}(x) + \sum_{\alpha=1}^{N} R_{\alpha}\eta(x)R_{\alpha}^{\dagger},$$

with solution $\eta(x) = \mathcal{P}e^{\int_y^x M_\rho(s)ds}R(y)\rho(y)$. We substitute this definition into (4.48) and further simplify the expression by rewriting it in terms of an auxiliary trace, as in (4.42), to obtain

$$\begin{aligned}&\mathrm{Tr}_{x,\ell/2}\left[\langle\omega_L|U_{\ell/2,x}\left(\eta(x)R^{\dagger}(x)\right)\otimes|\Omega\rangle\langle\Omega|U_{\ell/2,x}^{\dagger}|\omega_L\rangle\right]\\ &= \mathrm{tr}\left[\langle\Omega|_{x,\ell/2}U_{\ell/2,x}^{\dagger}|\omega_L\rangle\langle\omega_L|U_{\ell/2,x}|\Omega\rangle_{x,\ell/2}\left(R(x)\eta(x)R^{\dagger}(x)\right)\right] = \langle\sigma(x)R(x)|\eta(x)\rangle\end{aligned}$$

where $\sigma(x)$ is the left density matrix given by (4.26) and we have switched representations and flattened our matrices into vector form via the Jamiolkowski representation. To obtain our final form we now substitute for $\eta(x)$ and write the vectors as products of matrices and vectors. We have, for $x > y$,

$$\langle\sigma(x)R(x)|\mathcal{P}e^{\int_y^x M(s)ds}|R(y)\rho(y)\rangle = \langle\sigma(x)|\left(\mathbb{I}\otimes\overline{R}(x)\right)\mathcal{P}e^{\int_y^x M(s)ds}\left(R(y)\otimes\mathbb{I}\right)|\rho(y)\rangle.$$

The calculations for $y > x$ are analogous. The case $x = y$ is also accounted for by considering the same method outlined in the evaluation of the interaction energy, and (one half of) the result for $x = y$ can be directly seen from substitution into the above. We find that we can write the one particle correlation function as

$$\begin{aligned}\langle\Psi|\hat{\psi}^{\dagger}(x)\hat{\psi}(y)|\Psi\rangle =& \Theta(x-y)\langle\sigma(x)|\left(\mathbb{I}\otimes\overline{R}(x)\right)\mathcal{P}e^{\int_y^x M(s)ds}\left(R(y)\otimes\mathbb{I}\right)|\rho(y)\rangle \\ &+ \Theta(y-x)\langle\sigma(y)|\left(R(y)\otimes\mathbb{I}\right)\mathcal{P}e^{\int_x^y M(s)ds}\left(\mathbb{I}\otimes\overline{R(x)}\right)|\rho(x)\rangle\end{aligned} \tag{4.49}$$

Density-Density correlation function

Using similar techniques it can be shown that the density-density correlation function is given by

$$\begin{aligned}
&\langle\Psi|\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)\hat{\psi}(y)\hat{\psi}(x)|\Psi\rangle \\
&= \Theta(x-y)\langle\sigma(x)|\left(R(x)\otimes\overline{R(x)}\right)\mathcal{P}e^{\int_y^x M(s)ds}\left(R(y)\otimes\overline{R(y)}\right)|\rho(y)\rangle \\
&+ \Theta(y-x)\langle\sigma(y)|\left(R(y)\otimes\overline{R(y)}\right)\mathcal{P}e^{\int_x^y M(s)ds}\left(R(x)\otimes\overline{R(x)}\right)|\rho(x)\rangle
\end{aligned} \tag{4.50}$$

4.5 Gauge invariance

We now briefly report on the important property of gauge invariance within the class of cMPS. The term gauge invariance refers to the property that a whole class of parameterisations or representations, related by so-called gauge transformations, describe the same physical states. As a consequence, the same dynamics of a physical state can be obtained via different state representations. It is therefore beneficial to impose further constraints on the possible parameterisations of the state, linking each state $|\Psi(Q,\{R_\alpha\})\rangle$ in the variational manifold $\mathcal{V}$ to a unique representation via $Q(x)$ and $R_\alpha(x)$.

We briefly return to the relationship between MPS and cMPS, as discussed in section 4.2. It was shown that the MPS representation is not unique and has invariance under local gauge transformations $g(j)\in \mathrm{GL}(\mathbb{C},D_j), \forall j=1,\ldots,N$ where $\mathrm{GL}(\mathbb{C},D_j)$ is the general linear group over $\mathbb{C}$ of degree D_j, that is

$$|\Psi(\tilde{A})\rangle = |\Psi(A)\rangle \qquad \text{with} \qquad \tilde{A}_{i_j}(j) = g(j-1)A_{i_j}(j)g(j)^{-1} \qquad \forall i_j=1,\ldots,d_j, \forall j=1,\ldots,N$$

(see for example, [Haegeman, 2011, Haegeman et al., 2011a, Schollwock, 2011]). This representation redundancy motivated the study of similar gauge invariance properties within the class of cMPS. Indeed, the parameterisation of the cMPS via the matrices $\{Q(x),R_\alpha(x)\}$ does not lead to a unique representation of the state. Equivalent representations $\{Q(x),R_\alpha(x)\} \neq \left\{\tilde{Q}(x),\tilde{R}_\alpha(x)\right\}$ defined by the action of the group of local gauge transformations $G_{\mathrm{cMPS}} = \left\{g(x)|x\in[-\ell/2,\ell/2], g(x)\in\mathrm{GL}(\mathbb{C},D)\right\}$ exist. Thus, using the correspondence with MPS as in section 4.2, in particular the identifications (4.10), we find that

$$\begin{aligned}
\tilde{A}_0(j) &= g((j-1)\epsilon)A_0(j)g^{-1}(j\epsilon) = g((j-1)\epsilon)g^{-1}(j\epsilon) + \epsilon\, g((j-1)\epsilon)Q(j\epsilon)g^{-1}(j\epsilon) \\
&= \mathbb{I} + \epsilon\left(g(j\epsilon)Q(j\epsilon)g^{-1}(j\epsilon) - \left[\frac{dg(x)}{dx}g^{-1}(x)\right]_{x=j\epsilon}\right) + O(\epsilon^2) \\
\tilde{A}_1(j) &= g((j-1)\epsilon)A_1(j)g^{-1}(j\epsilon) = \sqrt{\epsilon}\left(g(j\epsilon)R(j\epsilon)g^{-1}(j\epsilon)\right) + O(\epsilon^{3/2})
\end{aligned}$$

such that the associated gauge transformations for the cMPS are given by

$$\tilde{Q}(x) = g(x)Q(x)g^{-1}(x) - \frac{dg(x)}{dx}g^{-1}(x), \qquad \tilde{R}(x) = g(x)R(x)g^{-1}(x).$$

The gauge transformation $g(x)$ should therefore be differentiable in order to obtain finite matrices $\tilde{Q}(x)$ and $\tilde{R}(x)$. The boundary matrix B must also be transformed as $g(-\ell/2)Bg(\ell/2)^{-1}$. If B is fixed, we need to restrict to $g(x)$ satisfying $g(-\ell/2) = g(\ell/2) = \mathbb{I}$ in the case of open boundary conditions, or $g(-\ell/2) = g(\ell/2)$ for periodic boundary conditions.

As was shown for MPS [Perez-Garcia et al., 2007], it is possible to specify gauge fixing constraints such that each state $|\Psi(Q,\{R_\alpha\})\rangle \in \mathcal{V}$ is linked to a unique parameterisation $\{Q,\{R_\alpha\}\}$. The cMPS is then said to be in canonical form. We consider the case of open boundary conditions, that is $B = |\omega_R\rangle\langle\omega_L|$, where we have the density matrices $\rho(x)$ and $\sigma(x)$ as defined in (4.23) and (4.26) at our disposal. Under the gauge transformation, $\tilde{\rho}(x) = g(x)\rho(x)g(x)^\dagger$ and $\tilde{\sigma}(x) = \left(g^{-1}(x)\right)^\dagger \sigma(x)g^{-1}(x)$. It is possible to specify the gauge transformations $g(x)$ in order to obtain a direct relationship between $Q(x)$ and $R_\alpha(x)$. By choosing $g(x) = \sigma(x)^{1/2}$ we find that $\tilde{\sigma}(x) = \mathbb{I}$. Since we know that $\tilde{\sigma}(x)$ satisfies the differential equation (4.27), namely

$$\frac{d\tilde{\sigma}(x)}{dx} = \tilde{\sigma}(x)\tilde{Q}(x) + \tilde{Q}^\dagger(x)\tilde{\sigma}(x) + \sum_{\alpha=1}^{N} \tilde{R}_\alpha^\dagger(x)\tilde{\sigma}(x)\tilde{R}_\alpha(x),$$

insertion of $\tilde{\sigma}(x) = \mathbb{I}$ leads us to conclude that

$$\tilde{Q}(x) + \tilde{Q}^\dagger(x) + \tilde{R}^\dagger(x)\tilde{R}(x) = 0.$$

Dropping the tildes and using the result that any matrix A can be written as a sum $A_h + A_a$ where $A_h = \frac{1}{2}(A + A^\dagger)$ is a hermitian matrix and $A_a = \frac{1}{2}(A - A^\dagger)$ is an antihermitian matrix, we can write our $Q(x)$ in this form by taking $Q_h(x) = -\frac{1}{2}R^\dagger(x)R(x)$ and $Q_a(x) = -iK(x)$ for some hermitian matrix $K(x)$ such that

$$Q(x) = -\frac{1}{2}R^\dagger(x)R(x) - iK(x), \tag{4.51}$$

implying that $Q(x)$ is of the same form as in (4.13). This constraint is equivalent to the left orthonormalisation condition of MPS [Perez-Garcia et al., 2007]. We can also use the choice of $g(x)$ to specify the form of $\rho(x)$, hence fixing the gauge completely. We note that since $\sigma(x) = \mathbb{I}$ and $g(x) = \sigma(x)^{1/2}$, this leads to $g(x)g^\dagger(x) = \mathbb{I}$ such that the gauge transformations are now arbitrary unitaries over $\mathbb{C}$ of degree D. Consequently, since the gauge transformation of $\rho(x)$ is given by $\tilde{\rho}(x) = g(x)\rho(x)g(x)^\dagger$ and $\rho(x)$ is hermitian, we can use the remaining degrees of freedom and diagonalise $\tilde{\rho}(x)$ at every point x. The combination of ensuring

$\sigma(x) = \mathbb{I}$, $Q(x) = -\frac{1}{2}R^\dagger(x)R(x) - iK(x)$ and $\rho(x)$ is diagonal means that the cMPS is in left-canonical form [1]. A parameterisation satisfying these constraints therefore uniquely determines the physical state.

The above multiplicative gauge transformations induce an additive gauge equivalence in the tangent plane. We do not explore this any further and instead refer to [Haegeman, 2011, Haegeman et al., 2011a].

4.6 Translational invariance and the thermodynamic limit

In the following we consider translationally invariant systems. Translational invariance enables a field theory with a continuous number of degrees of freedom to be parameterised by a discrete number of degrees of freedom, since the matrices parametrising the cMPS no longer depend on the continuous position coordinate x and all information is stored in the remaining discrete number of position independent entries specifying Q and R_α. In addition we also consider the so-called thermodynamic limit, where one takes the limit as volume and particle number approach infinity in constant ratio.

Definitions

When considering translationally invariant Hamiltonians, we take $Q(x) = Q$ and $R_\alpha(x) = R_\alpha$, $x \in [-\ell/2, \ell/2]$ to be constant $D \times D$ matrices in the definition of the cMPS given in (4.1). Although $\hat{H}_{\mathrm{cMPS}}(x) = Q \otimes \mathbb{I} + \sum_{\alpha=1}^{N} R_\alpha \otimes \hat{\psi}_\alpha^\dagger(x)$ remains x-dependent, the resulting cMPS is translationally invariant – the cMPS depends on the range over which the field and auxiliary system are interacted. As before we can choose to consider systems with periodic boundary conditions, where there are no boundary effects, or open boundary conditions. Open boundary conditions can have strong boundary effects that extend deeply into the bulk of the system. However, when considering very large systems we expect that the parameterisation matrices Q and R_α of the cMPS become site independent when sufficiently far from the boundaries. Thus, we can define these translationally invariant cMPS for both finite systems with periodic boundary conditions or for a system in the thermodynamic limit $\ell \to \infty$. We restrict to the latter.

When considering translational invariance and taking Q and R_α as constant matrices, the Lindblad generator $M(x)$ as defined in (4.30) is also constant $M(x) = M$. This leads to a

[1] Note that we could equally well have chosen to satisfy the conditions for the cMPS to be in right canonical form by setting $\rho(x) = \mathbb{I}$ and diagonalising $\sigma(x)$.

simplification of many of the calculations and quantities presented thus far. For example, when considering open boundary conditions and taking the thermodynamic limit, we have that the right and left density matrices, as introduced in (4.32) and (4.33), can be written

$$|\rho(x)\rangle = \lim_{\ell\to\infty} \mathcal{P} e^{\int_x^{\ell/2} M ds} |\omega_R\rangle|\omega_R\rangle = \lim_{\ell\to\infty} e^{(\ell/2-x)M}|\omega_R\rangle|\omega_R\rangle \tag{4.52}$$

$$\langle\sigma(x)| = \lim_{\ell\to\infty} \langle\omega_L|\langle\omega_L|\mathcal{P} e^{\int_{-\ell/2}^{x} M ds} = \langle\omega_L|\langle\omega_L| \lim_{\ell\to\infty} e^{(x+\ell/2)M}. \tag{4.53}$$

These expressions can be simplified further, in particular the x-dependence will vanish. Recalling the spectral decomposition of M, as given in (4.34), we find that

$$\begin{aligned} e^{\ell M} = e^{S\ell D S^{-1}} &= \sum_{i=0}^{\infty} \frac{(S\ell D S^{-1})^i}{i!} = \mathbb{I} + S\ell D S^{-1} + \frac{S\ell D S^{-1} S\ell D S^{-1}}{2} + \dots \\ &= S\mathbb{I}S^{-1} + S\ell D S^{-1} + \frac{S\ell^2 D^2 S^{-1}}{2} + \dots = S\left(\sum_{i=0}^{\infty} \frac{(\ell D)^i}{i!}\right) S^{-1} = S e^{\ell D} S^{-1}. \end{aligned}$$

Then, using that $m_0 = 0$ and all other eigenvalues $m_j, j > 0$ have negative real part, we have that in the thermodynamic limit $\ell \to \infty$, $e^{\ell M} = S|0\rangle\langle 0|S^{-1} = |\rho\rangle\langle\sigma|$ where $|\rho\rangle$ and $\langle\sigma|$ are the right and left eigenvectors corresponding to the zero eigenvalue of M respectively. These eigenvectors are position independent, since they satisfy the differential equations (4.25) and (4.27). It follows that (4.52) and (4.53) are given by

$$|\rho\rangle\langle\sigma|\omega_R\rangle|\omega_R\rangle = |\rho\rangle \tag{4.54}$$

$$\langle\omega_L|\langle\omega_L|\rho\rangle\langle\sigma| = |\sigma\rangle. \tag{4.55}$$

Gauge Invariance

Further restrictions and simplifications can be made when considering the gauge invariance for translationally invariant systems. Since position dependence is no longer present, the gauge transformations are restricted to global transformations $\tilde{Q} = gQg^{-1}$ and $\tilde{R}_\alpha = gR_\alpha g^{-1}$ with $g \in GL(\mathbb{C}, D)$ only. This transformation can be used to impose the left or right orthonormalisation conditions along with a further restriction to ensure that the canonical form is obtained, as described in section 4.5.

For the left orthonormalisation condition we fix the left eigenvector corresponding to the zero eigenvalue

$$\langle\sigma| = \langle\mathbb{I}|, \tag{4.56}$$

which requires that $Q = -iK - 1/2\sum_\alpha R_\alpha^\dagger R_\alpha$. The remaining gauge freedom can be used to diagonalise the matrix form r of the right eigenvector $|r\rangle$, such that Q and R_α are in left canonical form. The right canonical form is obtained analogously.

As stated in [Haegeman, 2011, Haegeman et al., 2011a], fixing of the gauge freedom in this way improves computational efficiency when performing numerical calculations with cMPS. An exact computation of the left and right eigenvectors $\langle\sigma|$ and $|\rho\rangle$ corresponding to the zero eigenvalue of M for general parameterisations Q, R_α is a computationally costly operation of $O(D^6)$. By ensuring left (or right) canonical form in terms of the hermitian matrix K and R_α, we know exactly that $m_0 = 0$ and $\langle\sigma| = \langle I|$. It is then possible to obtain $|\rho\rangle$ with an iterative solver with computational efficiency $O(D^3)$.

Expectation Values

We will now consider calculating expectation values and correlation functions of a translationally invariant Hamiltonian. The generic Hamiltonian (4.35) becomes translationally invariant when $v(x) = v$ and $w(x,y) = w(x-y)$ with $w(x) = w(-x)$ such that

$$\begin{aligned}\hat{H} &= \int_{-\ell/2}^{\ell/2} dx \left(\hat{t} + \hat{v} + \hat{w}\right) \\ &= \int_{-\ell/2}^{\ell/2} dx \frac{1}{2m} \frac{d\hat{\psi}^\dagger(x)}{dx} \frac{d\hat{\psi}(x)}{dx} + v \int_{-\ell/2}^{\ell/2} dx \hat{\psi}^\dagger(x)\hat{\psi}(x) \\ &+ \frac{1}{2} \int_{-\ell/2}^{\ell/2} dx \int_{-\ell/2}^{\ell/2} dy\, w(x-y)\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)\hat{\psi}(y)\hat{\psi}(x) \end{aligned} \tag{4.57}$$

The expectation values of the kinetic, potential and interaction energies, as presented in (4.46) and (4.47), are proportional to the size of the system and hence extensive properties. It is therefore more meaningful to calculate the expectation values of the kinetic, potential and interaction energy densities $\hat{t}$, $\hat{v}$ and $\hat{w}$. Applying the left orthonormalisation condition we find that in the thermodynamic limit

$$\begin{aligned}\langle\Psi|\hat{t}|\Psi\rangle &= \frac{1}{2m}\langle\mathbb{I}|\,[Q,R]\otimes\overline{[Q,R]}|\rho\rangle \\ \langle\Psi|\hat{v}|\Psi\rangle &= v\langle\mathbb{I}|R\otimes\overline{R}|\rho\rangle \\ \langle\Psi|\hat{w}|\Psi\rangle &= \int_0^\infty dz\, w(z)\langle\mathbb{I}|\left(R\otimes\overline{R}\right)e^{zM}\left(R\otimes\overline{R}\right)|\rho\rangle \\ &= \langle\mathbb{I}|\left(R\otimes\overline{R}\right)\mathcal{L}_z[w](-M)\left(R\otimes\overline{R}\right)|\rho\rangle\end{aligned}$$

where we introduce the variable $z = x - y$ and $\mathcal{L}_z[w](-M)$ is the Laplace transform of $w(z)$ defined by $\mathcal{L}_t[w](s) = \int_0^\infty w(t)e^{-st}dt$ for $\mathrm{Re}(s) \geq 0$. When calculating the expectation value of the interaction energy density the computational cost is $O(D^6)$ (having already obtained ρ and σ) due to the computation of $\mathcal{L}_z[w](-M)$. If only local interactions are present, i.e. $w(z) = w(x-y) \sim \delta(x-y)$, we have that $\mathcal{L}_z[w](-M) = \int_0^\infty \delta(z)e^{-zM}dz = \mathbb{I}$

and so the computational complexity reduces to $O(D^3)$, as is the case for the kinetic and potential energy densities. It is then also useful to employ the Jamiolkowski isomorphism and write the energy densities in terms of traces, namely

$$\langle\Psi|\hat{t}|\Psi\rangle = \frac{1}{2m}\langle\mathbb{I}|\,[Q,R]\,\rho\,[Q,R]^\dagger\rangle = \frac{1}{2m}\mathrm{tr}\left[[Q,R]\,\rho\,[Q,R]^\dagger\right] \tag{4.58}$$

$$\langle\Psi|\hat{v}|\Psi\rangle = v\ \langle\mathbb{I}|R\rho R^\dagger\rangle = v\ \mathrm{tr}\left[R\rho R^\dagger\right] \tag{4.59}$$

$$\langle\Psi|\hat{w}|\Psi\rangle = \langle\mathbb{I}|R^2\rho\left(R^\dagger\right)^2\rangle = \mathrm{tr}\left[R^2\rho\left(R^\dagger\right)^2\right]. \tag{4.60}$$

Finally, we note that the one particle and density-density correlation functions (4.49) and (4.50) for $x > y$ can be written

$$\langle\Psi|\hat{\psi}^\dagger(x)\hat{\psi}(y)|\Psi\rangle = \langle\mathbb{I}|\left(\mathbb{I}\otimes\overline{R}\right)e^{(x-y)M}\left(R\otimes\mathbb{I}\right)|\rho\rangle \tag{4.61}$$

$$\langle\Psi|\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)\hat{\psi}(y)\hat{\psi}(x)|\Psi\rangle = \langle\mathbb{I}|\left(R\otimes\overline{R}\right)e^{(x-y)M}\left(R\otimes\overline{R}\right)|\rho\rangle \tag{4.62}$$

in the translationally invariant setting.

4.7 Application of variational methods using cMPS

In this section we illustrate how the class of cMPS can be used as a variational class to simulate a continuous quantum system. We consider the paradigmatic Lieb-Liniger model and use techniques described in Chapter 2 to approximate the ground state energy. Since this model is in fact solvable, we are able to compare the results and substantiate that the family of cMPS are a suitable choice of variational class.

4.7.1 The Lieb-Liniger model

The Lieb-Liniger model [Lieb and Liniger, 1963] describes a one dimensional gas of particles satisfying Bose-Einstein statistics. The Hamiltonian describes N non-relativistic bosons of mass m in one dimension on the line $[-\ell/2,\ell/2]$, interacting via a two-body repulsive δ-potential and is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + 2c\sum_{i<j}\delta\left(x_i - x_j\right).$$

The constant $c > 0$ denotes the strength of the contact interaction. The limit $c \ll 1$ is the weak coupling limit and in this regime it is known that the Bogoliubov approximation, obtained by linearisation of the Gross-Pitaevskii equation (2.20), gives a good estimate of the ground state energy of the system [Lieb and Liniger, 1963]. For large c one approaches

the Tonks-Girardeau limit [Girardeau, 1960], where it can be shown that the ground state energy $E_{\mathrm{LL}} \to \pi^2/3$.

The model can be described in the second quantisation (see appendix A) using the quantum field annihilation and creation operators $\hat{\psi}(x)$ and $\hat{\psi}^\dagger(x)$ that obey the canonical commutation relations for bosonic particles

$$\left[\hat{\psi}(x), \hat{\psi}^\dagger(x')\right] = \delta(x - x'), \qquad \left[\hat{\psi}(x), \hat{\psi}(x')\right] = 0$$

where $-\ell/2 \leq x, y \leq \ell/2$ are position coordinates. The Lieb-Liniger Hamiltonian is then given by

$$\hat{H}_{\mathrm{LL}} = \int_{-\ell/2}^{\ell/2} dx \left(\frac{\hbar^2}{2m} \frac{d\hat{\psi}^\dagger(x)}{dx} \frac{d\hat{\psi}(x)}{dx} + c\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x) \right) = \int_{-\ell/2}^{\ell/2} dx \left(\hat{t}_{\mathrm{LL}} + \hat{w}_{\mathrm{LL}}(c) \right)$$

where the densities $\hat{t}_{\mathrm{LL}}$ and $\hat{w}_{\mathrm{LL}}(c)$ describe the kinetic energy and two particle interaction respectively.

Despite the seemingly simplicity of the Lieb-Liniger model, it has become a paradigmatic example of a continuous quantum system system since it has proved to have a striking richness. The ground state of this Hamiltonian was exactly determined by Lieb and Liniger in [Lieb and Liniger, 1963] using the Bethe ansatz. Its Bethe Ansatz equations can be explicitly derived and used to study equilibrium properties at zero and finite temperatures [Yang and Yang, 1969], and lie in accordance with previous approximations such as Bogolioubov's theory. More recently, a renewed interest in the Lieb-Liniger model has been triggered by its accurate experimental realisation [Kinoshita et al., 2004, Paredes et al., 2004]. The integrability, explicit analysis of the weak to strong coupling crossover and experimental feasibility of the model has set a precise point of reference for many-body techniques. Indeed, applications in Part II of this thesis use the Lieb-Liniger model as a test case to measure the success of the proposed variational algorithms.

4.7.2 Application of cMPS to Lieb-Liniger

Here we illustrate how the family of cMPS can be used as a variational ansatz for the simulation of the Lieb-Liniger model by using this class to approximate the ground state energy as a function of the interaction strength c. We perform a minimisation of the average energy, or in this translationally invariant case the average energy density, with respect to the variational parameters λ as given by (2.2) in Chapter 2, that is we calculate

$$\min_{\lambda} \left\{ E_{\mathrm{LL}}(c;\lambda) \right\} = \min_{\lambda} \left\{ \langle \Psi(\lambda) | \left(\hat{t}_{\mathrm{LL}} + \hat{w}_{\mathrm{LL}}(c) \right) | \Psi(\lambda) \rangle \right\}.$$

We take the variational class to be the family of translationally invariant, single-species (i.e $\alpha = 1$) cMPS as defined in (4.5). The variational parameters λ are included in the cMPS state representation via the matrices Q and R. We therefore minimise

$$E_{\mathrm{LL}}(c;Q,R) = \langle\Psi(\overline{Q},\overline{R})|\left(\hat{t}_{\mathrm{LL}} + \hat{w}_{\mathrm{LL}}(c)\right)|\Psi(Q,R)\rangle$$

where

$$|\Psi(Q,R)\rangle = \langle\omega_R|\mathcal{P}\exp\left(\int_{-\ell/2}^{\ell/2}\left(Q\otimes\mathbb{I} + R\otimes\hat{\psi}^\dagger(x)\right)dx\right)|\omega_L\rangle|\Omega\rangle$$

in order to determine the parameterisation $Q_{\mathrm{op}}, R_{\mathrm{op}}$ that best approximates the ground state. In Chapter 4, Eqs. (4.58) and (4.60) we found that the expectation values of the kinetic and interaction energy densities $\hat{t}$ and $\hat{w}$ with respect to the cMPS can be written

$$\langle\Psi(\overline{Q},\overline{R})|\hat{t}_{\mathrm{LL}}|\Psi(Q,R)\rangle = \mathrm{tr}\left[[Q,R]\,\rho\,[Q,R]^\dagger\right] \tag{4.63}$$

$$\langle\Psi(\overline{Q},\overline{R})|\hat{w}_{\mathrm{LL}}(c)|\Psi(Q,R)\rangle = c\ \mathrm{tr}\left[R^2\rho\left(R^\dagger\right)^2\right] \tag{4.64}$$

where tr denotes the trace over the cMPS auxiliary system, and ρ is the right density matrix of this system given by (4.23) and satisfying the master equation (4.25). We therefore have that

$$E_{LL}(c;Q,R) = \mathrm{tr}\left[[Q,R]\,\rho\,[Q,R]^\dagger + cR^2\rho\left(R^\dagger\right)^2\right]. \tag{4.65}$$

We apply a gradient descent algorithm to minimise this quantity by computing the gradient of the energy density $\nabla E_{LL}(c;Q,R)$ and iterating for each variational parameter λ_i

$$\lambda_i - \epsilon\left[\nabla E_{LL}(c;Q,R)\right]_i \ \rightarrow\ \tilde{\lambda}_i,$$

accompanied by an appropriate scaling procedure to ensure constant particle density and hence admissible energy densities, see section (5.2.3). The energy density is updated using the new parameters and the procedure repeated until the energy density reaches a fixed point. In Fig. 4.2 we have plotted $E_{\mathrm{LL}}(c;Q,R)$ at constant particle density $\langle\hat{\psi}^\dagger(x)\hat{\psi}(x)\rangle = 1$ for a range of the interaction strength c and dimensions $D = 2,4,7$. Since the eigenvalues of the model's Hamiltonian can, in principle, be calculated exactly we also include the exact solution given by the Bethe ansatz for comparison. With increasing dimension, the results become comparable to those of the exact calculation. By using more sophisticated minimisation procedures, e.g. conjugate gradients or the time-dependent variational principle with imaginary time evolution, it is expected that more precise results can be obtained. In fact, using the method above it was shown in [Verstraete and Cirac, 2010] that the expected

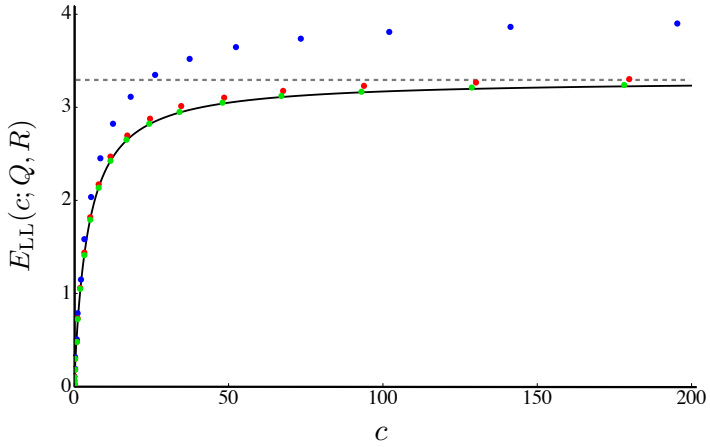

Figure 4.2: The (scaled) energy density $E_{\mathrm{LL}}(c;Q,R)$ as a function of the (scaled) interaction parameter c for $D=2,4,7$ (blue, red, green). The exact solution given by the Bethe ansatz is drawn for reference in black, with the dashed grey line showing the limiting value $\pi^2/3$ for $c\to\infty$.

energy density results obtained for $D=8$ are nearly indistinguishable from the exact Bethe ansatz solution. The class of cMPS are thus a suitable and expressive class of variational states, capable of capturing the ground state physics of continuous quantum systems. This is further supported in the next chapter.

Part II

Chapter 5

Simulating Quantum Fields with Cavity QED

Modelling interacting classical many-particle systems is a challenging yet tractable problem. However, in the quantum regime, it becomes rapidly intractable, due to the dramatic increase in the number of variables required to describe the system. Feynman [Feynman, 1982] realised that an alternate approach would be to exploit quantum mechanics to carry out simulations beyond the reach of classical computers. This idea was the basis of Lloyd's simulation algorithm [Lloyd, 1996], a procedure where a quantum computer simulates the dynamics of an interacting quantum system. Qubits are used to encode the state of the quantum system, and its unitary evolution is translated in terms of elementary quantum gates and implemented in a circuit based quantum computer. This approach is known as digital quantum simulation. In contrast, there is also an analogue approach to quantum simulation, where the controllable simulator's Hamiltonian is tailored to match that of the simulated system [Buluta and Nori, 2009]. The complementary aspects of the analogue and digital methods, reviewed in [Aspuru-Guzik and Walther, 2012, Bloch et al., 2012, Buluta and Nori, 2009, Johanning et al., 2009, Lewenstein et al., 2007], have led to a host of recent experiments [Barreiro et al., 2011, Friedenauer et al., 2008, Gerritsma et al., 2010, Haller et al., 2010, Kim et al., 2010, Simon et al., 2011].

To date, most experimental implementations of quantum simulation algorithms have been focussed on the task of simulating quantum lattice systems, with comparatively less attention paid to systems with continuous degrees of freedom. The archetypal example of a quantum system with a continuous degree of freedom is the quantum field. Currently, quantum simulations of quantum field theories have relied on discretisation of the dynamical degrees of freedom. One body of recent theoretical work is focussed on the analogue simulation of discretised quantum fields, using cold atoms in optical lattices [Bermudez et al., 2010, Cirac et al., 2010, Kapit and Mueller, 2011, Lepori et al., 2010] and coupled cavity arrays [Angelakis et al., 2007, Greentree et al., 2006, Hartmann et al., 2006]. Complementing

this are proposals for digital quantum simulation on a universal quantum computer of the zero-temperature [Byrnes and Yamamoto, 2006] and thermal [Temme et al., 2011] dynamics of non-abelian gauge theories and, more recently, a digital quantum simulation [Jordan et al., 2011, Jordan et al., 2012] of scattering processes of a discretized $\lambda\phi^4$ quantum field.

In this chapter we present an analogue algorithm to simulate the ground state physics of a one-dimensional interacting quantum field using the continuous output of a cavity QED apparatus. The method involves no discretisation of the dynamical degrees of freedom; the simulation register is the continuous electromagnetic output mode of the cavity. The variational wave function generated in this way therefore belongs to an extremely expressive class, namely the class of continuous matrix product states, as shown in Chapter 4. We argue that our approach is already realisable with state-of-the-art cavity QED technology.

The chapter is organised as follows. In section 5.1 we present the proposal, describing the types of quantum fields we seek to simulate, followed by the types of cavity systems we consider as simulators. The quantum simulation procedure is described, followed by a discussion of how to implement variational techniques in order to determine ground state properties. In section 5.2 we demonstrate that a paradigmatic cavity QED system is capable of simulating an equally paradigmatic quantum field. We discuss how the quantum simulation would proceed, and verify the proposal with classical simulation of variational calculations using cMPS. In section 5.3 we discuss extensions of the proposal and potential settings where the scheme could provide a practical advantage over classical computers in the simulation of quantum fields.

5.1 Setup and formulation

We consider simulating quantum fields modelling a one-dimensional collection of single-species interacting bosons. An important assumption is that the simulated field is translation-invariant, which we discuss shortly. Such systems can be described in second quantisation (see appendix A) using the quantum field annihilation and creation operators $\hat{\psi}(x)$ and $\hat{\psi}^\dagger(x)$ that obey the canonical commutation relations

$$[\hat{\psi}(x), \hat{\psi}^\dagger(y)] = \delta(x-y).$$

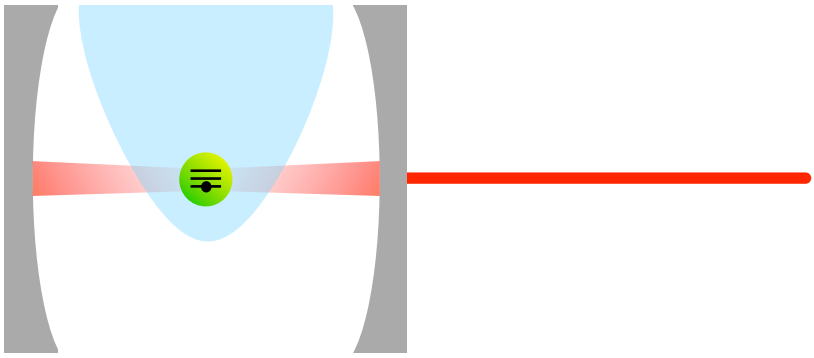

Figure 5.1: A schematic illustration of a cavity QED setup – some intracavity medium, for example an atom, is coupled to a single mode of the intracavity electromagnetic field. The right mirror of the cavity allows for transmission of light and here the output field is depicted.

where x, y are position coordinates. The prototypical form of a translation-invariant Hamiltonian was given in Eq. (4.57), namely

$$\hat{H} = \int dx \left(\hat{t} + \hat{v} + \hat{w}\right) = \int dx \frac{d\hat{\psi}^\dagger(x)}{dx}\frac{d\hat{\psi}(x)}{dx} + \mu \int dx \hat{\psi}^\dagger(x)\hat{\psi}(x) + \int dx \int dy\, w(x-y)\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)\hat{\psi}(y)\hat{\psi}(x) \tag{5.1}$$

where the densities $\hat{t}$, $\hat{w}$ and $\hat{v}$ describe the kinetic energy, two-particle interaction with potential $w(x-y)$, and the chemical potential term with chemical potential μ respectively. We have chosen units such that $\hbar = 2m = 1$. Although the Hamiltonians we consider are of this form, the approach works in principle for arbitrary translation-invariant Hamiltonians $\hat{H}$ that are finite sums of polynomials of creation and annihilation operators and their derivatives.

In order to determine the ground state physics of $\hat{H}$, we use the continuous output of a cavity QED device. In our setting, the proposed apparatus is a single-mode cavity coupled to the quantum degrees of freedom of some intracavity medium (Fig. 5.1). The proposal is not tied to the specific nature of the medium, so long as one or more tuneable nonlinear interactions are present that are sufficiently strong at the single-photon level. We consider the example of a single trapped atom coupled to the single field mode of the cavity via dipole transitions. The system is described by a Hamiltonian $\hat{H}_{\text{sys}}(\lambda)$ that depends on a set of controllable parameters λ. In particular, λ could include the atom-cavity field coupling or the frequency of the driving laser. When the cavity is driven, either directly through one of its mirrors or indirectly through the medium, the intracavity field relaxes to a stationary state, and the cavity emits a steady-state beam of photons in a well-defined mode. For an overview of such systems and cavity quantum electrodynamics, see Chapter 3.

In Chapter 4 we introduced a class of quantum field states known as continuous matrix product states (cMPS). We discussed how these states form a variational class of quantum field states that have proven to be capable of the classical simulation of both nonrelativistic and relativistic quantum fields [Haegeman et al., 2010, Osborne et al., 2010, Verstraete and Cirac, 2010]. Additionally we showed that quantum field states emerging from a cavity are of cMPS type. We therefore find that the stationary output of the cavity QED apparatus described in the above paragraph fulfills the necessary conditions for being a suitable and expressive class of variational quantum states, capable of capturing the ground state physics of interacting fields. The crucial idea underlying our simulation algorithm is thus to regard the steady-state cavity output as a continuous register recording a variational quantum state $|\Psi(\lambda)\rangle$ of a one-dimensional quantum field with control parameters λ as the variational parameters (see Chapter 2, section 2.1 for a description of variational states and parameters). In our setting the variational quantum state $|\Psi(\lambda)\rangle$ is a translationally invariant, single-species cMPS, as defined in Eq. (4.5). We have

$$|\Psi(\lambda)\rangle = |\Psi(Q(\lambda), R(\lambda))\rangle = \langle\omega_L|\mathcal{P}\exp\left(\int Q(\lambda)\otimes\mathbb{I} + R(\lambda)\otimes\hat{\psi}^\dagger(x)dx\right)|\omega_R\rangle|\Omega\rangle, \tag{5.2}$$

where Q, R are constant matrices acting on a D-dimensional auxiliary system, $\mathcal{P}\exp$ denotes the path ordered exponential, $|\omega_R\rangle$ and $\langle\omega_L|$ are vectors encoding the auxiliary system boundary conditions and $|\Omega\rangle$ is the field vacuum state annihilated by $\hat{\psi}(x)$. The representation of the state is chosen so that the spatial location x of the simulated translation-invariant field is identified with the value of the time-stationary cavity output mode exiting the cavity at time $t = x/s$. Since t can always be included in the set of parameters that define a variational manifold, the arbitrary scaling parameter s is included in our set of variational parameters λ. The full set of control parameters λ are encoded in the state representation via the matrices Q and R. We complete this identification by equating the annihilation operator $\hat{\psi}(x)$ of the simulated quantum field with the field operator $\hat{E}^+(t)$ for the positive-frequency electric field of the cavity output mode, as shown in (4.13) from Chapter 4, via

$$\hat{\psi}(x) = \frac{\hat{E}^+(t)}{\sqrt{s}} \tag{5.3}$$

where $\hat{E}^+(t)$ is as given in Eq. (4.11). We note that it is possible to choose units such that $\langle\hat{E}^-(t)\hat{E}^+(t)\rangle$ corresponds to the mean number of photons exiting the cavity per unit time. This choice has useful consequences, for example the energy expectation value of the chemical potential term in (5.1) can then be determined via an intensity measurement, see (5.7) below.

Given a variational quantum state $|\Psi(\lambda)\rangle$ we can perform variational techniques, as introduced in Chapter 2, to determine the ground state of the Hamiltonian $\hat{H}$. At this stage the set of parameters λ is not specified in terms of experimental parameters since they depend on the model under consideration. Our variational method proceeds by minimising the average energy, or in this translationally invariant setting the average energy density, of the variational state $|\Psi(\lambda)\rangle$

$$E(\lambda) = \langle\Psi(\lambda)| \left(\hat{t} + \imath\hat{w} + \hat{v}\right) |\Psi(\lambda)\rangle$$

over the variational parameters λ, in order to determine the set of parameters λ_0 that approximate the ground state. To calculate $E(\lambda)$ we can apply classical numerical techniques. For example, if $|\Psi(\lambda)\rangle$ is a cMPS then methods described in Chapter 4 can be used, see [Verstraete and Cirac, 2010]. However, such an algorithm requires a number of operations scaling exponentially with the number of field components, such that when considering more complex systems than the above the calculation becomes intractable.

A key point in our scheme is that, with the identification of the field operators $\hat{\psi}(x)$ and $\hat{E}^+(t)$ given in (5.3) at hand, the value of $E(\lambda)$ can be determined experimentally using standard optical measurements on the cavity output field, namely the measurement of Glauber correlation functions [Glauber, 1963], as presented in Chapter 3. This result is central for our proposal, and can easily be seen for the Hamiltonian (5.1). The linearity of the expectation value enables us to separately measure the individual expectation values

$$\langle\hat{v}\rangle = \mu\ \langle\hat{\psi}^\dagger(x)\hat{\psi}(x)\rangle \tag{5.4}$$

$$\langle\imath\hat{w}\rangle = \int dy\, w(x-y)\langle\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)\hat{\psi}(y)\hat{\psi}(x)\rangle \tag{5.5}$$

$$\langle\hat{t}\rangle = \Big\langle \frac{d\hat{\psi}^\dagger(x)}{dx}\frac{d\hat{\psi}(x)}{dx}\Big\rangle. \tag{5.6}$$

Using (5.3) we find that the expectation value of the chemical potential term $\hat{v}$ thus corresponds to the intensity of the output beam via

$$\langle\hat{v}\rangle\ \propto\ \langle\hat{\psi}^\dagger(x)\hat{\psi}(x)\rangle\ \rightarrow\ \frac{1}{s}\langle\hat{E}^-(t)\hat{E}^+(t)\rangle. \tag{5.7}$$

The expectation value of $\imath\hat{w}$ depends on two-point spatial correlation functions via

$$\langle\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)\hat{\psi}(y)\hat{\psi}(x)\rangle\ \rightarrow\ \frac{1}{s^2}\langle\hat{E}^-(t_1)\hat{E}^-(t_2)\hat{E}^+(t_2)\hat{E}^+(t_1)\rangle \tag{5.8}$$

which translates to measurements of

$$G^{(2)}(t_1,t_2) := \mathrm{Tr}\left[\rho\,\hat{E}^-(t_1)\hat{E}^-(t_2)\hat{E}^+(t_2)\hat{E}^+(t_1)\right],$$

where ρ is the quantum state of the cavity output, as defined in Eq. (3.70) of Chapter 3[1]. The kinetic energy term $\langle \hat{t} \rangle$ depends on the product of spatial derivatives of the simulated field annihilation and creation operators $\hat{\psi}(x)$ and $\hat{\psi}^\dagger(x)$, which under the identification (5.3) can be written

$$\frac{d\hat{E}^-(t)}{dt}\frac{d\hat{E}^+(t)}{dt} \approx \left[\frac{\hat{E}^-(t+\epsilon_1)-\hat{E}^-(t-\epsilon_1)}{2\epsilon_1}\right]\left[\frac{\hat{E}^+(t+\epsilon_2)-\hat{E}^+(t-\epsilon_2)}{2\epsilon_2}\right]$$

such that the kinetic energy density corresponds to the limit

$$\langle \hat{t} \rangle = \lim_{\epsilon_1,\epsilon_2 \to 0} \frac{1}{s^3\epsilon_1\epsilon_2}\Big(G^{(1)}(t+\epsilon_1,t+\epsilon_2)-G^{(1)}(t+\epsilon_1,t)-G^{(1)}(t,t+\epsilon_2)+G^{(1)}(t,t)\Big). \tag{5.9}$$

where $G^{(1)}$ is as defined in Eq. (3.68) of Chapter 3[2]. This quantity can be estimated by choosing a finite but small value for ϵ_1 and ϵ_2. We emphasise that the cavity output is a continuous quantum register, with a discretisation procedure entering only in the experimental measurement. The procedure of linearising the derivative therefore does not amount to a simple time discretisation of the cavity output itself, which in turn would lead to a space discretisation of the simulated field. Suitable timescales can be chosen such that possible errors become negligible, as discussed below. The detection schemes to estimate the terms (5.7), (5.8) and (5.9) are presented in Fig. 5.2. Measurement schemes $(2a)$ and $(2b)$ are the standard laboratory techniques of photon detection and Hanbury-Brown and Twiss interferometry. Measurement scheme $(2c)$ represents an interferometer with variable path length that is used to estimate the derivative of the quantum field in the kinetic term $\langle \hat{t} \rangle$. Length shifts on the millimeter scale correspond to picosecond values of ϵ_1 and ϵ_2 in the estimation of $\langle \hat{t} \rangle$. Since these values are six orders of magnitude smaller than the relevant timescales of the experiment, which are in the order of microseconds, we consider them to be sufficiently small such that the discretisation needed to estimate $\langle \hat{t} \rangle$ produces insignificant errors. Measurement setups corresponding to third [Koch et al., 2011] and higher order correlation functions can also be identified. This ultimately allows general Hamiltonians $\hat{H}(\hat{\psi}, \hat{\psi}^\dagger)$ to be measured.

Once $E(\lambda)$ has been experimentally estimated for a given λ, we can then apply a variational method to minimise $E(\lambda)$. Minimisation is carried out by adaptively tuning the

[1] Note that the position dependence found in (3.70) is omitted due to the symmetry of the setup in Fig. 5.2 $(2b)$. Furthermore, we have $t_1 = t_2 = t$ since the path lengths are identical.

[2] As before the absolute position can be neglected in this expression. The differing path lengths in Fig. 5.2 $(2c)$ are translated into differing times.

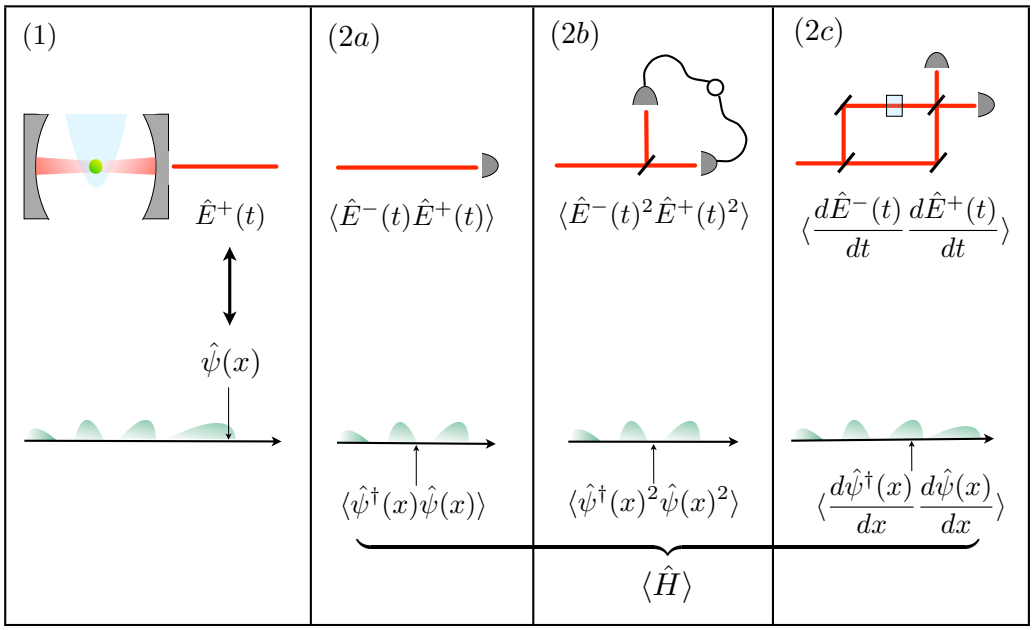

Figure 5.2: (1) The output field $\hat{E}^+(t)$ of a cavity QED system is identified with a bosonic quantum field $\hat{\psi}(x)$. Since optical detection schemes correspond to expectation values of quantum-field operators, $\langle \hat{H}\rangle$ can be estimated via independent measurements of the cavity field. For example, the operators $\hat{t}$, $\hat{w}$ and $\hat{v}$ of (5.1) are determined, respectively, from measurements of $(2a)$ the output-field intensity, $(2b)$ Hanbury Brown and Twiss correlations, and $(2c)$ an interferometer with variable path length.

parameters[3] λ to reduce $E(\lambda)$ using, for example, a standard numerical gradient descent method. The process is iterated until an energy minimum is attained. Once the optimum choice of λ is found, the resulting cavity output field is a variational approximation to the ground state of $\hat{H}$. Relevant observables of the field theory can then be directly measured using the detection schemes of Fig. 5.2. An important point to note is that the optimisation procedure may be performed experimentally without theoretically calculating the cavity QED system dynamics. In fact, it is not necessary to accurately characterise $\hat{H}_{\text{sys}}$ or its relation to the adjustable parameters λ.

5.2 Test case

With the identification of cavity QED output states and cMPS we now investigate whether a realistic system in the presence of decoherence can reproduce the relevant physics of an

[3] On a theoretical level we assume that we have sufficient control of the variational parameters to perform this tuning. When considering a physical implementation of the scheme the tuning will depend on the particular experiment of choice and its controllability.

interacting quantum field. As a test case, we demonstrate that the paradigmatic cavity QED system, comprising a single trapped atom coupled to a single mode of a high-finesse cavity, is capable of simulating the ground state physics of an equally paradigmatic field, namely, the Lieb-Liniger model [Lieb and Liniger, 1963]. As presented in section 4.7 of Chapter 4, this model describes hard-core bosons with a delta-function interaction and is given by (5.1) with $v = 0$ and $w(x-y) = c\delta(x-y)$, where c describes the interaction strength

$$\begin{aligned}\hat{H}_{\mathrm{LL}} \equiv \hat{H}_{\mathrm{LL}}(c) &= \int dx \left(\frac{d\hat{\psi}^\dagger(x)}{dx} \frac{d\hat{\psi}(x)}{dx} + c\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x) \right) \\ &= \int dx \left(\hat{t}_{\mathrm{LL}} + \hat{w}_{\mathrm{LL}}(c) \right) \end{aligned} \tag{5.10}$$

We have again chosen units such that $\hbar = 2m = 1$. Our simulator consists of a two-level atom interacting with one cavity mode, driven by a laser in order to obtain a stationary cavity-output state. As presented in Chapter 3, such a system in the interaction picture is described by the driven, on-resonance Jaynes-Cummings Hamiltonian (see (3.40) and (3.44) with $\Delta = 0$)

$$\hat{H}_{\mathrm{sys}} \equiv \hat{H}_{\mathrm{sys}}(g,\Omega) = g(\hat{\sigma}^+\hat{a} + \hat{\sigma}^-\hat{a}^\dagger) + \Omega(\hat{\sigma}^+ + \hat{\sigma}^-), \tag{5.11}$$

where $\hat{\sigma}^+$ is the atomic raising operator, $\hat{a}$ is the cavity photon annihilation operator, g the atom–cavity coupling and Ω the laser drive. Photons leak out of the cavity with leakage rate κ, and it is assumed that, in a real experiment, this output light can be measured by various detection setups. The experimentally tuneable parameters are therefore g and Ω, which we include in our set of variational parameters λ. In addition we also have a third variational parameter s, the scaling which links the position dependence of the field to the time dependence of the output beam. We discuss exactly how g, Ω and s function as variational parameters in 5.2.2.

In an experiment, to measure the variational energy density $E(\lambda)$, the output beam would be allowed to relax to a steady state and the intensity I, $G^{(1)}$, and $G^{(2)}$ functions estimated as depicted in Fig. 5.2. $E(\lambda)$ is then determined from post-processing this data. An application of the variational method follows to find the approximation to the ground state energy. However, the test model chosen here is simple enough to admit an entirely classical simulation [Astrakharchik and Giorgini, 2003, Verstraete and Cirac, 2010]. In the following we apply such methods, providing a proof-of-principle of our proposal by showing that the minimising variational parameters obtained via a completely classical simulation are in fact experimentally feasible. Naturally our aim is to achieve the simulation of more intricate

models. It is plausible that using more complex simulators will outperform the best classical methods, and we discuss such possibilities at the end of this chapter.

5.2.1 The variational method

To demonstrate the feasibility of our proposal we take the class of translationally invariant, single-species cMPS, see (5.2), as a variational class of states to determine the energy density of the Lieb-Liniger model

$$E_{\mathrm{LL}}(c;Q,R) = \langle\Psi(\overline{Q},\overline{R})|\ \hat{h}_{\mathrm{LL}}(c)\ |\Psi(Q,R)\rangle = \langle\Psi(\overline{Q},\overline{R})|\ \left(\hat{t}_{\mathrm{LL}} + \hat{w}_{\mathrm{LL}}(c)\right)\ |\Psi(Q,R)\rangle$$

and perform the variational minimisation procedure for a range of values for the interaction strength c. The variational parameters λ are included in the state representation via the matrices $Q = Q(\lambda)$ and $R = R(\lambda)$. We use a simple gradient-descent algorithm for clarity; it is expected that a more sophisticated optimisation procedure, such as conjugate gradients [Fletcher and Reeves, 1964] or the time-dependent variational principle with imaginary-time evolution, could be used, see section 2.3.6 of Chapter 2 and [Haegeman et al., 2011b]. It is required that the minimisation is performed maintaining constant particle density $\varrho = \langle\hat{\psi}^\dagger(x)\hat{\psi}(x)\rangle$. This is in order to ensure that the obtained energy densities are admissible values. We include this constraint by adding a chemical potential term $\hat{v}$ in the Hamiltonian with a chemical potential $-\mu$, which will be used to rescale the minimised energy densities to have constant particle density. We therefore consider the Hamiltonian

$$\begin{aligned}\hat{H}(c,\mu) &= \hat{H}_{\mathrm{LL}}(c) + \int dx\, \hat{v}(\mu) \\ &= \int dx \left(\frac{d\hat{\psi}^\dagger(x)}{dx}\frac{d\hat{\psi}(x)}{dx} + c\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x) - \mu\hat{\psi}^\dagger(x)\hat{\psi}(x) \right) \end{aligned} \tag{5.12}$$

and minimise the corresponding energy density

$$E_H(c,\mu;Q,R) = \langle\Psi(\overline{Q},\{\overline{R_\alpha}\})|\ \hat{h}(c,\mu)\ |\Psi(Q,\{R_\alpha\})\rangle,$$

where $\hat{h}(c,\mu) = \hat{t}_{\mathrm{LL}} + \hat{w}_{\mathrm{LL}}(c) + \hat{v}(\mu)$, using gradient descent. We compute the gradient of the energy density $\nabla E_H(c,\mu;Q,R)$ and iterate for each variational parameter λ_i

$$\lambda_i - \epsilon \left[\nabla E_H(c,\mu;Q,R)\right]_i \rightarrow \tilde{\lambda}_i.$$

The energy density is updated using these new parameters and the procedure repeated until the energy density reaches a fixed point.

Due to the addition of the chemical potential term this minimisation procedure will not produce the quantities that we are interested in, namely the minimum values of $E_{\mathrm{LL}}(c;Q,R)$. We therefore are required to modify the obtained energy minimum of the full Hamiltonian $\hat{H}(c,\mu)$ so as not to include the chemical potential energy density. We also use the chemical potential term to perform a scaling transformation to obtain the energy density at constant particle number. This modification and scaling transformation then gives us the Lieb-Liniger energy density minimum at constant particle density. We detail this scaling procedure below in section 5.2.3.

5.2.2 How the tuneable parameters are included in the cMPS formalism

We now discuss how the experimental parameters g and Ω, along with the scaling parameters s, are related to the cMPS formalism and included in the theoretical minimisation of $E_H(c,\mu;Q,R)$. We have already seen (see (5.7) - (5.9)) that each term of the expected energy density $E_{\mathrm{H}}(c;Q,R) = \langle \hat{t}_{\mathrm{LL}} \rangle + \langle i\hat{w}_{\mathrm{LL}}(c) \rangle + \langle \hat{v}(\mu) \rangle$ can be written in terms of the experimentally observed Glauber correlation functions $G^{(1)}$ and $G^{(2)}$ via the correspondence $\hat{\psi}(x) = \hat{E}^{+}(t)/\sqrt{s}$. In an experimental simulation, these correlation functions would be measured directly in the laboratory, and the results would be fed back into a classical computer performing the optimisation algorithm. However, for the purposes of our proof-of-principle simulation, we calculate the correlation functions directly. This can be achieved by using the cMPS formalism and results from Chapter 4, in particular Eqs. (4.58), (4.59) and (4.60). The same results can also be obtained by means of the input-output formalism. The cavity input-output relation given in Eq. (3.63) of Chapter 3 enables us to write

$$\hat{E}^{+}_{(\mathrm{out})}(t) = \hat{E}^{+}_{(\mathrm{in})}(t) + \sqrt{\kappa}\hat{a}(t),$$

where $\hat{E}^{+}_{(\mathrm{in})}(t)$ denotes the field impinging on the cavity at time t and κ is the cavity decay rate. It is assumed that this input field is in the vacuum state. This means that

$$\hat{E}^{+}_{\mathrm{out}}(t) = \sqrt{\kappa}\hat{a}(t), \tag{5.13}$$

which in turn will allow us to make a connection between the simulator field operator $\hat{E}^{+}_{\mathrm{out}}(t)$ and the cMPS formalism. We recall the link between the variational matrices R and Q and the cavity operators $\hat{a}$ and $\hat{H}_{\mathrm{sys}}$ as given in (4.13), namely

$$R = \sqrt{\frac{\kappa}{s}}\hat{a}, \qquad\qquad Q = -\frac{i}{s}\hat{H}_{\mathrm{sys}} - \frac{1}{2}R^{\dagger}R. \tag{5.14}$$

Since expectation values of operators are equivalent in different pictures, the relations (5.13) and (5.14) enable us to connect $\hat{E}^{+}_{\text{out}}(t)$ and R and thus calculate the expectation values directly using the cMPS matrices R and Q instead of performing measurements. We have that each term (5.7), (5.8) and (5.9) of the energy expectation can written in terms of experimentally observable and theoretical cMPS quantities via

$$\begin{aligned}
\langle \hat{v} \rangle &= -\frac{\mu}{s}\langle \hat{E}^{-}(t)\hat{E}^{+}(t)\rangle \equiv -\mu\langle R^{\dagger}R\rangle \\
\langle \hat{w} \rangle &= \frac{c}{s^{2}}\langle \hat{E}^{-}(t)\hat{E}^{-}(t)\hat{E}^{+}(t)\hat{E}^{+}(t)\rangle \equiv c\langle \left(R^{\dagger}\right)^{2}R^{2}\rangle \\
\langle \hat{t} \rangle &= \frac{1}{s^{3}}\langle \frac{dE^{-}(t)}{dt}\frac{dE^{+}(t)}{dt}\rangle \equiv \langle ([Q,R])^{\dagger}[Q,R]\rangle
\end{aligned} \tag{5.15}$$

where in the last line we have used the relation given in Chapter 4, Eq. (4.21), linking $\frac{d\hat{\psi}(x)}{dx}$ to $[Q,R]$. We can combine these terms to write the expected energy density of the full Hamiltonian in terms of the cMPS variational matrices

$$E_{H}(c,\mu;Q,R) = \langle ([Q,R])^{\dagger}[Q,R]\rangle + c\langle \left(R^{\dagger}\right)^{2}R^{2}\rangle - \mu\langle R^{\dagger}R\rangle \tag{5.16}$$

as presented in Chapter 4. The controllable variational parameters are included in R and Q as follows:

$$R \equiv R(s), \qquad Q \equiv Q(g,\Omega,s), \tag{5.17}$$

with the dependence of Q on g and Ω entering via the dependence of Q on $\hat{H}_{\text{sys}}(g,\Omega)$. The physical changes in an experiment that would allow variation of these controllable parameters will be discussed in section 5.2.6.

5.2.3 Scaling

We now describe the scaling procedure mentioned above in section 5.2.1. Recall that we add a chemical potential to the Lieb-Liniger Hamiltonian in order to keep the particle density constant and compute the energy density $E_{H}(c,\mu;Q,R)$. To remove the impact of this artificial potential and extract the Lieb-Liniger energy density $E_{\text{LL}}(c;Q,R)$ we first use the fact that the expectation value is linear, enabling us to separately calculate the average particle density $d = \langle \hat{v} \rangle = -\mu\langle R^{\dagger}R\rangle$. We add this result to $E_{H}(c,\mu;Q,R)$, such that the contribution of the chemical potential is removed and we have obtained an energy density for the Lieb-Liniger model. Then, we again use d to scale the energy density such that the resulting quantity is at constant particle density. The scaling of the Lieb-Liniger energy density is as follows. The state of the auxiliary system remains invariant under the transformation $Q' \to xQ$,

$R' \to \sqrt{x}R$ [Verstraete and Cirac, 2010]. This can be seen by substituting for Q', R' in Eq. (4.30) in Chapter 4 (as well as (5.22) and (5.23) below). Since the kinetic and interaction energies behave like $\langle [Q,R]^\dagger [Q,R] \rangle$ and $\langle (R^\dagger)^2 R^2 \rangle$ we have that under this transformation

$$E_{\mathrm{LL}}(c;Q',R') = x^3 \langle ([Q,R])^\dagger [Q,R] \rangle + cx^2 \langle \left(R^\dagger\right)^2 R^2 \rangle \tag{5.18}$$

$$= x^3 E_{\mathrm{LL}}(c/x;Q,R). \tag{5.19}$$

Under the same transformation the density term behaves as $d' = -\mu \langle (R')^\dagger R' \rangle \to -\mu x \langle R^\dagger R \rangle = xd$. Thus, by choosing $x = 1/d$ we have constant particle density $d' = 1$ and the scaling transformation

$$E_{\mathrm{LL}}(c;Q,R) \to \frac{E_{\mathrm{LL}}(cd;Q,R)}{d^3}; \tag{5.20}$$

follows. This means that the final minimised energy density of the Lieb-Liniger model is obtained by first minimising the full Hamiltonian with coupling constant c and fixed μ, followed by the addition (since μ is negative) of $\langle \hat{v} \rangle$ to cancel out the chemical potential term, then finally scaling as above to ensure that the final value corresponds to fixed density $d = 1$. It is worth emphasising that the final value does not correspond to the original coupling constant c, but the scaled quantity cd. The parameters that minimise $E_{\mathrm{LL}}(cd;Q,R)/d^3$ can subsequently be used to calculate other quantities of interest, such as correlation functions for the simulated ground state field, again corresponding to a coupling constant cd.

5.2.4 The classical algorithm in detail

We now present a general outline of the algorithm used to determine our optimum values of the variational parameters λ, for a given choice of c and μ. Using (5.14) we first specify our variational matrices R and Q. We have that

$$R(s) = \sqrt{\frac{\kappa}{s}} (\mathbb{I}_2 \otimes \hat{a}_n)$$

where κ is the photon leakage rate and is assumed to be fixed, $\mathbb{I}_2$ is the 2×2 identity matrix and $\hat{a}_n$ is the truncated cavity photon annihilation operator. We truncate the dimension of the annihilation operator $\hat{a}$ to n-th order, such that it is approximated by a $n \times n$ matrix

$$\hat{a}_n = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & \sqrt{2} & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \sqrt{n} \\ 0 & 0 & & 0 & 0 \end{pmatrix}.$$

In the cMPS formalism, the matrices R and Q act on the auxiliary system (the simulator), which in this case is the atom-cavity system. Since we model this system by a two level atom and a single mode of the electromagnetic field, the matrices R and Q therefore take the shape of a two dimensional system (the atom) tensored with a truncated n-dimensional system (representing the electromagnetic field mode). We therefore have that $\dim(R) = 2n$. We also define Q using (5.14) and have that

$$\begin{aligned} Q(g,\Omega,s) &= -i\hat{H}_{\text{sys}}(g,\Omega) - \frac{1}{2}R^\dagger(s)R(s) \\ &= -ig(\hat{\sigma}^+ \otimes \hat{a}_n + \hat{\sigma}^- \otimes \hat{a}_n^\dagger) + \Omega(\hat{\sigma}^+ + \hat{\sigma}^-) \otimes \mathbb{I}_n - \frac{\kappa}{s}\left(\mathbb{I}_2 \otimes \hat{a}_n^\dagger \hat{a}_n\right) \end{aligned} \tag{5.21}$$

where $\mathbb{I}_n$ is the $n \times n$ identity matrix, and $\hat{\sigma}^+, \hat{\sigma}^-$ are the 2×2 atomic raising and lowering operators introduced in Eq. (3.29) of section (3.2), given by

$$\hat{\sigma}^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad \hat{\sigma}^- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

Clearly, $\dim(Q) = 2n$. With these definitions in hand, we are able to proceed with calculating the expected energy density

$$\begin{aligned} E_H(c,\mu;Q,R) &= \langle ([Q,R])^\dagger [Q,R] \rangle + c\langle \left(R^\dagger\right)^2 R^2 \rangle - \mu \langle R^\dagger R \rangle \\ &= \text{tr}\left[([Q,R])^\dagger [Q,R]\rho\right] + c\ \text{tr}\left[\left(R^\dagger\right)^2 R^2\ \rho\right] - \mu\ \text{tr}\left[R^\dagger R \rho\right] \end{aligned}$$

where ρ is the unique steady state of the atom-cavity system, satisfying the master equation derived in Chapter 4, Eq. (4.25), namely

$$\frac{d\rho}{dt} = -i\left[\hat{H}_{\text{sys}}, \rho\right] - \frac{\kappa}{2}\hat{a}^\dagger \hat{a}\rho + \kappa \hat{a}\rho\hat{a}^\dagger - \frac{\kappa}{2}\rho\hat{a}^\dagger\hat{a} = 0. \tag{5.22}$$

It is convenient to write this master equation in the Jamiolkowski representation, see section (4.4.1), where operators are flattened into vector form via (4.28). In terms of this new notation (5.22) is written

$$\frac{d|\rho\rangle}{dt} = M|\rho\rangle,$$

where the matrix M is defined via

$$M := \left[Q \otimes \mathbb{I}_n + \mathbb{I}_n \otimes \overline{Q} + R \otimes \overline{R}\right] \tag{5.23}$$

and has $\dim(M) = (2n)^2$. The steady-state of the atom-cavity system is therefore the solution of this matrix equation, that is the eigenvector of M corresponding to the zero eigenvalue. As discussed in Chapter 4, this eigenvector is known to exist and furthermore it is unique.

To ensure that the eigenvector can be written as a legitimate density operator, we can scale the vector such that the matrix representation satisfies $\mathrm{tr}\left[\rho\right] = 1$. Once this eigenvector is obtained, we can directly calculate the expected energy density that we wish to minimise. We fix our chemical potential to $\mu = 1$ and thus minimise $E_H(c;Q,R) \equiv E_H(c,\mu=1;Q,R)$ using gradient descent. We first calculate the gradient of the energy function, estimated numerically for each component i of the parameter matrices R and Q via

$$\nabla E_H(c;Q,R) = \begin{pmatrix} \big(E_H(c;Q+\Delta_1,R+\Delta_1) - E_H(c;Q-\Delta_1,R-\Delta_1)\big)/2\Delta_1 \\ \vdots \\ \big(E_H(c;Q+\Delta_i,R+\Delta_i) - E_H(c;Q-\Delta_i,R-\Delta_i)\big)/2\Delta_i \\ \vdots \end{pmatrix}$$

for small values of Δ_i. We emphasise again that experimentally $\nabla E_H(c,\mu;Q,R)$ is found with the aid of measurements of $\langle\hat{t}\rangle$, $\langle i\hat{w}\rangle$, and $\langle\hat{v}\rangle$. The parameters are then adaptively tuned via

$$\lambda_i - \epsilon\left[\nabla E_H(c;Q,R)\right]_i \;\rightarrow\; \tilde{\lambda}_i. \tag{5.24}$$

The energy density is updated using these new parameters and the procedure repeated until a fixed point is reached. The general outline of the algorithm to determine the optimum values of the variational parameters λ for a given choice of μ and c is thus

Initialization

Choose a suitable distance δ for the energy convergence

Choose a suitable step size ϵ for the gradient descent

Initialise the set of variational parameters λ_{new} to an arbitrary real value

Iteration

Repeat

Set $\lambda_{old} = \lambda_{new}$

Calculate $\nabla E_H(c;Q_{old},R_{old})$

Update parameters as $\lambda_{new} = \lambda_{old} - \epsilon\nabla E_H(c;Q_{old},R_{old})$

Calculate $E_H(c;Q_{new},R_{new})$ and $E_H(c;Q_{old},R_{old})$

Until

$\left|E_H(c;Q_{new},R_{new}) - E_H(c;Q_{old},R_{old})\right| < \delta$

Once the algorithm has converged we take the final set of variational parameters - the optimal values - and calculate quantities of interest. For example, to obtain the ground state energy of the Lieb-Liniger model along with the corresponding interaction strength we take

the energy minimum obtained then simply perform the rescaling procedure described in section 5.2.1.

5.2.5 Results

Using the above algorithm with $n = 3$, we find the values of $\lambda = \{g, \Omega, s\}$ that minimise $E_H(c, \mu; Q, R)$ for $\mu = 1$ and a fixed value of c. This procedure is repeated over a range of values of interest for the parameter c. The corresponding optimised values of λ are then used to compute quantities of interest, such as spatial-correlation functions. We find that just these three variational parameters $\lambda = \{g, \Omega, s\}$, when varied in the experimentally feasible parameter regime of [Dubin et al., 2010, Stute et al., 2012] in the presence of losses, allow for a quantum simulation of Lieb-Liniger ground state physics.

After performing the scaling procedure given by (5.20) we obtain values of the expected ground state energy density of the Lieb-Liniger model for different values of the (now scaled) interaction strength. In Fig. 5.5 we compare the energy density $E_{\mathrm{LL}}(c; Q, R)$ obtained with a simulation of an ion-trap cavity experiment to that of a direct simulation of the Lieb-Liniger model with the cMPS formalism for dimensions D=2 and D=13 of the auxiliary system, corresponding to 8 and 338 variational parameters respectively. We find that our results for only 3 variational parameters $\{g, \Omega, s\}$ approximately reproduce those for 8 variational parameters when directly simulating the Lieb-Liniger model. We include the example of 338 parameters as a reference, highlighting that by increasing the dimension of the auxiliary system it is possible to obtain results compatible with known analytical methods for solving the Lieb-Liniger model. It was shown in [Verstraete and Cirac, 2010] that the expected energy density results obtained for $D > 12$ are nearly indistinguishable from the exact solution given by the Bethe Ansatz.

Using the optimal values of λ for a set of specific c the simulated two-photon correlation functions $G^{(2)}(t, t)$ were calculated and plotted in Fig. 5.5. In the same figure we plot the correlation functions $\langle \hat{\psi}^\dagger(0)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(0)\rangle$ calculated with a direct simulation of the Lieb-Liniger ground state for the same interaction strengths using 338 variational parameters. The Lieb-Liniger model is known to exhibit a transition between the superfluid regime for $c \approx 0$ and the Tonks-Girardeau regime for $c \gg 0$. This is seen in the value of the correlation function at $t = 0$, since the curves with highest interaction strengths (green and yellow) are approximately 0 at $t = 0$. Although there are visible differences between the two plots, with just three variational parameters $\{g, \Omega, s\}$ the transition in the correlation functions is approximately reproduced.

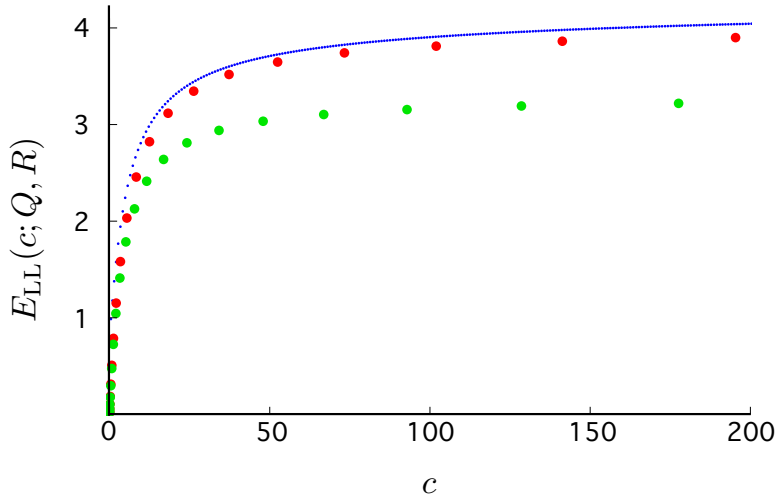

Figure 5.3: The (scaled) ground state energy density for different values of the interaction strength c are reproduced. The green and red show the directly simulated Lieb-Liniger ground state energy density as in [Verstraete and Cirac, 2010] using cMPS with 338 (green) and 8 (red) variational parameters [Haegeman, 2011]. The blue shows the (scaled) ground state energy density for an ion-trap cavity experiment with 3 variational parameters [Stute et al., 2012].

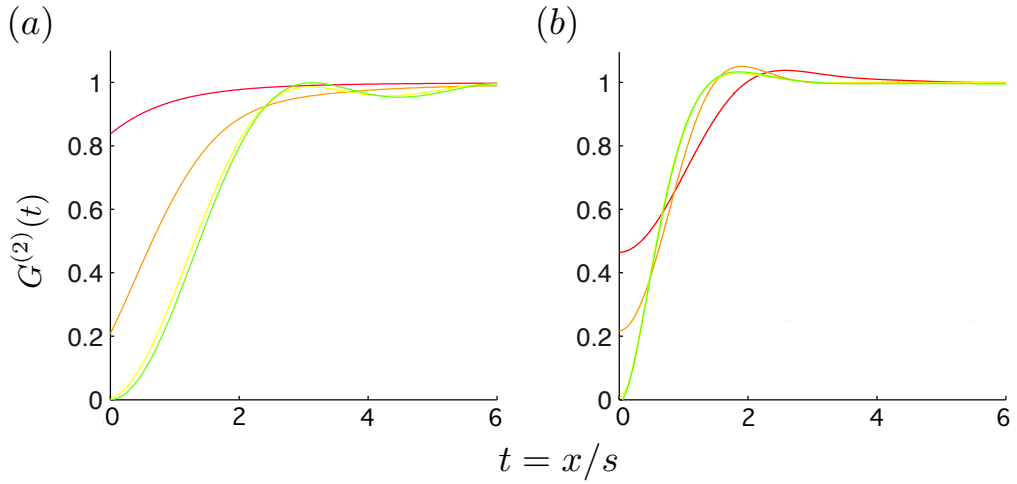

Figure 5.4: Two-particle correlations in the Lieb-Liniger model are reproduced in simulations of an ion-trap cavity experiment. (a) The Lieb-Liniger ground state is directly simulated for interaction strengths $c = \{0.07(\text{red}), 3.95(\text{orange}), 60.20(\text{yellow}), 625.95(\text{green})\}$, and correlation functions $\langle\hat{\psi}^\dagger(0)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(0)\rangle$ calculated by Haegeman in [Haegeman, 2011, Haegeman et al., 2011a] using 338 variational parameters. (b) Two-photon correlation functions $G^{(2)}(t)$ for an ion-trap cavity experiment with the parameters of [Stute et al., 2012].

It is worth emphasising how unusual it is for a variational calculation with only a few variational parameters to reproduce anything more than the coarsest features of a correlation function. We expect that our ground state approximation would improve by increasing the dimension of the auxiliary system and by allowing sufficiently general internal couplings and couplings to the field. In the context of atom-cavity systems, this could be achieved by making use of the level–structure of the atom and by introducing lasers to drive transitions between these levels.

5.2.6 Experimental considerations

The cavity QED Hamiltonian $\hat{H}_{\text{sys}}$ can be realised in various experimental architectures [Miller et al., 2005, Raimond et al., 2001]. We choose the example of a trapped calcium ion in an optical cavity, with which tuneable photon statistics have previously been demonstrated [Dubin et al., 2010]. The electronic structure of $^{40}Ca^{+}$ is actually modelled as a three level atom with ground, excited and metastable states $|1\rangle$, $|3\rangle$ and $|2\rangle$. A classical Raman field Ω' at frequency $\omega_{\Omega'}$ drives the $|1\rangle - |3\rangle$ transition, and the cavity is coupled with strength g_0 to the $|3\rangle - |2\rangle$ transition. The $|1\rangle - |2\rangle$ transition is driven directly via a laser with Rabi frequency Ω at frequency ω_{Ω}. The detuning of the $|1\rangle - |3\rangle$ transition from resonance is given by Δ (see Chapter 3, section 3.3.1). It can be shown that under the condition that the excited state $|3\rangle$ is weakly populated, adiabatic elimination of the state $|3\rangle$ allows the system Hamiltonian to be written in the form of (5.11), where the coupling strength g is given by

$$g = \Omega' g_0 / \Delta, \tag{5.25}$$

see, for example [Steck, 2011]. Tuning the variational parameters $g, \Omega \in \lambda$ thus consists of tuning the strengths of the two classical driving fields Ω' and Ω.

In addition to cavity decay at rate κ, a second decay channel in the experiment is spontaneous emission from the $|3\rangle$ state either to the $|2\rangle$ state, interpreted as spontaneous decay in the two-level system, or to the $|1\rangle$ state, interpreted as phase decoherence. Both channels can be included in the input-output formalism. There are also overall losses associated with scattering and absorption in cavity mirrors, optical losses in the detection path and photon-counter efficiency. Although these losses reduce the efficiency with which photon correlations are detected, they do not otherwise affect the system dynamics and thus are not included in the theoretical model. We have already demonstrated that the classical cMPS algorithm can reproduce characteristic features of Lieb-Liniger ground state physics. It remains to show that the minimising parameters obtained in this simulation are also

experimentally feasible. We compare our results with the experimental parameters of [Stute et al., 2012]. In this ion-cavity experiment the rates of the cavity coupling strength to the $|3\rangle - |2\rangle$ transition g_0, detuning Δ and cavity-field decay κ are given by

$$\begin{aligned} g_0 &= 2\pi \times 1.43 \text{ MHz}, \\ \Delta &= 2\pi \times 400 \text{ MHz} \\ \kappa &= 2\pi \times 0.05 \text{ MHz}. \end{aligned} \tag{5.26}$$

Typical values of the classical driving fields Ω and Ω' lie within the ranges

$$\begin{aligned} \Omega' &\in 2\pi \times (1 - 100) \text{ MHz} \\ \Omega &\in 2\pi \times (0.001 - 5) \text{ MHz}. \end{aligned} \tag{5.27}$$

Using (5.25) we therefore find that the permissible values of the coupling strength $g = \Omega' g_0/\Delta$ are given by

$$g \in 2\pi \times (0.003575 - 0.3575) \text{ MHz}. \tag{5.28}$$

We now compare these values to the values obtained from our simulation. Recall that the cavity-decay rate κ is fixed in the experiment, and the algorithm varies over s via $\Gamma = \sqrt{\kappa/s}$. To make the comparison we therefore rescale the parameters obtained in the simulation according to

$$(\widetilde{g}_{\text{sim}}, \widetilde{\Omega}_{\text{sim}}, \Gamma) \to (g_{\text{sim}}, \Omega_{\text{sim}}, \kappa)$$

with $g_{\text{sim}} = \frac{\kappa}{\Gamma}\widetilde{g}_{\text{sim}}$ and $\Omega_{\text{sim}} = \frac{\kappa}{\Gamma}\widetilde{\Omega}_{\text{sim}}$ to obtain the minimising parameters at $\kappa = 2\pi \times 0.05$ MHz. These parameter values that minimise the energy density for different c obtained in the variational algorithm are presented in Fig. 5.5. We find that the values obtained lie comfortably within the experimentally feasible parameter regime of [Stute et al., 2012].

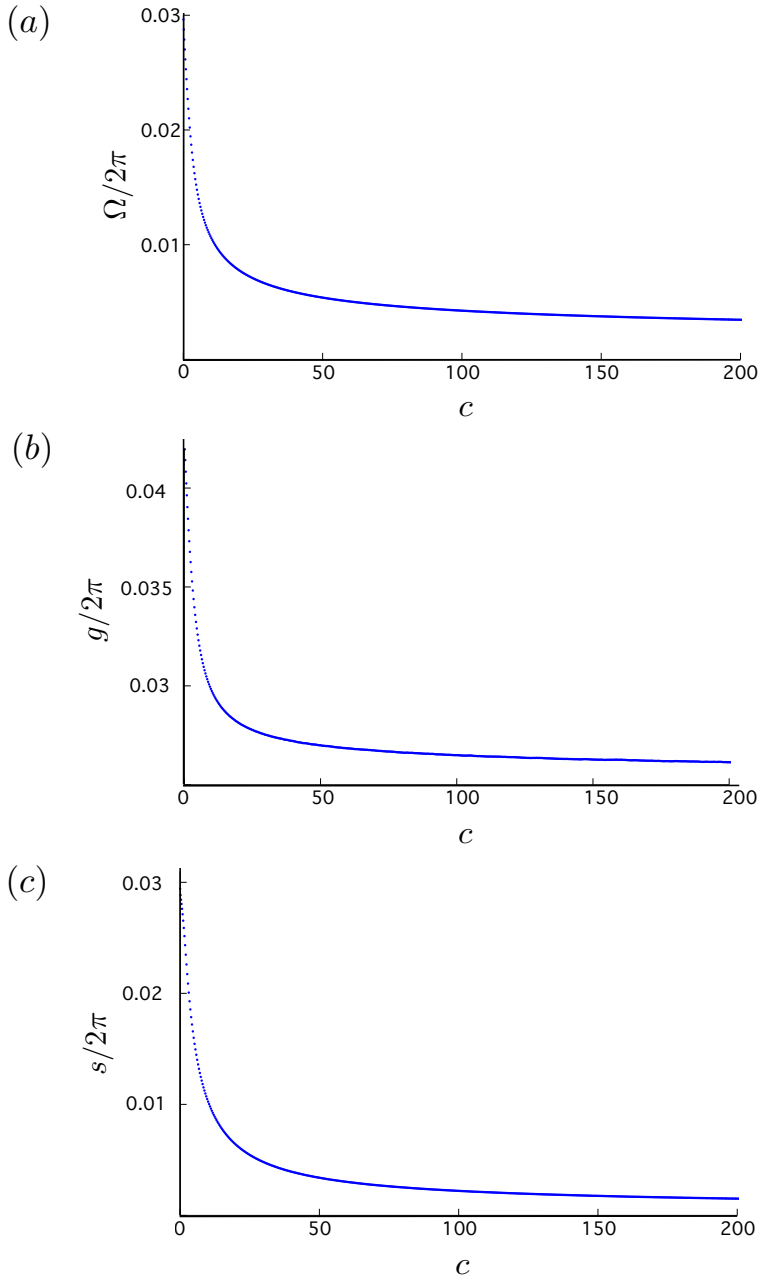

Figure 5.5: Minimising scaled variational parameters for varying interaction strength c and fixed $\kappa = 2\pi \times 0.05$ MHZ obtained via the variational algorithm. (a) Ω in MHz, (b) g in MHz, (c) the scaling parameter s.

5.3 Extensions and outlook

As mentioned earlier, the test model we considered is simple enough to admit an entirely classical simulation. A natural extension is to consider under which conditions our scheme would provide a practical advantage over classical computers in the simulation of quantum fields. We expect this to be the case in particular for the simulation of fields with multiple components, or species of particles. Consider simulating a translational invariant quantum field with multiple bosonic components indexed via $\alpha = 1, \ldots, N$. Such a system is described in second quantisation using the quantum field-annihilation and creation operators $\hat{\psi}_\alpha(x)$ and $\hat{\psi}^\dagger_\alpha(x)$, which obey the canonical commutation relations

$$\left[\hat{\psi}_\alpha(x), \hat{\psi}_\beta(y)\right] = 0, \qquad \left[\hat{\psi}_\alpha(x), \hat{\psi}^\dagger_\beta(y)\right] = \delta_{\alpha,\beta}\delta(x-y) \tag{5.29}$$

described by an arbitrary translational invariant field-theoretic Hamiltonian $\hat{H} = \int dx \hat{h}$ that consists of finite sums of polynomials of the creation and annihilation operators and their derivatives.

To determine the ground state physics of such a Hamiltonian we take a cavity QED device consisting of an N-mode cavity coupled to the quantum degrees of freedom of some intracavity medium. The cavity system is described by a Hamiltonian $\hat{H}_{\text{sys}}(\lambda)$ dependent on some set of controllable parameters λ. The existence of sufficiently strong, tuneable nonlinear interactions is essential in order to provide such tuneable parameters. As before, the simulation algorithm does not depend on the specific nature of the chosen apparatus, it is not even necessary to accurately characterise $\hat{H}_{\text{sys}}(\lambda)$ or its relation to the adjustable parameters λ. When the cavity is driven, either directly through one of its mirrors or indirectly through say the intracavity medium, the intracavity field relaxes to a stationary state and the cavity emits a steady-state beam of photons in each mode $\alpha = 1, \ldots, N$.

Again it is this stationary output state that can be used to simulate the ground state physics of the field. Since quantum field states, including multi-component field states, emerging from a cavity are of cMPS type, we view the output state as a continuous register recording a variational quantum state that has the form of a translational invariant, multi-component cMPS, defined by

$$|\Psi(Q, \{R_\alpha\})\rangle = \langle \omega_L | \mathcal{P} \exp\left(\int Q \otimes \mathbb{I} + \sum_{\alpha=1}^{N} R_\alpha \otimes \hat{\psi}^\dagger_\alpha(x) dx \right) |\omega_R\rangle |\Omega\rangle.$$

The adjustable parameters λ are encoded in the state representation via the matrices Q and R_α and, together with the arbitrary scaling parameter s, make up the variational parameters.

The correspondence between the cavity output and the cMPS representation is completed by identifying the annihilation operators $\hat{\psi}_\alpha(x)$ of the simulated quantum field with the field operators $\hat{E}^+_\alpha(t)$ for the positive frequency electric field of the cavity output modes via

$$\hat{\psi}_\alpha(x) = \frac{\hat{E}^+_\alpha(t)}{\sqrt{s}}, \qquad \alpha = 1, \ldots, N. \tag{5.30}$$

As with the single component case, this identification enables the average energy density of the variational state to be obtained experimentally from standard optical measurements on the cavity output field, namely the Glauber correlation functions of first, second and higher orders. As discussed and depicted in Fig. 5.2 earlier, measurement setups corresponding to such correlation functions can be identified, such that general field-theoretic Hamiltonians can be measured. Generalisations are straightforward for multi-component fields and higher order correlation functions via introducing, for example, more beam splitters and detectors.

Once the average energy density $E(\lambda)$ has been experimentally estimated for a given λ, we can employ the same variational techniques, for example an application of a gradient descent algorithm, to minimise it. As before, the quantity $\nabla E(\lambda)$ would be found with the aid of measurements of the density of the hamiltonian. In some settings, it is possible to efficiently calculate the value of $E(\lambda)$ classically. We would take the class of cMPS as the variational class of states to calculate

$$E(\lambda) \equiv E(Q, R_\alpha) = \langle \Psi(\overline{Q}, \{\overline{R_\alpha}\}) | \hat{h} | \Psi(Q, \{R_\alpha\}) \rangle.$$

This can be done employing the techniques presented in Chapter 4, section 4.4. As before the input-output relation enables us to calculate the correlation functions directly, providing a link between the experimentally observable electric fields and the theoretical cMPS formalism. Under the assumption that the input field is in the vacuum state, we find that

$$\hat{E}^+_{(\text{out})}(t) = \sum_{\alpha=1}^{N} \sqrt{\kappa_\alpha}\, \hat{a}_\alpha(t),$$

such that the connection between $\hat{E}^+(t)$ and the cMPS notation can be made. Using Eq. (4.13), namely $R_\alpha = \sqrt{\frac{\kappa_\alpha}{s}}\hat{a}_\alpha$ and $Q = -\frac{i}{s}\hat{H}_{\text{sys}} - \frac{1}{2}\sum_{\alpha=1}^{N} R^\dagger_\alpha R_\alpha$, we have $\frac{\hat{E}^+_\alpha(t)}{\sqrt{s}} = \sqrt{\frac{\kappa_\alpha}{s}}\hat{a}_\alpha(t) = R_\alpha$, enabling us to make the connections as in (5.15).

In cases involving the study and simulation of fields with multiple components, classical variational calculations using cMPS fail, as the number of variational parameters must scale as $D \sim 2^N$. However, in a cavity QED quantum simulation multiple output fields are naturally accessible via polarisation or higher order cavity modes, and at the same time large

system Hilbert space dimensions can be achieved, e.g., with trapped ions or atoms. With $N \gtrsim 10$, substantial practical speedups are already expected with respect to the classical cMPS algorithm, which requires a number of operations scaling as $2^{3\times N}$.

In addition to this generalisation, we expect that since the input-output and cMPS formalisms generalise in a natural way to fermionic settings [Bi Sun and Milburn, 1999, Gardiner, 2004,Search et al., 2002], our simulation procedure may be applicable to cavity-like microelectronic settings involving fermionic degrees of freedom.

5.4 Chapter summary

We have presented a variational method exploiting the natural physics of cavity QED architectures to simulate interacting quantum fields. The output of a cavity QED apparatus admits an innate interpretation as a variational class of quantum-field states, capable of capturing the ground state physics of interacting fields. We have demonstrated that this interpretation allows an analogue quantum simulation procedure of such systems. By linking the annihilation operators $\hat{\psi}(x)$ of the simulated field with the observable field $\hat{E}^{+}(t)$ we showed that quantities of interest such as the average energy density can be determined experimentally via measurement of Glauber correlation functions. Subsequent minimisation of the energy density in order to obtain a ground state approximation was achieved via a simple gradient descent method.

We illustrated the power of our approach by performing a classical simulation of Lieb-Liniger ground state physics using the cMPS formalism. We found that the minimising parameters obtained lie within an experimentally feasible range and reproduce known features of the model, thus demonstrating that existing cavity devices can simulate models of interacting bosons. We also discussed potential extensions of the model, including the simulation of multi-component fields and generalisation to fermionic systems. Our approach offers a new perspective for all cavity QED systems that exhibit sufficiently strong nonlinearities at the single-photon level, not only optical cavities coupled to atoms, since such architectures could also be used to simulate interacting continuous quantum systems.

Chapter 6

Simulating Continuous Quantum Random Systems

In recent years the study of quantum systems whose Hamiltonians depend on random parameters, that is classical random variables, has attracted much attention. Particularly in the study of magnetic systems, the presence of such randomness, or disorder, has gone from being considered a ubiquitous nuisance, disparaged as dirt, to an essential ingredient producing fascinating phenomena and insights [Fisher et al., 1988]. Its applications are far reaching, a selection of settings including the study of phase transitions in spin chains, the Quantum Hall effect and superconductivity [Fisher, 1995, Gusev et al., 2010, Huse and Fisher, 1992]. The simulation of interacting quantum systems is not easy, and simulating such fields under the action of an impurity, or random potential, involves further complications. The Hamiltonian of a quantum random system generally depends on one or more parameters that are classical random variables. The exact simulation of such physical systems thus requires the study of the system behaviour under different Hamiltonians, corresponding to each realisation of the random variables. The number of such required simulations scales exponentially with the number of random parameters.

To date, much focus has been on the task of simulating discrete quantum random systems on a lattice, where the system Hamiltonian depends on a finite set of discrete random variables. One body of recent work presented an algorithm mapping the problem of simulating a quantum random lattice system to that of simulating a corresponding, non-random interacting lattice problem, for which efficient methods are known [Paredes et al., 2005]. In this approach the system of interest is interacted with an auxiliary system, where the different realisations of the set of classical discrete random parameters are encoded quantum mechanically in a superposition state of this auxiliary system. Choosing the interaction between the system and the auxiliary system appropriately allows for all possible evolutions to be simulated in parallel.

In this chapter we present an algorithm to simulate the dynamics of a continuous quantum

random system (cQRS). The algorithm is a generalisation of [Paredes et al., 2005] to the continuous setting. As in [Paredes et al., 2005], we establish a mapping between a cQRS and an interacting, non-random continuous system, which takes us from the task of simulating a disordered quantum field to that of simulating two interacting quantum fields. Mapping the simulation task in this way opens up a new set of simulation methods and tools. Indeed, problems similar to this have been treated successfully using numerical methods inspired by variational methods and cMPS techniques [Haegeman, 2011, Haegeman et al., 2011a, Verstraete and Cirac, 2010]. One contribution of this chapter, other than establishing the aforementioned mapping, is the proposal of an efficient simulation procedure based on techniques presented in Chapters 2 and 4 and [Haegeman, 2011, Haegeman et al., 2011a, Verstraete and Cirac, 2010]. We develop an extension of the time-dependent variational principle for multi-component fields using cMPS, deriving equations of motion for the time evolution of the cMPS variational parameters.

The chapter is organised as follows. In section 6.1 we present the proposal, describing the type of system we seek to simulate and the difficulties in doing so, followed by a description of the interacting field system we actually simulate. In section 6.1.4 we state the equivalence of the simulation tasks, which we prove first for a discrete system with continuous randomness and then for the case of quantum fields by describing the necessary scaling procedure. In section 6.2.1 we present an illustrative example detailing how the simulation of the Lieb-Liniger model with a random external potential can be achieved. The method relies on an extension of the TDVP, which we describe in full in section 6.2. Following this analysis we perform an analytical implementation for a simple one-dimensional case, and obtain equations of motion that verify our results. In section 6.3 we discuss potential extensions of the proposal and experimental considerations.

6.1 Setup and formulation

6.1.1 What we want to simulate

We consider the simulation of quantum fields modelling a one-dimensional collection of interacting, single-species bosons that are subject to an external random potential. Such a system can be described in second quantisation using the quantum field annihilation and creation operators $\hat{\psi}(x)$ and $\hat{\psi}^\dagger(y)$ that obey the canonical commutation relations

$$\left[\hat{\psi}(x), \hat{\psi}^\dagger(y)\right] = \delta(x-y),$$

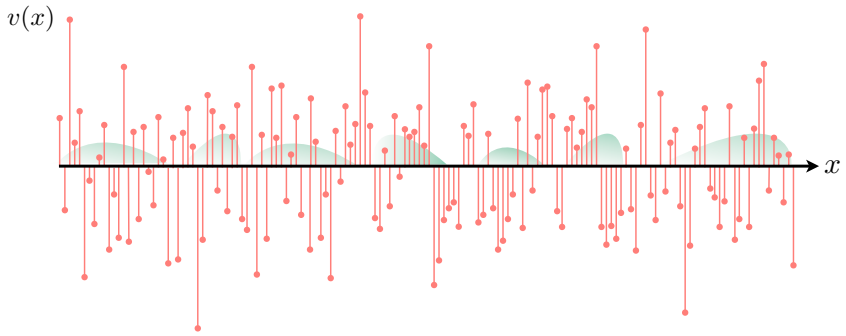

Figure 6.1: Depiction of the quantum field (green) subject to a continuous random potential $v(x)$ (red).

where $-\ell/2 \leq x, y \leq \ell/2$ are space coordinates. The prototypical form of a Hamiltonian for a cQRS is given by

$$\begin{aligned}\hat{H}_{\text{cQRS}}(v(x)) = &\int_{-\ell/2}^{\ell/2} dx \frac{d\psi^\dagger(x)}{dx}\frac{d\psi(x)}{dx} + J\int_{-\ell/2}^{\ell/2} dx\, v(x)\psi^\dagger(x)\psi(x) \\ &+\frac{1}{2}\int_{-\ell/2}^{\ell/2} dx \int_{-\ell/2}^{\ell/2} dy\, w(x,y)\psi^\dagger(x)\psi^\dagger(y)\psi(y)\psi(x),\end{aligned} \tag{6.1}$$

where the first term describes the kinetic energy, the second the potential energy with external random potential $v(x)$ of strength J, to be specified later, and the third a two-particle interaction with potential $w(x,y)$. We have chosen units such that $\hbar = 2m = 1$. Although the Hamiltonians we consider are of this form, the approach works, in principle, for arbitrary field theoretic Hamiltonians that are finite sums of polynomials of field creation and annihilation operators and their derivatives. The main object of interest is the term containing the random potential $v(x)$, whose values at every point x are chosen according to some underlying probability distribution. In a physical setting this random potential could be due to an externally applied magnetic field, about which we do not have precise knowledge of its strength. We could intuitively view $v(x)$ as a derivative of a Brownian motion. For illustrative purposes we depict the quantum field with random potential in Fig. 6.1.

6.1.2 Difficulties in simulating cQRS

The simulation of random systems typically requires the evaluation of dynamical properties averaged over all possible realisations of the randomness. The central quantity of interest is the density operator of the system averaged over the disorder

$$\rho(t) = \mathbb{E}_{v(x)}\left[e^{-it\hat{H}_{\text{cQRS}}(v(x))}|\psi(0)\rangle\langle\psi(0)|e^{it\hat{H}_{\text{cQRS}}(v(x))}\right], \tag{6.2}$$

where each evolved state

$$|\Psi(t)\rangle = e^{-it\hat{H}_{\mathrm{cQRS}}(v(x))}|\Psi(0)\rangle \tag{6.3}$$

corresponds to the evolution of the system under a single realisation of $v(x)$. With $\rho(t)$ we can obtain expectation values of observables $\hat{O}$ averaged over all possible realisations of the random potential via

$$\langle\langle\hat{O}\rangle\rangle = \mathrm{Tr}\left[\hat{O}\rho(t)\right]. \tag{6.4}$$

However, exact determination of (6.2) is often an intractable task, since in many cases we would be required to perform a number of simulations corresponding to the number of possible realisations of the random potential $v(x)$. In a discrete setting, where the random potential consists of a finite set of random variables $r_1, \ldots r_n$ with $r_i \in \Gamma_i = \left\{\lambda_1^i, \ldots \lambda_{m_i}^i\right\}$, the number of simulations needed to exactly simulate the evolution under a random Hamiltonian would be $\prod_{i=1}^{n} m_i$. Clearly in the continuous setting, where the possible realisations Γ_i form an infinite set, the goal of the exact simulation of (6.2) fails.

As in [Paredes et al., 2005], we show that to circumvent this problem we can instead map the task of simulating the random system to that of simulating a non-random, interacting field system. These simulation tasks prove to be equivalent in the sense that the expectation values of physical observables obtained for the two setups are equal. We can therefore instead consider the simulation of the interacting field system.

Recently, numerical techniques based on the time-dependent variational principle (TDVP), see Chapter 2, have been implemented using the class of continuous matrix product states (cMPS), see Chapter 4, as a variational class for finding the ground states, simulating dynamics and studying excitations of one-dimensional continuous quantum systems [Haegeman et al., 2010, Haegeman et al., 2012]. We derive an extension of the TDVP for interacting quantum fields using cMPS with multiple field components, the details of which will be provided in subsequent sections. Firstly, to provide a more straightforward derivation of the aforementioned equivalence, we now proceed by introducing the setup of two quantum fields interacting via a specifically chosen interaction. We then show how this system can be used to simulate the quantum field with external random potential.

6.1.3 What we do to circumvent this difficulty

We now consider two interacting one-dimensional continuous quantum systems, or quantum fields, of length ℓ. The primary field, indexed via α, is described in second quantisation using the quantum field annihilation and creation operators $\hat{\psi}_\alpha(x)$ and $\hat{\psi}_\alpha^\dagger(x)$ that obey the

commutation relation $\left[\hat{\psi}_\alpha(x), \hat{\psi}^\dagger_\alpha(y)\right] = \delta(x-y)$ with x, y position coordinates. In addition to this primary field we consider a second field, the auxiliary field. This auxiliary field, indexed via β, is described in second quantisation using the quantum field annihilation and creation operators $\hat{\psi}_\beta(x)$ and $\hat{\psi}^\dagger_\beta(x)$ that obey the canonical commutation relations

$$\left[\hat{\psi}_\alpha(x), \hat{\psi}^\dagger_\beta(y)\right] = \delta_{\alpha\beta}\delta(x-y).$$

The two fields interact according to the potential $\left(\hat{\psi}_\beta(x) + \hat{\psi}^\dagger_\beta(x)\right)$. As we shall see shortly, this particular choice of field-field interaction forms a crucial part of the algorithm for simulating the cQRS described by (6.1). We are not interested in the specific dynamics of the auxiliary field, it is the interaction between the auxiliary field and the primary field that is of importance. The Hamiltonian $\hat{H}_{\text{int}}$ for the combined system therefore does not include the auxiliary field dynamics and is given by

$$\begin{aligned}\hat{H}_{\text{int}} = &\int_{-\ell/2}^{\ell/2} dx \frac{d\hat{\psi}^\dagger_\alpha(x)}{dx}\frac{d\hat{\psi}_\alpha(x)}{dx} + \int_{-\ell/2}^{\ell/2} dx \frac{\left(\hat{\psi}_\beta(x) + \hat{\psi}^\dagger_\beta(x)\right)}{\sqrt{2}}\hat{\psi}^\dagger_\alpha(x)\hat{\psi}_\alpha(x) \\ &+ \frac{1}{2}\int_{-\ell/2}^{\ell/2} dx \int_{-\ell/2}^{\ell/2} dy\, w(x,y)\hat{\psi}^\dagger_\alpha(x)\hat{\psi}^\dagger_\alpha(y)\hat{\psi}_\alpha(y)\hat{\psi}_\alpha(x), \end{aligned} \tag{6.5}$$

where we have again chosen units such that $\hbar = 2m = 1$. Since we treat the α field as our primary field, this Hamiltonian describes particles interacting with each other through a two-particle interaction $w(x,y)$ and additionally interacting with the auxiliary field β according to the potential $\left(\hat{\psi}_\beta(x) + \hat{\psi}^\dagger_\beta(x)\right)$. This field interaction term can intuitively be thought of as a field position operator

$$\hat{z}(x) = \frac{\left(\hat{\psi}_\beta(x) + \hat{\psi}^\dagger_\beta(x)\right)}{\sqrt{2}},$$

motivated by the relation between the position operator and harmonic oscillator creation and annihilation operators $\hat{z}_j = \left(\hat{a}_j + \hat{a}^\dagger_j\right)/\sqrt{2}$ (see also section 3.1). An essential part of the scheme is that the auxiliary field is prepared in a field coherent state $|\phi\rangle$, as described in section 2.3.2 of Chapter 2.

6.1.4 The equivalence of expectation values

We are now ready to state the mapping between the cQRS and the interacting quantum fields system described above. To summarise, we have that the cQRS evolves accordingly to the Hamiltonian $\hat{H}_{\text{cQRS}}(v(x))$ given in (6.1), where $v(x)$ is a random potential. We have not

specified $v(x)$ thus far, this is to come in the determination of the mapping. The object of interest is the density operator of the system averaged over the disorder, namely

$$\rho(t) = \mathbb{E}_{v(x)}\left[e^{-itH_{\mathrm{cQRS}}(v(x))}|\psi\rangle\langle\psi|e^{itH_{\mathrm{cQRS}}(v(x))}\right], \tag{6.6}$$

where the expectation value $\mathbb{E}_{v(x)}$ is taken with respect to all realisations of the random potential $v(x)$ and $|\psi\rangle$ is the initial state of the field. Determining this expectation value will facilitate the calculation of the expected values of physical observables $\hat{O}$ averaged over the disorder, as we shall see shortly.

Recall that the interacting field system, consisting of the primary field indexed via α and auxiliary field indexed via β, evolves according to the Hamiltonian $\hat{H}_{\mathrm{int}}(\hat{z}(x))$ given by (6.5), where $\hat{z}(x) = (\hat{\psi}_\beta(x) + \hat{\psi}^\dagger_\beta(x))/\sqrt{2}$. The auxiliary field is prepared in the field coherent state $|\phi\rangle$, obtained by taking the continuum limit of the coherent state $|\alpha\rangle$ satisfying $|\langle\alpha|z\rangle|^2 = e^{-z^2/2\gamma}$ with $|z\rangle$ a position eigenstate, see Eq. (2.17). Calculation of the reduced density operator of the primary field α at time t after the evolution of the interacting system under $H_{\mathrm{int}}(\hat{z}(x))$ requires the evaluation of

$$\rho_\alpha(t) = \mathrm{tr}_\beta\left[e^{-itH_{\mathrm{int}}(\hat{z}(x))}|\psi\rangle\langle\psi|_\alpha \otimes |\phi\rangle\langle\phi|_\beta e^{itH_{\mathrm{int}}(\hat{z}(x))}\right], \tag{6.7}$$

where tr_β denotes the trace over the auxiliary field β. We wish to show that the two expectation values (6.6) and (6.7) for the time-evolved states are in fact equivalent, facilitating the simulation of the cQRS via techniques for the simulation of interacting quantum systems. We derive such a method in section 6.2.

Argument

To establish the equivalence of (6.6) and (6.7) we evaluate both expressions in the discrete setting. This is to avoid the cumbersome task of calculating with path ordered integrals. We therefore derive the corresponding discrete Hamiltonians by approximating the continuum by a one-dimensional lattice $\mathcal{L}$ with lattice spacing ϵ. This allows us to prove the equivalence of (6.6) and (6.7) in the discrete setting, whereupon, by ensuring an appropriate scaling for the random potential with respect to ϵ, we can then deduce the equivalence also holds in the continuous setting $\epsilon \to 0$.

The discrete setting of a one-dimensional quantum field of length ℓ is a one-dimensional lattice $\mathcal{L}$. described in section 2.3.2. The creation and annihilation operators $\hat{a}^\dagger_j$ and $\hat{a}_j$ appearing in (2.13) are the discrete forms of the field creation and annihilation operators

$\hat{\psi}^\dagger(x)$ and $\hat{\psi}(x)$, obtained from taking the limit $\epsilon \to 0$ via

$$\hat{\psi}(x) \mapsto \hat{\psi}(j\epsilon) = \hat{a}_j/\sqrt{\epsilon}.$$

The derivative of the field operator is therefore given by

$$\frac{d\hat{\psi}(x)}{dx} = \frac{\hat{\psi}(x+\epsilon)-\hat{\psi}(x)}{\epsilon} \mapsto \frac{\psi(j\epsilon+\epsilon)-\psi(j\epsilon)}{\epsilon} = \frac{\hat{a}_{j+1}-\hat{a}_j}{\epsilon\sqrt{\epsilon}}.$$

We then see that the kinetic term in (6.1) and (6.5) can be written

$$\int_{-\ell/2}^{\ell/2} dx \frac{d\hat{\psi}^\dagger(x)}{dx}\frac{d\hat{\psi}(x)}{dx} \mapsto \epsilon \sum_{j=1}^{N} \frac{(\hat{a}_{j+1}^\dagger - \hat{a}_j^\dagger)(\hat{a}_{j+1}-\hat{a}_j)}{\epsilon^3}.$$

For the particle-particle interaction term we have

$$\frac{1}{2}\int_{-\ell/2}^{\ell/2} dx \int_{-\ell/2}^{\ell/2} dy\, w(x,y)\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(y)\hat{\psi}(y)\hat{\psi}(x) \mapsto \frac{\epsilon^2}{2}\sum_{i,j=1}^{N} w(i\epsilon, j\epsilon)\frac{(\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_i)}{\epsilon^2}.$$

For the interaction potential term of (6.5) we have

$$\begin{aligned}\int_{-\ell/2}^{\ell/2} dx \frac{\left(\hat{\psi}_\beta(x)+\hat{\psi}_\beta^\dagger(x)\right)}{\sqrt{2}}\hat{\psi}_\alpha^\dagger(x)\hat{\psi}_\alpha(x) &\mapsto \epsilon\sum_{j=1}^{N}\left(\frac{\hat{b}_j+\hat{b}_j^\dagger}{\sqrt{2\epsilon}}\right)\frac{\hat{a}_j^\dagger\hat{a}_j}{\epsilon} \\ &= \epsilon\sum_{j=1}^{N}\left(\frac{\hat{z}_j}{\sqrt{\epsilon}}\right)\frac{\hat{a}_j^\dagger\hat{a}_j}{\epsilon}, \end{aligned} \tag{6.8}$$

where $\hat{z}_j = (\hat{b}_j + \hat{b}_j^\dagger)/\sqrt{2}$ is the position operator satisfying $\hat{z}_j|z_j\rangle = z_j|z_j\rangle$ with $|z_j\rangle$ the position eigenstate providing a basis for the auxiliary system with $\int dz_j |z_j\rangle\langle z_j| = \mathbb{I}$. We therefore find that the Hamiltonian for the discrete interacting quantum system is given by

$$\hat{H}_{\text{int}}(\hat{z}(x)) = \epsilon\sum_{j=1}^{N}\frac{(\hat{a}_{j+1}^\dagger-\hat{a}_j^\dagger)(\hat{a}_{j+1}-\hat{a}_j)}{\epsilon^3} + \frac{\epsilon^2}{2}\sum_{i,j=1}^{N} w(i\epsilon,j\epsilon)\frac{(\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_j\hat{a}_i)}{\epsilon^2} + \epsilon\sum_{j=1}^{N}\frac{\hat{z}_j}{\sqrt{\epsilon}}\frac{\hat{a}_j^\dagger\hat{a}_j}{\epsilon}. \tag{6.9}$$

We now consider the random potential term of (6.1). In the discrete setting the random potential $v(x)$ comprises a finite set $\underline{v} = \{v_1, \ldots, v_N\}$ of random variables whose values are chosen according to some probability distribution. We take $\underline{v}$ to be a set of Gaussian random variables with probability density function $f(v_j) = \frac{1}{\sqrt{2\pi\gamma}}e^{-v_j^2/2\gamma}$ for each $j \in \{1,\ldots,N\}$, satisfying

$$\mathbb{E}\left[v_j\right] = 0, \qquad \mathbb{E}\left[v_j^2\right] = \gamma \qquad \text{and} \qquad \mathbb{E}\left[v_j v_k\right] = 0, \ \ \forall j \neq k.$$

When considering the limit $\epsilon \to 0$ we must apply an appropriate scaling procedure such that the resulting sample $v(x)$ behaves sufficiently well, that is we require finite expectation

values for the gain in potential strength, defined by $V_k = \sum_{j=1}^{k} v_j$, with $1 \leq k \leq N$, and also for how much the potential strength changes from one position to the next, that is how jagged the potential path is, measured by the sum of the quadratic variations $\sum_{j=1}^{N-1}(v_{j+1} - v_j)^2$. Using linearity of the expectation value we find that the expectation value of the increase in potential strength is given by

$$\mathbb{E}[V_k] = \mathbb{E}\left[\sum_{j=1}^{k} v_j\right] = \sum_{j=1}^{k} \mathbb{E}\left[v_j\right] = 0.$$

The expectation value for the gain in potential strength is therefore always finite. For the quadratic variation we obtain

$$\begin{aligned}\mathbb{E}\left[\sum_{j=1}^{N-1}\left(v_{j+1} - v_j\right)^2\right] &= \mathbb{E}\left[\sum_{j=1}^{N-1}\left(v_{j+1}^2 + v_j^2 - 2v_{j+1}v_j\right)\right] \\ &= \sum_{j=1}^{N-1}\mathbb{E}\left[v_{j+1}^2\right] + \sum_{j=1}^{N-1}\mathbb{E}\left[v_j^2\right] - 2\sum_{j=1}^{N-1}\underbrace{\mathbb{E}\left[v_{j+1}v_j\right]}_{=0} = 2(N-1)\gamma.\end{aligned}$$

Using that $\ell = N\epsilon$ we thus find that γ must scale as $\gamma \sim \epsilon$ to ensure that we obtain a finite value. Since $\mathbb{E}\left[v_j^2\right] = \gamma$ this means we have to use the scaled random variables $\frac{v_j}{\sqrt{\epsilon}}$.

We note that this process of determining the correct scaling is the usual procedure when defining a Wiener process or Brownian motion as a limit of random walks. We therefore find that the Hamiltonian for the discrete quantum random system is given by

$$\hat{H}_{\mathrm{QRS}}(\underline{v}) = \epsilon\sum_{j=1}^{N}\frac{(\hat{a}_{j+1}^\dagger - \hat{a}_j^\dagger)(\hat{a}_{j+1} - \hat{a}_j)}{\epsilon^3} + \frac{\epsilon^2}{2}\sum_{i,j=1}^{N} w(i\epsilon, j\epsilon)\frac{(\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_j\hat{a}_i)}{\epsilon^2} + \epsilon\sum_{j=1}^{N}\frac{v_j}{\sqrt{\epsilon}}\frac{\hat{a}_j^\dagger\hat{a}_j}{\epsilon}. \tag{6.10}$$

The density operator of the system averaged over the disorder, as given by (6.6), is then

$$\begin{aligned}\rho(t) &= \mathbb{E}_{\underline{v}}\left[e^{-it\hat{H}_{\mathrm{QRS}}(\underline{v})}|\psi(0)\rangle\langle\psi(0)|e^{it\hat{H}_{\mathrm{QRS}}(\underline{v})}\right] \\ &= \int d\underline{v}\; f(\underline{v})e^{-it\hat{H}_{\mathrm{QRS}}(\underline{v})}|\psi(0)\rangle\langle\psi(0)|e^{it\hat{H}_{\mathrm{QRS}}(\underline{v})} \\ &= \frac{1}{(2\pi\gamma)^{N/2}}\int d\underline{v}\; e^{-\underline{v}^2/\gamma}e^{-it\hat{H}_{\mathrm{QRS}}(\underline{v})}|\psi(0)\rangle\langle\psi(0)|e^{it\hat{H}_{\mathrm{QRS}}(\underline{v})}.\end{aligned} \tag{6.11}$$

where $\int d\underline{v}e^{-\underline{v}^2/\gamma} = \int dv_1 \ldots \int dv_N e^{-{v_1}^2/\gamma}\ldots e^{-{v_N}^2/\gamma}$. Having rewritten (6.6) we proceed with a similar treatment of (6.7), so that we can show they are in fact equivalent. For the discrete interacting quantum system the Hamiltonian is given by (6.9). Treatment of (6.7) requires that we evaluate

$$\rho_\alpha(t) = \mathrm{tr}_\beta\left[e^{-it\hat{H}(\hat{z})}|\psi(0)\rangle\langle\psi(0)| \otimes (|\alpha\rangle\langle\alpha|)_\beta^{\otimes N} e^{it\hat{H}(\hat{z})}\right]. \tag{6.12}$$

Using the resolution of identity via the position eigenbasis of the auxiliary system, that is $\int d\underline{z}|z\rangle\langle z|^{\otimes N} = \mathbb{I}$, we find that

$$\begin{aligned}\rho_\alpha(t) &= \mathrm{tr}_\beta\left[e^{-itH(\hat{z})}|\psi(0)\rangle\langle\psi(0)|\otimes(|\alpha\rangle\langle\alpha|)_\beta^{\otimes N}e^{itH(\hat{z})}\right]\\ &= \mathrm{tr}_\beta\left[e^{-itH(\hat{z})}|\psi(0)\rangle\langle\psi(0)|\otimes(|\alpha\rangle\langle\alpha|)_\beta^{\otimes N}e^{itH(\hat{z})}\left(\mathbb{I}\otimes\int d\underline{z}|z\rangle\langle z|^{\otimes N}\right)\right]\\ &= \int d\underline{z}\,\mathbb{I}\otimes(\langle z|)^{\otimes N}\left(e^{-itH(\hat{z})}|\psi(0)\rangle\langle\psi(0)|\otimes(|\alpha\rangle\langle\alpha|)_\beta^{\otimes N}e^{itH(\hat{z})}\right)\mathbb{I}\otimes(|z\rangle)^{\otimes N}.\end{aligned}$$

Since $\hat{z}|z\rangle = z|z\rangle$ it is straightforward to show, via series expansion of $e^{itH(\hat{z})}$ and decomposition of $H(\hat{z})$ into a sum of tensor products on the separate systems, that $e^{itH(\hat{z})}(\mathbb{I}\otimes|z\rangle^{\otimes N}) = e^{itH(\underline{z})}(\mathbb{I}\otimes|z\rangle^{\otimes N})$, enabling the replacement of operators $\hat{z}$ with real numbers $\underline{z}$. We can therefore write that

$$\begin{aligned}&\int d\underline{z}\,\mathbb{I}\otimes(\langle z|)^{\otimes N}\left(e^{-itH(\hat{z})}|\psi(0)\rangle\langle\psi(0)|\otimes(|\alpha\rangle\langle\alpha|)_\beta^{\otimes N}e^{itH(\hat{z})}\right)\mathbb{I}\otimes(|z\rangle)^{\otimes N}\\ &= \int d\underline{z}\,e^{-itH(\underline{z})}\left(|\psi(0)\rangle\langle\psi(0)|\otimes\langle z|^{\otimes N}|\alpha\rangle\langle\alpha|_\beta^{\otimes N}|z\rangle^{\otimes N}\right)e^{itH(\underline{z})}\\ &= \frac{1}{(2\pi\gamma)^{N/2}}\int d\underline{z}\,e^{-\underline{z}^2/\gamma}e^{-itH(\underline{z})}|\psi(0)\rangle\langle\psi(0)|e^{itH(\underline{z})},\end{aligned}\tag{6.13}$$

where in the last line we have used that $|\langle\alpha|z\rangle|^2 = \frac{1}{\sqrt{2\pi\gamma}}e^{-z^2/\gamma}$. We have thus proven (6.11) and (6.13) to be equivalent. Since we have shown that the continuous setting can be obtained by taking the limit $\epsilon\to 0$ with the above scaling procedure, we can therefore write that

$$\mathrm{tr}_\beta\left[e^{-itH_{\mathrm{int}}(\hat{z}(x))}|\psi\rangle\langle\psi|_\alpha\otimes|\phi\rangle\langle\phi|_\beta e^{itH_{\mathrm{int}}(\hat{z}(x))}\right] = \mathbb{E}_{v(x)}\left[e^{-itH_{\mathrm{cQRS}}(v(x))}|\psi\rangle\langle\psi|e^{itH_{\mathrm{cQRS}}(v(x))}\right],\tag{6.14}$$

where the Hamiltonians $H_{\mathrm{int}}(\hat{z}(x))$ and $H_{\mathrm{cQRS}}(v(x))$ are the continuous quantum system Hamiltonians given by (6.1) and (6.5). In Fig.6.2 we illustrate this equivalence and the corresponding analogies.

6.1.5 How to proceed

We have shown that to determine the expectation value over all realisations of the cQRS time-evolved states we can instead consider the time-evolved state of a corresponding interacting quantum field system. We are thus faced with the task of simulating this time-evolved state, obtained via time evolution of the initial product state under the interaction Hamiltonian $H_{\mathrm{int}(\hat{z})}$, which we achieve by applying the TDVP using cMPS.

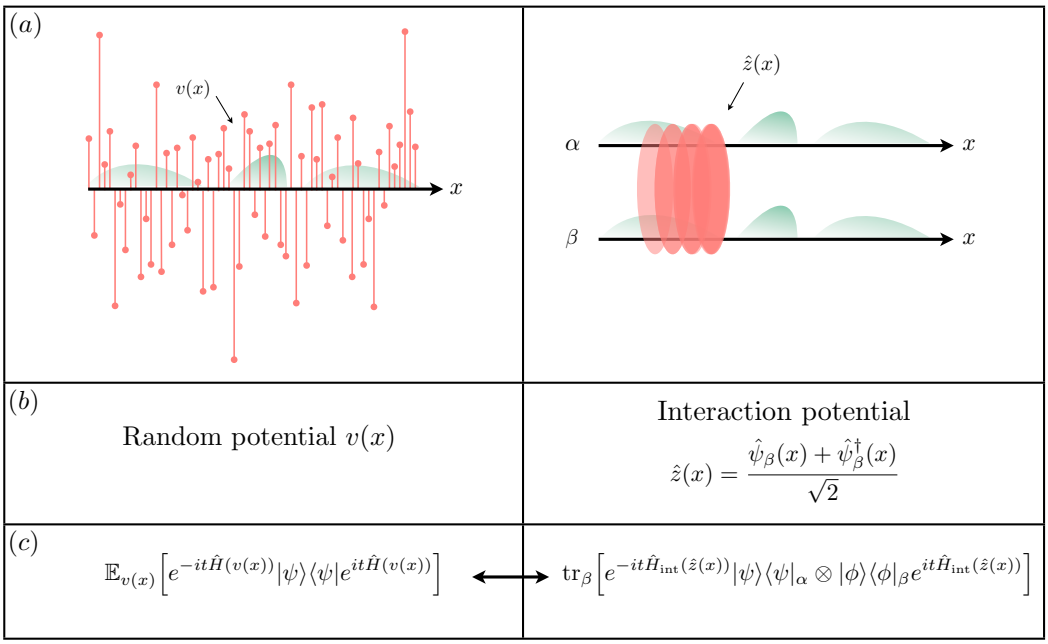

Figure 6.2: Identification of corresponding quantities in the mapping between the cQRS and interacting quantum fields. (a) Depiction of the corresponding systems: (left) the quantum field (green) subject to a random potential (red), (right) the quantum fields (green) interacting via the field position operator (red). (b) The corresponding (left) random potential, (right) field interaction. (c) The equivalent expectation values.

6.2 The time-dependent variational principle for multi-component fields

Recall from Chapter 2 that the TDVP is a method used to approximate the dynamics of quantum systems that are governed by the time-dependent Schrödinger equation,

$$\frac{d}{dt}|\Psi(z(t))\rangle = -i\hat{H}(t)|\Psi(z(t))\rangle$$

whilst remaining within some variational class $\mathcal{V}$, here parameterised by a set of parameters $z(t)$, embedded in the system Hilbert space. The exact evolution of the state will generally leave the variational class. The best approximation within $\mathcal{V}$ is therefore found by approximating the actual evolution $-i\hat{H}(t)|\Psi(z(t))\rangle$ by the tangent vector $\frac{d}{dt}|\Psi(z(t))\rangle$ that minimises

$$\left|\frac{d}{dt}|\Psi(z(t))\rangle + i\hat{H}(t)|\Psi(z(t))\rangle\right|^2. \tag{6.15}$$

This is equivalent to finding optimal equations of motion for $z(t)$, since writing $\frac{d}{dt}|\Psi(z(t))\rangle = \dot{z}^j|\partial_j\Psi(z)t))\rangle$ and differentiating (6.15) with respect to $\dot{\bar{z}}^j$ shows that the minimum occurs

when the tangent vector is parameterised by $z(t)$ satisfying

$$\begin{aligned}\dot{z}^k(t) &= -i\langle\partial_{\bar{j}}\Psi(\overline{z})|\partial_k\Psi(z)\rangle^{-1}\langle\partial_{\bar{j}}\Psi(z(t))|\hat{H}(t)|\Psi(z(t))\rangle \\ &= -iG_{\bar{j}k}(\overline{z},z)^{-1}L_{\bar{j}}(\overline{z},z)\end{aligned} \tag{6.16}$$

where we have defined $G_{\bar{j},k}(\overline{z},z)$ and $L_{\bar{j}}(\overline{z},z)$ as in (2.27) and (2.26) respectively, see section 2.3, particularly 2.3.4, for a detailed presentation of the method.

We apply the TDVP using the class of multi-component translationally invariant cMPS given by (6.21) as our variational manifold

$$\mathcal{V} = \left\{ |\Psi(Q,R_\alpha,R_\beta\rangle \,\middle|\, \forall Q,R_\alpha,R_\beta \in \mathbb{C}^{D\times D} \right\}.$$

This class of states is parameterised via the $D\times D$ matrices Q,R_α and R_β. The $3D^2$ entries of these matrices form our set of variational parameters $z(t)=\left\{z^1(t),z^2(t),\ldots,z^{3D^2}(t)\right\}$. To obtain the optimal set of $z(t)$ satisfying (6.16) we therefore must compute the $3D^2\times 3D^2$ matrix G, as defined above in (6.16), whose jk-th entry is given by the overlap of the tangent vectors $|\partial_{\bar{j}}\Psi(\overline{z})\rangle$ and $\langle\partial_k\Psi(z)|$, namely

$$G_{jk} = \langle\partial_{\bar{j}}\Psi(\overline{z})|\partial_k\Psi(z)\rangle \tag{6.17}$$

along with the $3D^2\times 1$ projection matrix L, as defined above in (6.16), whose j-th entry given by

$$L_j = \langle\partial_{\bar{j}}\Psi(\overline{z})|\hat{H}|\Psi(z)\rangle. \tag{6.18}$$

6.2.1 Implementation of the scheme

As an illustrative example we study the dynamics of the Lieb-Liniger model subject to an external random potential. As presented in section 4.7 of Chapter 4, the Lieb-Liniger model describes a one-dimensional system of bosons interacting via a two-body delta-potential and is described in second quantisation by the Hamiltonian

$$\hat{H}_{\mathrm{LL}} = \int_{-\ell/2}^{\ell/2} dx \left(\frac{d\psi_\alpha^\dagger(x)}{dx}\frac{d\psi_\alpha(x)}{dx} + c\psi_\alpha^\dagger(x)\psi_\alpha^\dagger(x)\psi_\alpha(x)\psi_\alpha(x) \right),$$

where ℓ is the system length and c describes the interaction strength. The addition of an external random potential means we study the dynamics of the system governed by

$$\tilde{H}_{v(x)} = \hat{H}_{\mathrm{LL}} + J\int_{-\ell/2}^{\ell/2} dx\, v(x)\psi_\alpha^\dagger(x)\psi_\alpha(x), \tag{6.19}$$

where $v(x)$ is considered to be the random potential with strength J, obtained via a limiting procedure and scaling of Gaussian random potentials on the lattice, as described in section 6.1.

Exact simulation of the dynamics of $\hat{H}(v(x))$ would require an infinite number of simulations corresponding to each realisation of $v(x)$. However, following the above algorithm we can avoid this unattainable task as follows. We include an auxiliary field system, described in second quantisation via the field operators $\hat{\psi}_\beta(x)$ and $\hat{\psi}^\dagger_\beta(x)$, that is initially prepared in a field coherent state $|\phi\rangle$. We then evolve the composite system, consisting of the primary field indexed via α and the auxiliary field indexed via β, under the interaction Hamiltonian

$$\tilde{H}_{\text{int}} = \int_{-\ell/2}^{\ell/2} dx \left[\left(\frac{d\psi^\dagger_\alpha(x)}{dx} \frac{d\psi_\alpha(x)}{dx} \otimes \mathbb{I} \right) + \left(c\psi^\dagger_\alpha(x)\psi^\dagger_\alpha(x)\psi_\alpha(x)\psi_\alpha(x) \otimes \mathbb{I} \right) + \frac{J}{\sqrt{2}} \left(\psi^\dagger_\alpha(x)\psi_\alpha(x) \otimes \left(\hat{\psi}_\beta(x) + \psi^\dagger_\beta(x) \right) \right) \right]. \tag{6.20}$$

To simulate the dynamics according to $\tilde{H}_{v(x)}$ we thus study the dynamics of this interacting system using methods introduced in [Haegeman, 2011, Haegeman et al., 2011a, Haegeman et al., 2010], namely application of the time-dependent variational principle in conjunction with cMPS, as we show below.

The interaction Hamiltonian $\hat{H}_{\text{int}}$ acts on the composite system consisting of two quantum fields indexed via α and β. We therefore take the initial state $|\Psi(0)\rangle = |\psi(0)\rangle_\alpha \otimes |\phi\rangle_\beta$ to be the translationally invariant continuous matrix product state (cMPS), as defined in section 4.1 of Chapter 4, with two field components, that is

$$\begin{aligned} |\Psi(0)\rangle &= |\Psi(Q, R_\alpha, R_\beta)\rangle \\ &= \langle \omega_L | \mathcal{P} \exp \left(\int_{-\ell/2}^{\ell/2} Q \otimes \mathbb{I} \otimes \mathbb{I} + R_\alpha \otimes \hat{\psi}^\dagger_\alpha(x) \otimes \mathbb{I} + R_\beta \otimes \mathbb{I} \otimes \hat{\psi}^\dagger_\beta(x) dx \right) |\omega_R\rangle |\Omega\rangle_\alpha |\Omega\rangle_\beta, \end{aligned} \tag{6.21}$$

where Q, R_α and R_β are constant matrices acting on a D-dimensional auxiliary system (not to be confused with the auxiliary field system introduced in (6.20)), $|\Omega\rangle_\alpha$ and $|\Omega\rangle_\beta$ are the field vacuum states and $|\omega_R\rangle$ and $\langle\omega_L|$ are vectors encoding the auxiliary system boundary conditions. Evolution of the cMPS under the Hamiltonian $\hat{H}_{\text{int}}$ can be simulated via application of the TDVP for multiple species of bosons. As described above and in Chapter 2, the TDVP provides an approximation to the actual time evolved state. We therefore lose the exact simulation of the cQRS at this stage. However, since we employ the class of cMPS, which have proven to be an expressive variational class capable of simulating quantum fields [Haegeman, 2011, Haegeman et al., 2011a, Verstraete and Cirac, 2010], we are optimistic that the obtained approximation is more than adequate. We justify our conjecture by considering a simple analytical example for $D = 1$ in section 6.2.10.

The necessary formula required for an application of the TDVP using the multi-component cMPS will be computed below. So far, applications of the TDVP using cMPS have been

restricted to single-species bosonic particles. We therefore include a detailed description of the generalisation to multiple species.

6.2.2 Computing the Gram matrix

To specify the Gram matrix (6.17) we must evaluate derivatives of the cMPS (6.21) with respect to each variational parameter z^j. In appendix B.1 we detailed the calculation of a general tangent vector to the cMPS $|\Psi(Q,\{R_\alpha\})\rangle$, that is a linear combination of all $3D^2$ derivatives of the cMPS with respect to each variational parameter. We follow the same procedure presented there to begin the evaluation of the Gram matrix G. We have that, henceforth omitting the arguments Q, R_α and R_β in the state $|\Psi(Q,R_\alpha,R_\beta)\rangle$,

$$|\partial_j\Psi\rangle = \langle\omega_L|\partial_j U_{\ell/2,-\ell/2}|\omega_R\rangle|\Omega\rangle_\alpha|\Omega\rangle_\beta \tag{6.22}$$

where, as in eq. (4.2), we have labelled the path ordered integral

$$U_{\ell/2,-\ell/2} = \mathcal{P}\exp\left(\int_{-\ell/2}^{\ell/2} Q\otimes\mathbb{I}\otimes\mathbb{I} + R_\alpha\otimes\hat{\psi}^\dagger_\alpha(x)\otimes\mathbb{I} + R_\beta\otimes\mathbb{I}\otimes\hat{\psi}^\dagger_\beta(x)dx\right).$$

From appendix B.1 we know that

$$\partial_j\left(U_{\ell/2,-\ell/2}\right) = \int_{-\ell/2}^{\ell/2}\left(U_{\ell/2,s}\partial_j\left(\hat{H}_{\text{cMPS}}(s)\right)U_{s,-\ell/2}\right)ds$$

where

$$\hat{H}_{\text{cMPS}}(s) = Q\otimes\mathbb{I}\otimes\mathbb{I} + R_\alpha\otimes\psi^\dagger_\alpha(s)\otimes\mathbb{I} + R_\beta\otimes\mathbb{I}\otimes\psi^\dagger_\beta(s)$$

as defined in (4.3). Now, since the variational parameters z^j enter the cMPS representation via the matrices $Q = Q(z^1,\ldots,z^{D^2})$, $R_\alpha = R_\alpha(z^{D^2+1},\ldots,z^{2D^2})$ and $R_\beta = R_\beta(z^{2D^2+1},\ldots,z^{3D^2})$ we have that

$$\partial_j\left(\hat{H}_{\text{cMPS}}(s)\right) = \begin{cases} \partial_j(Q\otimes\mathbb{I}\otimes\mathbb{I}) & \text{if } 1\le j\le D^2; \\ \partial_j(R_\alpha\otimes\psi^\dagger_\alpha(s)\otimes\mathbb{I}) & \text{if } D^2+1\le j\le 2D^2; \\ \partial_j(R_\beta\otimes\mathbb{I}\otimes\psi^\dagger_\beta(s)) & \text{if } 2D^2+1\le j\le 3D^2. \end{cases}$$

Therefore the derivative of the cMPS with respect to the variational parameter z^j is given by

$$|\partial_j\Psi\rangle = \begin{cases} \int ds\langle\omega_L|U_{\ell/2,s}(q^j\otimes\mathbb{I}\otimes\mathbb{I})U_{s,-\ell/2}|\omega_R\rangle|\Omega\rangle_{\alpha,\beta} & \text{if } 1\le j\le D^2; \\ \int ds\langle\omega_L|U_{\ell/2,s}(r^j_\alpha\otimes\psi^\dagger_\alpha(s)\otimes\mathbb{I})U_{s,-\ell/2}|\omega_R\rangle|\Omega\rangle_{\alpha,\beta} & \text{if } D^2+1\le j\le 2D^2; \\ \int ds\langle\omega_L|U_{\ell/2,s}(r^j_\beta\otimes\mathbb{I}\otimes\psi^\dagger_\beta(s))U_{s,-\ell/2}|\omega_R\rangle|\Omega\rangle_{\alpha,\beta} & \text{if } 2D^2+1\le j\le 3D^2. \end{cases} \tag{6.23}$$

where $q_j = \partial_j Q$, $r^j_\alpha = \partial_j R_\alpha$ and $r^j_\beta = \partial_j R_\beta$. The computation of a general entry $G_{jk} = \langle \partial_{\bar{j}} \Psi | \partial_k \Psi \rangle$ of the Gram matrix is dependent on where j and k are in $\{1, \ldots, 3D^2\}$. There are nine separate cases, or blocks of the matrix, to consider. We present a detailed calculation for one of these cases, before specifying the Gram matrix in full. For more information on how to compute the other block entries of the Gram matrix, see appendix C.

6.2.3 Block 5 of G

We consider the block matrix entry obtained when $D^2 + 1 \leq j, k \leq 2D^2$. We choose to present this calculation in full since, unlike the other cases, it is burdened by the additional complexity of the presence of two field operators of the same type. We first rewrite the matrix entry as a trace rather than the overlap of tangent vectors,

$$G_{jk} = \langle \partial_{\bar{j}} \Psi | \partial_k \Psi \rangle = \mathrm{Tr}\left[|\partial_k \Psi\rangle\langle \partial_{\bar{j}} \Psi| \right]$$

then insert the corresponding form of the tangent vectors given in (6.23) for $D^2 + 1 \leq j, k \leq 2D^2$. Note that in the following we make notation more compact by writing $\omega_R \equiv |\omega_R\rangle\langle\omega_R|$, $\Omega \equiv |\Omega\rangle\langle\Omega|_{\alpha,\beta}$ and $(r^k_\alpha \otimes \psi^\dagger_\alpha(s)) \equiv (r^k_\alpha \otimes \psi^\dagger_\alpha(s) \otimes \mathbb{I})$. We evaluate

$$\mathrm{Tr}\left[|\partial_k \Psi\rangle\langle \partial_{\bar{j}} \Psi| \right] = \int_{-\ell/2}^{\ell/2} \int_{-\ell/2}^{\ell/2} ds\, ds'\, \mathrm{Tr}\Big[\langle \omega_L | U_{\ell/2,s}(r^k_\alpha \otimes \psi^\dagger_\alpha(s)) U_{s,-\ell/2}(\omega_R \otimes \Omega) U^\dagger_{s',-\ell/2} \times (r^j_\alpha \otimes \psi^\dagger_\alpha(s'))^\dagger U^\dagger_{\ell/2,s'} |\omega_L\rangle \Big] \tag{6.24}$$

where Tr denotes the field trace only, the trace over the auxiliary system is implicit. It now becomes more convenient to break the integral up into pieces for $s \leq s'$ and $s > s'$

$$\int_{-\ell/2}^{\ell/2} \int_{-\ell/2}^{\ell/2} ds\, ds' = \int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} ds + \int_{-\ell/2}^{\ell/2} ds \int_{-\ell/2}^{s} ds'$$

We consider both integrals separately and in turn.

Evaluation of (6.24) for $s \leq s'$

We evaluate

$$\int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} ds\, \mathrm{Tr}\left[\langle \omega_L | U_{\ell/2,s}(r^k_\alpha \otimes \psi^\dagger_\alpha(s)) U_{s,-\ell/2}(\omega_R \otimes \Omega) U^\dagger_{s',-\ell/2}(r^{j\dagger}_\alpha \otimes \psi_\alpha(s')) U^\dagger_{\ell/2,s'} |\omega_L\rangle \right] \tag{6.25}$$

by eliminating the field operators $\psi_\alpha, \psi^\dagger_\alpha$ using techniques and results from chapter 4, section 4.3. We have that the field operator ψ_α annihilates the field vacuum $|\Omega\rangle_\alpha$, namely

$\psi_\alpha(x)|\Omega\rangle_\alpha = \langle\Omega|_\alpha \psi^\dagger_\alpha(x) = 0$. This allows us to replace certain products of operators that are adjacent to the field vacuum with a commutator. Using the cyclic rule of trace we have that the integrand in (6.25) is equivalent to

$$\mathrm{Tr}\left[(\omega_R\otimes\Omega)\left[U^\dagger_{s',-\ell/2}(r^{j\dagger}_\alpha\otimes\psi_\alpha(s'))U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}\ ,\ (\mathbb{I}\otimes\psi^\dagger_\alpha(s))\right]\left(r^k_\alpha\otimes\mathbb{I}\right)U_{s,-\ell/2}\right].$$

where we have replaced the product

$$\begin{aligned}&(\omega_R\otimes\Omega)\left(U^\dagger_{s',-\ell/2}(r^{j\dagger}_\alpha\otimes\psi_\alpha(s'))U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(\mathbb{I}\otimes\psi^\dagger_\alpha(s))\right)\\ &\to(\omega_R\otimes\Omega)\left[U^\dagger_{s',-\ell/2}(r^{j\dagger}_\alpha\otimes\psi_\alpha(s'))U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}\ ,\ (\mathbb{I}\otimes\psi^\dagger_\alpha(s))\right].\end{aligned}$$

The commutator can be expanded as follows

$$\begin{aligned}&\left[U^\dagger_{s',-\ell/2}(r^{j\dagger}_\alpha\otimes\psi_\alpha(s'))U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}\ ,\ (\mathbb{I}\otimes\psi^\dagger_\alpha(s))\right]\\ &=\left[\mathbb{I}\otimes\psi_\alpha(s)\ ,\ U^\dagger_{\ell/2,s}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s'}(r^j_\alpha\otimes\psi^\dagger_\alpha(s'))U_{s',-\ell/2}\right]^\dagger\\ &=\Big(U^\dagger_{\ell/2,s}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s'}\left[\psi_\alpha(s)\ ,\ \psi^\dagger_\alpha(s')\right](r^j_\alpha\otimes\mathbb{I})U_{s',-\ell/2}\\ &\quad+\ U^\dagger_{\ell/2,s}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s'}(r^j_\alpha\otimes\psi^\dagger_\alpha(s'))\left[\mathbb{I}\otimes\psi_\alpha(s)\ ,\ U_{s',-\ell/2}\right]\Big)^\dagger\end{aligned}\tag{6.26}$$

and simplified using the commutation relations (4.16), namely $\left[\psi_\alpha(s), U_{\ell/2,-\ell/2}\right] = U_{\ell/2,s}R_\alpha U_{s,-\ell/2}$, and $\left[\psi_\alpha(s),\psi^\dagger_\alpha(s')\right]=\delta(s-s')$. We have that (6.26) can be written

$$\begin{aligned}&\left[U^\dagger_{s',-\ell/2}(r^{j\dagger}_\alpha\otimes\psi_\alpha(s'))U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}\ ,\ (\mathbb{I}\otimes\psi^\dagger_\alpha(s))\right]\\ &=U^\dagger_{s',-\ell/2}(r^j_\alpha\otimes\delta(s-s'))^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}\\ &+U^\dagger_{s,-\ell/2}R^\dagger_\alpha U^\dagger_{s',s}(r^{j\dagger}_\alpha\otimes\psi_\alpha(s'))U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}.\end{aligned}$$

Substitution into (6.25) gives

$$\begin{aligned}&\int_{-\ell/2}^{\ell/2}ds'\int_{-\ell/2}^{s'}ds\ \mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s}(r^k_\alpha\otimes\psi^\dagger_\alpha(s))U_{s,-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}(r^{j\dagger}_\alpha\otimes\psi_\alpha(s'))U^\dagger_{\ell/2,s'}|\omega_L\rangle\right]\\ &=\int_{-\ell/2}^{\ell/2}ds'\int_{-\ell/2}^{s'}ds\ \Big(\mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s}\left(r^k_\alpha\otimes\mathbb{I}\right)U_{s,-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}(r^j_\alpha\otimes\delta(s-s'))^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\right]\\ &+\mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s}\left(r^k_\alpha\otimes\mathbb{I}\right)U_{s,-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{s,-\ell/2}R^\dagger_\alpha U^\dagger_{s',s}(r^{j\dagger}_\alpha\otimes\psi_\alpha(s'))U^\dagger_{\ell/2,s'}|\omega_L\rangle\right]\Big)\\ &=(*)+(**)\end{aligned}\tag{6.27}$$

In an endeavour to keep the calculation simple to follow, we continue the evaluation of terms $(*)$ and $(**)$ separately.

The term $(**)$

The remaining field operator in term $(**)$ can be eliminated by applying the same procedure, this time making the replacement

$$\begin{aligned}&(\mathbb{I}\otimes\psi_\alpha(s'))U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}\left(r^k_\alpha\otimes\mathbb{I}\right)U_{s,-\ell/2}(\omega_R\otimes\Omega)\\&\rightarrow\left[(\mathbb{I}\otimes\psi_\alpha(s'))\,,\,U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}\left(r^k_\alpha\otimes\mathbb{I}\right)U_{s,-\ell/2}\right](\omega_R\otimes\Omega).\end{aligned}$$

The commutator can be expanded and simplified using (4.16) to give

$$\begin{aligned}&\left[(\mathbb{I}\otimes\psi_\alpha(s'))\,,\,U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}\left(r^k_\alpha\otimes\mathbb{I}\right)U_{s,-\ell/2}\right]\\&=U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s'}R_\alpha U_{s',s}\left(r^k_\alpha\otimes\mathbb{I}\right)U_{s,-\ell/2}\end{aligned}$$

The integrand in term $(**)$ in (6.27) can therefore be written

$$\mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s'}R_\alpha U_{s',s}\left(r^k_\alpha\otimes\mathbb{I}\right)U_{s,-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{s,-\ell/2}R^\dagger_\alpha U^\dagger_{s',s}(r^{j\dagger}_\alpha\otimes\mathbb{I})U^\dagger_{\ell/2,s'}|\omega_L\rangle\right]. \quad (6.28)$$

This expression can be further simplified using results from chapter 4 concerning the auxiliary system associated with the cMPS representation in which the variational matrices Q, R_α and R_β act. Recall from (4.23) in section (4.4) that $\rho(s)$ is the state of the auxiliary system after $U_{s,-\ell/2}$ has been applied to the initial composite state $|\omega_R\rangle\langle\omega_R|\otimes\Omega$, namely

$$\rho(s)=\mathrm{Tr}_{-\ell/2,s}\left[U_{s,-\ell/2}\left(|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|_{[-\ell/2,s]}\right)U^\dagger_{s,-\ell/2}\right]$$

satisfying the differential equation in Jamiolkowski form (4.30)

$$\frac{d}{ds}|\rho(s)\rangle=\left[Q\otimes\mathbb{I}+\mathbb{I}\otimes\overline{Q}+R_\alpha\otimes\overline{R}_\alpha+R_\beta\otimes\overline{R}_\beta\right]|\rho(s)\rangle=:M|\rho(s)\rangle \quad (6.29)$$

with solution $|\rho(s)\rangle=e^{(s+\ell/2)M}|\omega_R\rangle|\omega_R\rangle$. The choice of representation of this equation in Jamiolkowski form (see (4.28)), where matrices such as $\rho(s)$ are flattened in vector form $|\rho(s)\rangle$, is convenient for our purposes and shall become clear shortly. In the thermodynamic limit $\ell\rightarrow\infty$, see section 4.6 of Chapter 4, the solution can be written $|\rho(s)\rangle=|\rho\rangle$ where $|\rho\rangle$ is the right eigenvector corresponding to the zero eigenvalue of M. See (4.52) through (4.54). Separating the complete field trace into two regions $\mathrm{Tr}_{-\ell/2,\ell/2}=\mathrm{Tr}_{-\ell/2,s}\mathrm{Tr}_{s,\ell/2}$ we can therefore rewrite (6.28)

$$\begin{aligned}&\mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s'}R_\alpha U_{s',s}\left(r^k_\alpha\otimes\mathbb{I}\right)U_{s,-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{s,-\ell/2}R^\dagger_\alpha U^\dagger_{s',s}(r^{j\dagger}_\alpha\otimes\mathbb{I})U^\dagger_{\ell/2,s'}|\omega_L\rangle\right]\\&=\mathrm{Tr}_{s,\ell/2}\left[\langle\omega_L|U_{\ell/2,s'}R_\alpha U_{s',s}\left(r^k_\alpha\rho R^\dagger_\alpha\otimes\Omega_{s,\ell/2}\right)U^\dagger_{s',s}r^{j\dagger}_\alpha U^\dagger_{\ell/2,s'}|\omega_L\rangle\right] \quad (6.30)\end{aligned}$$

where $\Omega_{s,\ell/2}$ denotes the field vacuum on $(s,\ell/2]$ only. Separating the trace once more into regions $[s,s']$ and $[s',\ell/2]$ we repeat the procedure above. We define $\tau(s')$ to be the state of the auxiliary system after $U_{s',s}$ has been applied to the state $\left(r_\alpha^k \rho R_\alpha^\dagger \otimes \Omega_{s,\ell/2}\right)$, namely

$$\tau(s') = \mathrm{Tr}_{s,s'}\left[U_{s',s}\left(r_\alpha^k \rho R_\alpha^\dagger \otimes \Omega_{s,\ell/2}\right) U_{s',s}^\dagger\right].$$

Using similar techniques to those presented in appendix B.2 it can be shown that $\tau(s')$ satisfies the differential equation in Jamiolkowski form

$$\frac{d}{dx}|\tau(s')\rangle = \left[Q\otimes\mathbb{I} + \mathbb{I}\otimes\overline{Q} + R_\alpha \otimes \overline{R}_\alpha + R_\beta \otimes \overline{R}_\beta\right]|\tau(s')\rangle =: M|\tau(s')\rangle \tag{6.31}$$

with solution $|\tau(s')\rangle = e^{(s'-s)M}|r_\alpha^k \rho R_\alpha^\dagger\rangle$. Substitution into (6.30) gives

$$\begin{aligned}&\mathrm{Tr}_{s,\ell/2}\left[\langle\omega_L|U_{\ell/2,s'} R_\alpha U_{s',s}\left(r_\alpha^k \rho(s) R_\alpha^\dagger \otimes \Omega_{s,\ell/2}\right) U_{s',s}^\dagger r_\alpha^{j\dagger} U_{\ell/2,s'}^\dagger|\omega_L\rangle\right]\\ &= \mathrm{Tr}_{s,\ell/2}\left[\langle\omega_L|U_{\ell/2,s'}\left(R_\alpha \tau(s) r_\alpha^{j\dagger} \otimes \Omega_{s,\ell/2}\right) U_{\ell/2,s'}^\dagger|\omega_L\rangle\right].\end{aligned} \tag{6.32}$$

To simplify this expression further it is beneficial to rearrange the argument of the field trace to explicitly include the trace over the auxiliary system, denoted by tr, and implicitly include the field trace. This results in an object consisting of cMPS auxiliary system operators only. We apply the formula $\mathrm{Tr}_{II}\left[\langle A|_{I,II}(B_I\otimes|C\rangle\langle C|_{II})|A\rangle_{I,II}\right] = \mathrm{tr}_I\left[\langle C|_I|A\rangle\langle A|_{I,II}|C\rangle_{II} B_I\right]$, where in this case I and II denote the auxiliary and field systems respectively, $|A\rangle_{I,II} = U_{\ell/2,s'}^\dagger|\omega_L\rangle$, $B_I = R_\alpha \tau(s) r_\alpha^{j\dagger}$ and $C_{II} = |\Omega\rangle$. We therefore have that (6.32) can be written

$$\begin{aligned}&\mathrm{Tr}_{s,\ell/2}\left[\langle\omega_L|U_{\ell/2,s'}\left(R_\alpha\tau(s) r_\alpha^{j\dagger}\otimes\Omega_{s,\ell/2}\right) U_{\ell/2,s'}^\dagger|\omega_L\rangle\right]\\ &= \mathrm{tr}\left[\langle\Omega|_{s',\ell/2} U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s'}|\Omega\rangle_{s',\ell/2} R_\alpha \tau(s) r_\alpha^{j\dagger}\right]\\ &= \mathrm{tr}\left[\sigma(s') R_\alpha \tau(s) r_\alpha^{j\dagger}\right]\end{aligned} \tag{6.33}$$

where in the last line we have used the definition of $\sigma(s')$ given in (4.26), namely

$$\sigma(s') = \langle\Omega|_{s',\ell/2} U_{\ell/2,s'}^\dagger (|\omega_L\rangle\langle\omega_L|\otimes\mathbb{I}) U_{\ell/2,s'}|\Omega\rangle_{s',\ell/2}, \tag{6.34}$$

satisfying the differential equation

$$\frac{d}{ds'}|\sigma(s')\rangle = \left[\mathbb{I}\otimes Q^T + Q^\dagger\otimes\mathbb{I} + R_\alpha^\dagger\otimes R_\alpha^T + R_\beta^\dagger\otimes R_\beta^T\right]|\sigma(s')\rangle = M^\dagger|\sigma(s')\rangle$$

with solution $\langle\sigma(s')| = \langle\omega_L|\langle\omega_L|e^{(\ell/2-s')M}$. As in the case of $|\rho(s)\rangle$, in the limit $\ell\to\infty$ this solution can be written $\langle\sigma(s')| = \langle\sigma|$ where $\langle\sigma|$ is the left eigenvector corresponding to the zero eigenvalue of M, see (4.55). Furthermore, by imposing the gauge fixing conditions

described in section 4.5 we can set $\langle\sigma(s')| = \langle\mathbb{I}|$, where $\langle\mathbb{I}|$ is the flattened identity matrix, see (4.56). We thus have that

$$\mathrm{tr}\left[\sigma(s')R_\alpha\tau(s)r_\alpha^{j\dagger}\right] = \mathrm{tr}\left[R_\alpha\tau(s)r_\alpha^{j\dagger}\right].$$

We now substitute this much simpler expression into the main equation (6.27). We have that term $(**)$ of (6.27) can be written

$$(**) = \int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} ds\, \mathrm{tr}\left(R_\alpha\tau(s)r_\alpha^{j\dagger}\right) = \int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} ds\, \langle R_\alpha^\dagger r_\alpha^j|\tau(s)\rangle$$

where we have again used the Jamiolkowski representation to flatten matrices into vector form and write $\mathrm{Tr}[AB] = \langle A^\dagger|B\rangle$. We now substitute for $|\tau(s)\rangle$ as given in (6.31), resulting in

$$\langle R_\alpha^\dagger r_\alpha^j| \left(\int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} e^{(s'-s)M} ds \right) |r_\alpha^k \rho R_\alpha^\dagger\rangle \tag{6.35}$$

We now evaluate this integral. The matrix M satisfies some important properties, as discussed at the end of section 4.4.1. It is know that the matrix is diagonalisable, such that we can decompose the integrand as follows

$$e^{(s'-s)M} = e^{(s'-s)m_0}|u_0\rangle\langle v_0| + \sum_{\alpha=1}^{D^2-1} e^{(s'-s)m_\alpha}|u_\alpha\rangle\langle v_\alpha|$$

where m_α and $|u_\alpha\rangle, |v_\alpha\rangle$ are the eigenvalues and left and right eigenvectors respectively. The eigenvalues are assumed to be arranged in decreasing real part, and we have separated the zero eigenvalue $m_0 = 0$ contribution since we have already specified the eigenvectors corresponding to m_0, namely $|\rho\rangle$ and $\langle\sigma| = \langle\mathbb{I}|$. We therefore calculate

$$\int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} e^{(s'-s)M} ds = \int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} \left(|\rho\rangle\langle\mathbb{I}| + \sum_{\alpha=1}^{D^2-1} e^{(s'-s)m_\alpha}|u_\alpha\rangle\langle v_\alpha| \right) ds.$$

We first evaluate the integral with respect to s:

$$\int_{-\ell/2}^{s'} \left(|\rho\rangle\langle\mathbb{I}| + \sum_{\alpha=1}^{D^2-1} e^{(s'-s)m_\alpha}|u_\alpha\rangle\langle v_\alpha| \right) ds = \left[s|\rho\rangle\langle\mathbb{I}| - \sum_{\alpha=1}^{D^2-1} \frac{e^{(s'-s)m_\alpha}}{m_\alpha}|u_\alpha\rangle\langle v_\alpha| \right]_{-\ell/2}^{s'}$$

$$= s'|\rho\rangle\langle\mathbb{I}| + \frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| + \sum_{\alpha=1}^{D^2-1} \left(-\frac{\mathbb{I}}{m_\alpha} + \frac{e^{(s'+\frac{\ell}{2})m_\alpha}}{m_\alpha} \right) |u_\alpha\rangle\langle v_\alpha|$$

followed by the integral with respect to s'

$$\int_{-\ell/2}^{\ell/2} \left(s'|\rho\rangle\langle\mathbb{I}| + \frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| + \sum_{\alpha=1}^{D^2-1} -\frac{\mathbb{I}}{m_\alpha} + \frac{e^{(s'+\frac{\ell}{2})m_\alpha}}{m_\alpha}|u_\alpha\rangle\langle v_\alpha| \right) ds'$$

$$= \left[\frac{s'^2}{2}|\rho\rangle\langle\mathbb{I}| + \frac{s'\ell}{2}|\rho\rangle\langle\mathbb{I}| + \sum_{\alpha=1}^{D^2-1} -\frac{s'}{m_\alpha} + \frac{e^{(s'+\frac{\ell}{2})m_\alpha}}{m_\alpha^2}|u_\alpha\rangle\langle v_\alpha| \right]_{-\ell/2}^{\ell/2}$$

We therefore find that

$$\int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} e^{(s'-s)M} ds = \ell \left(\frac{\ell}{2} |\rho\rangle\langle\mathbb{I}| + \sum_{\alpha=1}^{D^2-1} \left[-\frac{\mathbb{I}}{m_\alpha} + \frac{e^{\ell m_\alpha} - \mathbb{I}}{\ell m_\alpha^2} \right] |u_\alpha\rangle\langle v_\alpha| \right).$$

In the infinite size limit $\ell \to \infty$ the second term in the summation evaluates to zero. We can also replace $\sum_{\alpha>0} \left(\frac{\mathbb{I}}{m_\alpha}\right) |u_\alpha\rangle\langle v_\alpha|$ by the pseudoinverse of M, denoted by $\mathbb{I}/M$, such that

$$\int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} e^{(s'-s)M} ds = \ell \left(\frac{\ell}{2} |\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M} \right)$$

Substituting this into main calculation (6.35) gives

$$(**) = \langle R_\alpha^\dagger r_\alpha^j | \int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} e^{(s'-s)M} ds | r_\alpha^k \rho R_\alpha^\dagger \rangle = \ell \langle R_\alpha^\dagger r_\alpha^j | \left(\frac{\ell}{2} |\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M} \right) | r_\alpha^k \rho R_\alpha^\dagger \rangle. \quad (6.37)$$

We now have fully evaluated the term $(**)$ in (6.27).

The term $(*)$

We now consider the second term $(*)$ of (6.27). We have

$$(*) = \int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} ds \, \mathrm{Tr} \left[\langle \omega_L | U_{\ell/2,s} (r_\alpha^k \otimes \mathbb{I}) U_{s,-\ell/2} (\omega_R \otimes \Omega) U_{s',-\ell/2}^\dagger (r_\alpha^{j\dagger} \otimes \delta(s-s')) U_{\ell/2,s'}^\dagger | \omega_L \rangle \right].$$

Since there are no field operators remaining in this expression, unlike term $(**)$ of (6.27), our first step is to integrate out the delta function. Following this we repeat the process of systematically performing the field trace in sections, resulting in the addition of auxiliary system operators ρ and σ as in (6.30) and (6.33). First taking the trace from $[-\ell/2, s]$ yields

$$\int_{-\ell/2}^{\ell/2} ds \mathrm{Tr}_{s,\ell/2} \left[\langle \omega_L | U_{\ell/2,s} r_\alpha^k \rho r_\alpha^{j\dagger} \otimes |\Omega\rangle\langle\Omega|_{s,\ell/2} U_{\ell/2,s}^\dagger | \omega_L \rangle \right].$$

This equation is of the same form as (6.32), and the calculation proceeds as before, with the exception that no integration of an exponential term appears. We find that

$$\begin{aligned} \int_{-\ell/2}^{\ell/2} ds \mathrm{Tr}_{s,\ell/2} \left[\langle \omega_L | U_{\ell/2,s} r_\alpha^k \rho r_\alpha^{j\dagger} \otimes |\Omega\rangle\langle\Omega|_{s,\ell/2} U_{\ell/2,s}^\dagger | \omega_L \rangle \right] &= \int_{-\ell/2}^{\ell/2} ds' \langle \mathbb{I} | r_\alpha^k \rho r_\alpha^{j\dagger} \rangle \\ &= \ell \langle \mathbb{I} | r_\alpha^k \rho r_\alpha^{j\dagger} \rangle \end{aligned} \quad (6.38)$$

Combining equations (6.37) and (6.38) we can specify (6.27), and in turn complete the evaluation of (6.25). We find that for $s \leq s'$ we have a contribution toward the total matrix entry of G_{jk} given by

$$\ell \left[\langle R_\alpha^\dagger r_\alpha^j | \left(\frac{\ell}{2} |\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M} \right) | r_\alpha^k \rho R_\alpha^\dagger \rangle + \langle \mathbb{I} | r_\alpha^k \rho r_\alpha^{j\dagger} \rangle \right]$$

Using (4.29) from chapter 4 it is practical to single out the vectors $|\rho\rangle$ and $\langle\mathbb{I}|$ and write this expression in an equivalent form

$$\begin{aligned}&\ell\left[\langle R_\alpha^\dagger r_\alpha^j|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)|r_\alpha^k\rho R_\alpha^\dagger\rangle+\langle\mathbb{I}|r_\alpha^k\rho\, r_\alpha^{j\dagger}\rangle\right]\\&=\ell\left[\langle\mathbb{I}|\left(R_\alpha\otimes\overline{r}_\alpha^j\right)\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)\left(r_\alpha^k\otimes\overline{R}_\alpha\right)|\rho\rangle+\langle\mathbb{I}|r_\alpha^k\otimes\overline{r}_\alpha^j|\rho\rangle\right],\end{aligned}\tag{6.39}$$

such that when combining the above result with the case $s<s'$ simplifications can clearly be made.

Evaluation of (6.24) for $\mathbf{s>s'}$

We now consider $s>s'$ and evaluate

$$\int_{-\ell/2}^{\ell/2}ds\int_{-\ell/2}^{s}ds'\mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s}(r_\alpha^k\otimes\psi_\alpha^\dagger(s))U_{s,-\ell/2}(\omega_R\otimes\Omega)\,U_{s',-\ell/2}^\dagger(r_\alpha^{j\dagger}\otimes\psi_\alpha(s'))U_{\ell/2,s'}^\dagger|\omega_L\rangle\right]\tag{6.40}$$

The procedure is analogous to the case $s<s'$. We adopt the same notational conventions and as before begin by eliminating the field operators. We replace the product

$$\begin{aligned}&(\mathbb{I}\otimes\psi_\alpha(s'))U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(r_\alpha^k\otimes\psi_\alpha^\dagger(s))U_{s,-\ell/2}(\omega_R\otimes\Omega)\\&\to\left[(\mathbb{I}\otimes\psi_\alpha(s'))\,,\;U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(r_\alpha^k\otimes\psi_\alpha^\dagger(s))U_{s,-\ell/2}\right](\omega_R\otimes\Omega)\end{aligned}$$

which can be expanded and simplified using (4.16). We find that

$$\begin{aligned}&\left[(\mathbb{I}\otimes\psi_\alpha(s'))\,,\;U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(r_\alpha^k\otimes\psi_\alpha^\dagger(s))U_{s,-\ell/2}\right]\\&=U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(r_\alpha^k\otimes\psi_\alpha^\dagger(s))\left[(\mathbb{I}\otimes\psi_\alpha(s'))\,,\;U_{s,-\ell/2}\right]\\&=U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(r_\alpha^k\otimes\psi_\alpha^\dagger(s))U_{s,s'}R_\alpha U_{s',-\ell/2}.\end{aligned}$$

Substitution into (6.40) allows us to write the integrand as

$$\begin{aligned}&\mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s}(r_\alpha^k\otimes\psi_\alpha^\dagger(s))U_{s,-\ell/2}(\omega_R\otimes\Omega)\,U_{s',-\ell/2}^\dagger(r_\alpha^{j\dagger}\otimes\psi(s'))U_{\ell/2,s'}^\dagger|\omega_L\rangle\right]\\&=\mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s}(r_\alpha^k\otimes\psi_\alpha^\dagger(s))U_{s,s'}R_\alpha U_{s',-\ell/2}(\omega_R\otimes\Omega)\,U_{s',-\ell/2}^\dagger(r_\alpha^{j\dagger}\otimes\mathbb{I})U_{\ell/2,s'}^\dagger|\omega_L\rangle\right].\end{aligned}\tag{6.41}$$

The remaining field operator $\psi_\alpha^\dagger(s)$ can be eliminated by applying the same procedure, this time making the replacement

$$\begin{aligned}&(\omega_R\otimes\Omega)\,U_{s',-\ell/2}^\dagger(r_\alpha^{j\dagger}\otimes\mathbb{I})U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(r_\alpha^k\otimes\psi_\alpha^\dagger(s))\\&\to(\omega_R\otimes\Omega)\left[U_{s',-\ell/2}^\dagger(r_\alpha^{j\dagger}\otimes\mathbb{I})U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(r_\alpha^k\otimes\mathbb{I})\,,\;\mathbb{I}\otimes\psi_\alpha^\dagger(s))\right]\end{aligned}$$

where the commutator evaluates to

$$(\omega_R \otimes \Omega)\left[U^\dagger_{s',-\ell/2}(r^{j\dagger}_\alpha \otimes \mathbb{I})U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(r^k_\alpha \otimes \mathbb{I})\,,\ \mathbb{I}\otimes\psi^\dagger(s))\right]$$
$$= U^\dagger_{s',-\ell/2}(r^{j\dagger}_\alpha \otimes \mathbb{I})U^\dagger_{s,s'}R^\dagger_\alpha U^\dagger_{\ell/2,s}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(r^k_\alpha \otimes \mathbb{I}).$$

Substitution into (6.41) gives

$$\mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s}(r^k_\alpha\otimes\psi^\dagger(s))U_{s,s'}R_\alpha U_{s',-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}(r^{j\dagger}_\alpha\otimes\mathbb{I})U^\dagger_{\ell/2,s'}|\omega_L\rangle\right]$$
$$= \mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s}(r^k_\alpha\otimes\mathbb{I})U_{s,s'}R_\alpha U_{s',-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}(r^{j\dagger}_\alpha\otimes\mathbb{I})U^\dagger_{s,s'}R^\dagger_\alpha U^\dagger_{\ell/2,s}|\omega_L\rangle\right] \quad (6.42)$$

The procedure for evaluating (6.40) using (6.42) is identical to before, we thus omit presentation of the calculations. We find that for $s > s'$ we have a contribution toward the total matrix entry of G_{jk} given by

$$\ell\left[\langle r^{k\dagger}_\alpha R_\alpha|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|R_\alpha\rho\, r^{j\dagger}_\alpha\rangle\right] = \ell\left[\langle\mathbb{I}|\left(r^k_\alpha\otimes\overline{R}_\alpha\right)\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)\left(R_\alpha\otimes\overline{r}^j_\alpha\right)|\rho\rangle\right]. \quad (6.43)$$

Having covered both parts of the integral $\int\int ds\,ds' = \int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} ds + \int_{-\ell/2}^{\ell/2} ds \int_{-\ell/2}^{s} ds'$ we can now write a complete evaluation of equation (6.24). Using (6.39) and (6.43) we have that, for $D^2+1 \le j,k \le 2D^2$,

$$G_{jk} = \langle\partial_{\bar{j}}\Psi|\partial_k\Psi\rangle = \ell\Big[\langle\mathbb{I}|\left(r^k_\alpha\otimes\overline{R}_\alpha\right)\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)\left(R_\alpha\otimes\overline{r}^j_\alpha\right)|\rho\rangle \quad (6.44)$$
$$+\langle\mathbb{I}|\left(R_\alpha\otimes\overline{r}^j_\alpha\right)\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)\left(r^k_\alpha\otimes\overline{R}_\alpha\right)|\rho\rangle + \langle\mathbb{I}|r^k_\alpha\otimes\overline{r}^j_\alpha|\rho\rangle\Big]$$
$$= \ell\Big[\ell\langle\mathbb{I}|\left(r^k_\alpha\otimes\overline{R}_\alpha\right)|\rho\rangle\langle\mathbb{I}|\left(R_\alpha\otimes\overline{r}^j_\alpha\right)|\rho\rangle - \langle\mathbb{I}|\left(r^k_\alpha\otimes\overline{R}_\alpha\right)\frac{\mathbb{I}}{M}\left(R_\alpha\otimes\overline{r}^j_\alpha\right)|\rho\rangle$$
$$-\langle\mathbb{I}|\left(R_\alpha\otimes\overline{r}^j_\alpha\right)\frac{\mathbb{I}}{M}\left(r^k_\alpha\otimes\overline{R}_\alpha\right)|\rho\rangle + \langle\mathbb{I}|r^k_\alpha\otimes\overline{r}^j_\alpha|\rho\rangle\Big]. \quad (6.45)$$

There are two important points to note having completed this evaluation. Firstly, we note that the overall factor ℓ will not lead to a divergence in the thermodynamic limit $\ell\to\infty$ when considering the main TDVP equation (6.16), see below. Secondly, we observe that the first term in the brackets is in fact diverging in the limit $\ell\to\infty$. However if necessary this divergence can be removed by imposing gauge fixing conditions on the tangent vectors $|\partial_j\Psi\rangle$, as described in [Haegeman, 2011, Haegeman et al., 2011a]. We discuss this further below when G has been specified in full.

6.2.4 G in full

As mentioned previously, the calculations for specifying the remaining block entries of the complete Gram matrix (6.17) follow a similar pattern to the above, and we omit presentation

of the derivations due to their repetitiveness. We now specify a general entry of the Gram matrix

$$\begin{aligned} G_{jk} = \ell \Big[& \ell \langle \mathbb{I}| \left(\mathbb{I} \otimes \overline{q}^j + R_\alpha \otimes \overline{r}^j_\alpha + R_\beta \otimes \overline{r}^j_\beta \right) |\rho\rangle \langle \mathbb{I}| \left(q_k \otimes \mathbb{I} + r^k_\alpha \otimes \overline{R}_\alpha + r^k_\beta \otimes \overline{R}_\beta \right) |\rho\rangle \\ & - \langle \mathbb{I}| \left(q_k \otimes \mathbb{I} + r^k_\alpha \otimes \overline{R}_\alpha + r^k_\beta \otimes \overline{R}_\beta \right) \frac{\mathbb{I}}{M} \left(\mathbb{I} \otimes \overline{q}^j + R_\alpha \otimes \overline{r}^j_\alpha + R_\beta \otimes \overline{r}^j_\beta \right) |\rho\rangle \\ & - \langle \mathbb{I}| \left(\mathbb{I} \otimes \overline{q}^j + R_\alpha \otimes \overline{r}^j_\alpha + R_\beta \otimes \overline{r}^j_\beta \right) \frac{\mathbb{I}}{M} \left(q_k \otimes \mathbb{I} + r^k_\alpha \otimes \overline{R}_\alpha + r^k_\beta \otimes \overline{R}_\beta \right) |\rho\rangle \\ & + \langle \mathbb{I}| r^k_\alpha \otimes \overline{r}^j_\alpha |\rho\rangle + \langle \mathbb{I}| r^k_\beta \otimes \overline{r}^j_\beta |\rho\rangle \Big]. \end{aligned} \tag{6.46}$$

As mentioned above, the overall factor ℓ will not lead to a divergence in the limit $\ell \to \infty$. Since both G and L contain the same prefactor, when substituting into the main TDVP equation (6.16) we find they cancel out since we invert G. The first term inside the brackets on the right hand side is divergent when taking the thermodynamic limit. However, this divergence can be removed if we impose gauge fixing conditions as developed in [Haegeman, 2011, Haegeman et al., 2011a]. In Chapter 4, section 4.5, we discussed how within the cMPS formalism, classes of parameterisations, related by so-called gauge transformations, describe the same physical states. We showed that by imposing constraints on the possible parameterisations, each state $|\Psi(Q, \{R_\alpha\})\rangle$ can be linked to a unique representation via Q and R. These gauge transformations induce a gauge equivalence in the tangent plane also. It was shown in [Haegeman, 2011, Haegeman et al., 2011a] that this gauge can be fixed by imposing

$$\langle \mathbb{I}| \left(q_k \otimes \mathbb{I} + r^k_\alpha \otimes \overline{R}_\alpha + r^k_\beta \otimes \overline{R}_\beta \right) = 0. \tag{6.47}$$

In addition, it can be shown that this condition also imposes orthogonality of tangent vectors with respect to the cMPS providing norm preservation [Haegeman, 2011, Haegeman et al., 2011a]. Parameterisations that respect (6.47) can easily be found, for example the above fixing is satisfied by the parameterisation $q^k = -R^\dagger_\alpha r^k_\alpha - R^\dagger_\beta r^k_\beta$ where r^k_α and r^k_β can be chosen freely. Imposing the gauge fixing requirement (6.47) eliminates the first two terms of (6.46), removing the diverging term.

It is instructive to also write G in matrix form. We have that

$$G = \ell \begin{pmatrix} \ell\langle \mathbb{I}|\mathbb{I}\otimes\overline{q}^j|\rho\rangle\langle\mathbb{I}|q_k\otimes\mathbb{I}|\rho\rangle & \ell\langle\mathbb{I}|\mathbb{I}\otimes\overline{q}^j|\rho\rangle\langle\mathbb{I}|r^k_\alpha\otimes\overline{R}_\alpha|\rho\rangle & \ell\langle\mathbb{I}|\mathbb{I}\otimes\overline{q}^j|\rho\rangle\langle\mathbb{I}|r^k_\beta\otimes\overline{R}_\beta|\rho\rangle \\ -\langle\mathbb{I}|\mathbb{I}\otimes\overline{q}^j\tfrac{\mathbb{I}}{M}q_k\otimes\mathbb{I}|\rho\rangle & -\langle\mathbb{I}|\mathbb{I}\otimes\overline{q}^j\tfrac{\mathbb{I}}{M}r^k_\alpha\otimes\overline{R}_\alpha|\rho\rangle & -\langle\mathbb{I}|\mathbb{I}\otimes\overline{q}^j\tfrac{\mathbb{I}}{M}r^k_\beta\otimes\overline{R}_\beta|\rho\rangle \\ -\langle\mathbb{I}|q_k\otimes\mathbb{I}\tfrac{\mathbb{I}}{M}\mathbb{I}\otimes\overline{q}^j|\rho\rangle & -\langle\mathbb{I}|r^k_\alpha\otimes\overline{R}_\alpha\tfrac{I}{M}\mathbb{I}\otimes\overline{q}^j|\rho\rangle & -\langle\mathbb{I}|r^k_\beta\otimes\overline{R}_\beta\tfrac{I}{M}\mathbb{I}\otimes\overline{q}^j|\rho\rangle \\ \ell\langle\mathbb{I}|R_\alpha\otimes\overline{r}^j_\alpha|\rho\rangle\langle\mathbb{I}|q_k\otimes\mathbb{I}|\rho\rangle & \ell\langle\mathbb{I}|R_\alpha\otimes\overline{r}^j_\alpha|\rho\rangle\langle\mathbb{I}|r^k_\alpha\otimes\overline{R}_\alpha|\rho\rangle & \ell\langle\mathbb{I}|R_\alpha\otimes\overline{r}^j_\alpha|\rho\rangle\langle\mathbb{I}|r^k_\beta\otimes\overline{R}_\beta|\rho\rangle \\ -\langle\mathbb{I}|R_\alpha\otimes\overline{r}^j_\alpha\tfrac{\mathbb{I}}{M}q_k\otimes\mathbb{I}|\rho\rangle & -\langle\mathbb{I}|R_\alpha\otimes\overline{r}^j_\alpha\tfrac{\mathbb{I}}{M}r^k_\alpha\otimes\overline{R}_\alpha|\rho\rangle & -\langle\mathbb{I}|R_\alpha\otimes\overline{r}^j_\alpha\tfrac{\mathbb{I}}{M}r^k_\beta\otimes\overline{R}_\beta|\rho\rangle \\ -\langle\mathbb{I}|q_k\otimes\mathbb{I}\tfrac{\mathbb{I}}{M}R_\alpha\otimes\overline{r}^j_\alpha|\rho\rangle & -\langle\mathbb{I}|r^k_\alpha\otimes\overline{R}_\alpha\tfrac{\mathbb{I}}{M}R_\alpha\otimes\overline{r}^j_\alpha|\rho\rangle & -\langle\mathbb{I}|r^k_\beta\otimes\overline{R}_\beta\tfrac{\mathbb{I}}{M}R_\alpha\otimes\overline{r}^j_\alpha|\rho\rangle \\ & +\langle\mathbb{I}|r^k_\alpha\otimes\overline{r}^j_\alpha|\rho\rangle & \\ \ell\langle\mathbb{I}|R_\beta\otimes\overline{r}^j_\beta|\rho\rangle\langle\mathbb{I}|q_k\otimes\mathbb{I}|\rho\rangle & \ell\langle\mathbb{I}|R_\beta\otimes\overline{r}^j_\beta|\rho\rangle\langle\mathbb{I}|r^k_\alpha\otimes\overline{R}_\alpha|\rho\rangle & \ell\langle\mathbb{I}|R_\beta\otimes\overline{r}^j_\beta|\rho\rangle\langle\mathbb{I}|r^k_\beta\otimes\overline{R}_\beta|\rho\rangle \\ -\langle\mathbb{I}|R_\beta\otimes\overline{r}^j_\beta\tfrac{\mathbb{I}}{M}q_k\otimes\mathbb{I}|\rho\rangle & -\langle\mathbb{I}|R_\beta\otimes\overline{r}^j_\beta\tfrac{\mathbb{I}}{M}r^k_\alpha\otimes\overline{R}_\alpha|\rho\rangle & -\langle\mathbb{I}|R_\beta\otimes\overline{r}^j_\beta\tfrac{\mathbb{I}}{M}r^k_\beta\otimes\overline{R}_\beta|\rho\rangle \\ -\langle\mathbb{I}|q_k\otimes\mathbb{I}\tfrac{\mathbb{I}}{M}R_\beta\otimes\overline{r}^j_\beta|\rho\rangle & -\langle\mathbb{I}|r^k_\alpha\otimes\overline{R}_\alpha\tfrac{\mathbb{I}}{M}R_\beta\otimes\overline{r}^j_\beta|\rho\rangle & -\langle\mathbb{I}|r^k_\beta\otimes\overline{R}_\beta\tfrac{\mathbb{I}}{M}R_\beta\otimes\overline{r}^j_\beta|\rho\rangle \\ & & +\langle\mathbb{I}|r^k_\beta\otimes\overline{r}^j_\beta|\rho\rangle \end{pmatrix} \tag{6.48}$$

6.2.5 Computing the projection matrix

We now turn our attention to calculating the $3D^2\times 1$ projection matrix (6.18), whose j-th row element is given by

$$L_j = \langle\partial_{\overline{j}}\Psi(\overline{z})|\hat{H}_{\text{int}}|\Psi(z)\rangle$$

where $\hat{H}_{\text{int}}$ is the non-random, interaction Hamiltonian given by (6.20), namely

$$\begin{aligned}\hat{H}_{\text{int}} &= \hat{T}+\hat{W}+\hat{V}\\ &= \int_{-\ell/2}^{\ell/2} dx\left[\left(\frac{d\psi^\dagger_\alpha(x)}{dx}\frac{d\psi_\alpha(x)}{dx}\otimes\mathbb{I}\right)+\left(c\psi^\dagger_\alpha(x)\psi^\dagger_\alpha(x)\psi_\alpha(x)\psi_\alpha(x)\otimes\mathbb{I}\right)\right.\\ &\quad\left.+\frac{1}{\sqrt{2}}\left(\psi^\dagger_\alpha(x)\psi_\alpha(x)\otimes\left(\hat{\psi}_\beta(x)+\psi^\dagger_\beta(x)\right)\right)\right].\end{aligned}$$

We separate the terms of the Hamiltonian $\hat{T}$, $\hat{W}$ and $\hat{V}$ and present their contribution to L separately. Furthermore, as with the Gram matrix, the entries of the projection matrix depend on the derivatives of the cMPS with respect to the variational parameters z^j, namely

$$|\partial_j\Psi\rangle = \begin{cases} \int ds\langle\omega_L|U_{\ell/2,s}(q^j\otimes\mathbb{I}\otimes\mathbb{I})U_{s,-\ell/2}|\omega_R\rangle|\Omega\rangle_{\alpha,\beta} & \text{if } 1\le j\le D^2;\\ \int ds\langle\omega_L|U_{\ell/2,s}(r^j_\alpha\otimes\psi^\dagger_\alpha(s)\otimes\mathbb{I})U_{s,-\ell/2}|\omega_R\rangle|\Omega\rangle_{\alpha,\beta} & \text{if } D^2+1\le j\le 2D^2;\\ \int ds\langle\omega_L|U_{\ell/2,s}(r^j_\beta\otimes\mathbb{I}\otimes\psi^\dagger_\beta(s))U_{s,-\ell/2}|\omega_R\rangle|\Omega\rangle_{\alpha,\beta} & \text{if } 2D^2+1\le j\le 3D^2.\end{cases}$$

The computation of a general entry is therefore dependent on where j is in $\left[1,3D^2\right]$, and there are three cases to consider. We derive the contribution of the density term $\hat{V}$ of $\hat{H}_{\text{int}}$ in the case $D^2+1 \leq j \leq 2D^2$. The calculations for other terms are similar and lengthy, we thus omit them from this chapter and state the final form of L. Derivations of other contributions for the kinetic and interaction terms can be found in Appendix C.

6.2.6 Projection of the density

The projection of the density term of the Hamiltonian $\hat{V}$ requires the evaluation of

$$\langle \partial_{\bar{j}} \Psi(\overline{z}) | \hat{V} | \Psi(z) \rangle = \int_{-\ell/2}^{\ell/2} ds \; \langle \partial_{\bar{j}} \Psi(\overline{z}) | \frac{J}{\sqrt{2}} \left(\psi_\alpha^\dagger(s) \psi_\alpha(s) \otimes \left(\hat{\psi}_\beta(s) + \psi_\beta^\dagger(s) \right) \right) | \Psi(z) \rangle$$

for the different cases $1 \leq j \leq D^2$, $D^2+1 \leq j \leq 2D^2$, and $2D^2+1 \leq j \leq 3D^2$. As noted, we will detail only one of these cases, a pattern for calculating the different cases is soon established. We choose $D^2+1 \leq j \leq 2D^2$, since this case has the additional complexity of a field operator appearing in the derivative of the tangent vector

$$|\partial_j \Psi\rangle = \int_{-\ell/2}^{\ell/2} ds \langle \omega_L | U_{\ell/2,s} (r_\alpha^j \otimes \psi_\alpha^\dagger(s) \otimes \mathbb{I}) U_{s,-\ell/2} | \omega_R \rangle | \Omega \rangle_{\alpha,\beta}, \qquad D^2+1 \leq j \leq 2D^2$$

(note that we could have chosen $2D^2+1 \leq j \leq 3D^2$ for the same reason).

Derivations for $\mathbf{D^2+1 \leq j \leq 2D^2}$

We adopt the same notational conventions as before, for convenience temporarily excluding the factor $J/\sqrt{2}$ in $\hat{V}$, and evaluate

$$\begin{aligned} &\langle \partial_{\bar{j}} \Psi(\overline{z}) | \hat{V} | \Psi(z) \rangle = \mathrm{Tr} \left[\hat{V} | \Psi(z) \rangle \langle \partial_{\bar{j}} \Psi(\overline{z}) | \right] \qquad (6.49) \\ &= \int_{-\ell/2}^{\ell/2} \int_{-\ell/2}^{\ell/2} ds\, ds' \mathrm{Tr} \Big[\langle \omega_L | \left(\mathbb{I} \otimes \psi_\alpha^\dagger(s) \psi_\alpha(s) \otimes \left(\hat{\psi}_\beta(s) + \psi_\beta^\dagger(s) \right) \right) U_{\ell/2,-\ell/2} \\ &\qquad \times (\omega_R \otimes \Omega) U_{s',-\ell/2}^\dagger \left(r_\alpha^{j\dagger} \otimes \psi_\alpha(s') \otimes \mathbb{I} \right) U_{\ell/2,s'}^\dagger | \omega_L \rangle \Big]. \end{aligned}$$

We first break the expression into two terms by splitting $\hat{V}$ and writing

$$\begin{aligned} &\left(\mathbb{I} \otimes \psi_\alpha^\dagger(s) \psi_\alpha(s) \otimes \left(\hat{\psi}_\beta(s) + \psi_\beta^\dagger(s) \right) \right) \\ &= \left(\mathbb{I} \otimes \psi_\alpha^\dagger(s) \otimes \mathbb{I} \right) \left(\mathbb{I} \otimes \psi_\alpha(s) \otimes \psi_\beta(s) \right) + \left(\mathbb{I} \otimes \psi_\alpha^\dagger(s) \otimes \psi_\beta^\dagger(s) \right) \left(\mathbb{I} \otimes \psi_\alpha(s) \otimes \mathbb{I} \right) \end{aligned}$$

so that the operator is normally ordered. We therefore evaluate

$$\begin{aligned}
&\langle \partial_{\bar{j}} \Psi(\overline{z})|\hat{V}|\Psi(z)\rangle \\
&= \int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2} ds\, ds' \mathrm{Tr}\Big[\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\psi_\beta(s)\right)U_{\ell/2,-\ell/2} \\
&\qquad\qquad \times(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\Big] \\
&+ \int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2} ds\, ds' \mathrm{Tr}\Big[\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\psi_\beta^\dagger(s)\right)\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}\right)U_{\ell/2,-\ell/2} \\
&\qquad\qquad \times(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\Big] \\
&= (*)+(**)
\end{aligned} \tag{6.50}$$

We consider the terms $(*)$ and $(**)$ separately in an attempt to keep calculations clear.

The term $(**)$

We evaluate

$$\begin{aligned}
\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2} ds\, ds' \mathrm{Tr}\Big[&\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}\right)U_{\ell/2,-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right) \\
&\times U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\psi_\beta^\dagger(s)\right)\Big]
\end{aligned} \tag{6.51}$$

where we have used the cyclic rule of trace to move the term $\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\psi_\beta^\dagger(s)\right)$ to the right hand side of the field vacuum Ω. We now begin the procedure of eliminating the field operators. As before, we use that $\psi_\alpha|\Omega\rangle_\alpha = 0$ to replace products of operators with commutators. To remove $\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}$ we make the replacement

$$\begin{aligned}
\left(\mathbb{I}\otimes\psi(s)\otimes\mathbb{I}\right)U_{\ell/2,-\ell/2}(\omega_R\otimes\Omega) &\rightarrow \Big[\left(\mathbb{I}\otimes\psi(s)\otimes\mathbb{I}\right)\,,\,U_{\ell/2,-\ell/2}\Big](\omega_R\otimes\Omega) \\
&= U_{\ell/2,s}\left(R_\alpha\otimes\mathbb{I}\otimes\mathbb{I}\right)U_{s,-\ell/2}
\end{aligned} \tag{6.52}$$

where in the last line we have employed Eq. (4.17) of section 4.3. For the product on the right hand side of the field vacuum, we write

$$\begin{aligned}
&(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\psi_\beta^\dagger(s)\right) \\
&\rightarrow(\omega_R\otimes\Omega)\Big[U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\,,\,\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\psi_\beta^\dagger(s)\right)\Big] \\
&=(\omega_R\otimes\Omega)\Big[U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\,,\,\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\Big]\left(\mathbb{I}\otimes\mathbb{I}\otimes\psi_\beta^\dagger(s)\right) \\
&+(\omega_R\otimes\Omega)\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\Big[U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\,,\,\left(\mathbb{I}\otimes\mathbb{I}\otimes\psi_\beta^\dagger(s)\right)\Big].
\end{aligned}$$

The second term equates to zero, since the $\psi^\dagger_\alpha(s)$ annihilates the field vacuum Ω. We therefore consider the first term only, and evaluate the commutator

$$\begin{aligned}
&\left[U^\dagger_{s',-\ell/2}\left(r^{j\dagger}_\alpha\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\,,\,\left(\mathbb{I}\otimes\psi^\dagger_\alpha(s)\otimes\mathbb{I}\right)\right]\\
=&\Theta(s-s')U^\dagger_{s',-\ell/2}\left(r^{j\dagger}_\alpha\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{s,s'}R^\dagger_\alpha U^\dagger_{\ell/2,s}|\omega_L\rangle\langle\omega_L| &(6.53)\\
+&\Theta(s'-s)U^\dagger_{s,-\ell/2}R_\alpha U^\dagger_{s',s}\left(r^{j\dagger}_\alpha\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L| &(6.54)\\
+&U^\dagger_{s',-\ell/2}\left(r^{j\dagger}_\alpha\otimes\mathbb{I}\otimes\mathbb{I}\right)\left(\mathbb{I}\otimes\delta(s'-s)\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L| &(6.55)
\end{aligned}$$

where $\Theta(s-s')$ is the heaviside step function, defined via

$$\Theta(s-s')=\begin{cases}1 & s<s'\\ 1/2 & s=s'\\ 0 & s>s'\end{cases}. \tag{6.56}$$

We have thus eliminated the field operator $\psi^\dagger_\alpha(s)$. We then substitute each term (6.53), (6.54) and (6.55) back into (6.51) and evaluate the resulting expression in turn.

Substitution of (6.53) into (6.51)

Substituting for (6.53), along with (6.52), in (6.51) gives

$$\begin{aligned}
\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2}ds\,ds'\Theta(s-s')\mathrm{Tr}\Big[&\langle\omega_L|\left(\mathbb{I}\otimes\mathbb{I}\otimes\psi^\dagger_\beta(s)\right)U_{\ell/2,s}\left(R_\alpha\otimes\mathbb{I}\otimes\mathbb{I}\right)U_{s,-\ell/2}(\omega_R\otimes\Omega)\\
&\times U^\dagger_{s',-\ell/2}\left(r^{j\dagger}_\alpha\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{s,s'}\left(R^\dagger_\alpha\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s}|\omega_L\rangle\Big].
\end{aligned} \tag{6.57}$$

$\psi^\dagger_\beta(x)$ can be eliminated by repeating the procedure above. We replace the product

$$\begin{aligned}
&U^\dagger_{s',-\ell/2}\left(r^{j\dagger}_\alpha\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{s,s'}\left(R^\dagger_\alpha\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s}|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\mathbb{I}\otimes\psi^\dagger_\beta(s)\right) &(6.58)\\
\rightarrow&\left[U^\dagger_{s',-\ell/2}\left(r^{j\dagger}_\alpha\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{s,s'}\left(R^\dagger_\alpha\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s}|\omega_L\rangle\langle\omega_L|\,,\,\left(\mathbb{I}\otimes\mathbb{I}\otimes\psi^\dagger_\beta(s)\right)\right] &(6.59)
\end{aligned}$$

and expand and evaluate the commutator. Keeping the overall factor of $\Theta(s-s')$ in mind, we find that we can make the substitution

$$\begin{aligned}
&U^\dagger_{s',-\ell/2}\left(r^{j\dagger}_\alpha\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{s,s'}\left(R^\dagger_\alpha\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s}\left(\mathbb{I}\otimes\mathbb{I}\otimes\psi^\dagger_\beta(s)\right) &(6.60)\\
\rightarrow&U^\dagger_{s',-\ell/2}\left(r^{j\dagger}_\alpha\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{s,s'}\left(\left\{R^\dagger_\alpha,R^\dagger_\beta\right\}\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s} &(6.61)
\end{aligned}$$

where $\left\{R_\alpha^\dagger, R_\beta^\dagger\right\}$ denotes the anticommutator $R_\alpha^\dagger R_\beta^\dagger + R_\beta^\dagger R_\alpha^\dagger$. We thus find that (6.57) can be written

$$\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2} ds\, ds' \Theta(s-s') \mathrm{Tr}\Big[\langle\omega_L| U_{\ell/2,s}(R_\alpha \otimes \mathbb{I}\otimes\mathbb{I}) U_{s,-\ell/2}(\omega_R\otimes\Omega) U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right) \times U^\dagger_{s,s'}\left(\left\{R_\alpha^\dagger, R_\beta^\dagger\right\}\otimes\mathbb{I}\otimes\mathbb{I}\right) U^\dagger_{\ell/2,s}|\omega_L\rangle\Big] \tag{6.62}$$

We have now eliminated the creation operator $\psi_\beta^\dagger$ and must repeat the process to remove $\psi_\alpha(s)$. We make the replacement

$$\begin{aligned}
&\left(\mathbb{I}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right) U^\dagger_{s,s'}\left(\left\{R_\alpha^\dagger, R_\beta^\dagger\right\}\otimes\mathbb{I}\otimes\mathbb{I}\right) U^\dagger_{\ell/2,s}|\omega_L\rangle\langle\omega_L| U_{\ell/2,s}(R_\alpha\otimes\mathbb{I}\otimes\mathbb{I}) U_{s,-\ell/2}\\
&\to \left[\left(\mathbb{I}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)\ ,\ U^\dagger_{s,s'}\left(\left\{R_\alpha^\dagger, R_\beta^\dagger\right\}\otimes\mathbb{I}\otimes\mathbb{I}\right) U^\dagger_{\ell/2,s}|\omega_L\rangle\langle\omega_L| U_{\ell/2,s}(R_\alpha\otimes\mathbb{I}\otimes\mathbb{I}) U_{s,-\ell/2}\right]\\
&= U^\dagger_{s,s'}\left(\left\{R_\alpha^\dagger, R_\beta^\dagger\right\}\otimes\mathbb{I}\otimes\mathbb{I}\right) U^\dagger_{\ell/2,s}|\omega_L\rangle\langle\omega_L| U_{\ell/2,s}(R_\alpha\otimes\mathbb{I}\otimes\mathbb{I}) U_{s,s'} R_\alpha U_{s',-\ell/2},
\end{aligned}$$

which removes all field operators from (6.62) such that (6.57) can be written

$$\begin{aligned}
&\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2} ds\, ds' \Theta(s-s') \mathrm{Tr}\Big[\langle\omega_L| U_{\ell/2,s}(R_\alpha\otimes\mathbb{I}\otimes\mathbb{I}) U_{s,s'} R_\alpha U_{s',-\ell/2}(\omega_R\otimes\Omega) U^\dagger_{s',-\ell/2}\\
&\qquad\qquad \times\left(r_\alpha^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right) U^\dagger_{s,s'}\left(\left\{R_\alpha^\dagger, R_\beta^\dagger\right\}\otimes\mathbb{I}\otimes\mathbb{I}\right) U^\dagger_{\ell/2,s}|\omega_L\rangle\Big]\\
&= \int_{-\ell/2}^{\ell/2} ds \int_{-\ell/2}^{s} ds' \mathrm{Tr}\Big[\langle\omega_L| U_{\ell/2,s}(R_\alpha\otimes\mathbb{I}\otimes\mathbb{I}) U_{s,s'} R_\alpha U_{s',-\ell/2}(\omega_R\otimes\Omega) U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)\\
&\qquad\qquad \times U^\dagger_{s,s'}\left(\left\{R_\alpha^\dagger, R_\beta^\dagger\right\}\otimes\mathbb{I}\otimes\mathbb{I}\right) U^\dagger_{\ell/2,s}|\omega_L\rangle\Big]
\end{aligned} \tag{6.63}$$

The integrand in this equation is of the form (6.28), and so to continue our evaluation we follow an identical procedure to the evaluation of (6.28), see (6.28) through (6.37). We find that we have a contribution towards term $(**)$ in (6.50), and in turn for the final expression for $\langle\partial_{\bar{j}}\Psi(\overline{z})|\hat{V}|\Psi(z)\rangle$ with $D^2+1\le j\le 2D^2$, written in the Jamiolkowski representation, of

$$\ell\langle R_\alpha^\dagger\left\{R_\alpha, R_\beta\right\}|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|R_\alpha\rho\, r_\alpha^{j\dagger}\rangle \tag{6.64}$$

where ρ is the matrix form of the right eigenvector corresponding to the zero eigenvalue of the matrix M, see (6.29).

Substitution of (6.54) into (6.51)

The procedure following the substitution of (6.54) is analogous to the above. We omit presentation of the derivation to avoid repetition and simply state that we obtain a contribution

of

$$\ell\langle R_\alpha^\dagger r_\alpha^j|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)|R_\alpha\rho\left\{R_\alpha,R_\beta\right\}^\dagger\rangle. \tag{6.65}$$

Substitution of (6.55) into (6.51)

The evaluation of (6.51) having substituted (6.55) is somewhat easier. Including (6.52), we find that (6.51) can be written

$$\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2} ds\,ds'\mathrm{Tr}\Big[\langle\omega_L|\left(\mathbb{I}\otimes\mathbb{I}\otimes\psi_\beta^\dagger(s)\right)U_{\ell/2,s}\left(R_\alpha\otimes\mathbb{I}\otimes\mathbb{I}\right)U_{s,-\ell/2}(\omega_R\otimes\Omega)U_{s',-\ell/2}^\dagger \\ \times\left(r_\alpha^{j\dagger}\otimes\delta(s'-s)\otimes\mathbb{I}\right)U_{\ell/2,s}^\dagger|\omega_L\rangle\Big]. \tag{6.66}$$

We first integrate out the delta function, then replace the product

$$U_{s,-\ell/2}^\dagger\left(r_\alpha^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)U_{\ell/2,s}^\dagger|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\mathbb{I}\otimes\psi_\beta^\dagger(s)\right)$$

$$\to\left[U_{s,-\ell/2}^\dagger\left(r_\alpha^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)U_{\ell/2,s}^\dagger|\omega_L\rangle\langle\omega_L|\,,\,\left(\mathbb{I}\otimes\mathbb{I}\otimes\psi_\beta^\dagger(s)\right)\right] \tag{6.67}$$

$$=U_{s,-\ell/2}^\dagger\left(\left\{r_\alpha^{j\dagger},R_\beta^\dagger\right\}\otimes\mathbb{I}\otimes\mathbb{I}\right)U_{\ell/2,s}^\dagger|\omega_L\rangle\langle\omega_L|. \tag{6.68}$$

We thus find that (6.66) can be written

$$\int_{-\ell/2}^{\ell/2} ds\,\mathrm{Tr}\Big[\langle\omega_L|U_{\ell/2,s}\left(R_\alpha\otimes\mathbb{I}\otimes\mathbb{I}\right)U_{s,-\ell/2}(\omega_R\otimes\Omega)U_{s,-\ell/2}^\dagger\left(\left\{r_\alpha^{j\dagger},R_\beta^\dagger\right\}\otimes\mathbb{I}\otimes\mathbb{I}\right)U_{\ell/2,s}^\dagger|\omega_L\rangle\Big]. \tag{6.69}$$

The integrand of this equation is of the form (6.28), and so to continue the evaluation of (6.69) we follow an identical procedure to that of (6.28), see (6.28) through (6.38). We find that we have a contribution towards term (∗∗) in (6.50), and in turn for the final expression for $\langle\partial_{\overline{j}}\Psi(\overline{z})|\hat{V}|\Psi(z)\rangle$ with $D^2+1\le j\le 2D^2$, written in Jamiolkowski representation, of

$$\ell\langle\mathbb{I}|R_\alpha\rho\left\{r_\alpha^{j\dagger},R_\beta^\dagger\right\}\rangle \tag{6.70}$$

Combining all contributions, namely equations (6.64), (6.65) and (6.70) we find that the term (∗∗) of equation (6.50) is given by

$$\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2} ds\,ds'\mathrm{Tr}\Big[\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\psi_\beta^\dagger(s)\right)\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}\right)U_{\ell/2,-\ell/2} \\ \times(\omega_R\otimes\Omega)U_{s',-\ell/2}^\dagger\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U_{\ell/2,s'}^\dagger|\omega_L\rangle\Big]$$

$$=\ell\Big[\langle R_\alpha^\dagger\left\{R_\alpha,R_\beta\right\}|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)|R_\alpha\rho r_\alpha^{j\dagger}\rangle+\langle R_\alpha^\dagger r_\alpha^j|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)|R_\alpha\rho\left\{R_\alpha,R_\beta\right\}^\dagger\rangle \\ +\langle\mathbb{I}|R_\alpha\rho\left\{r_\alpha^{j\dagger},R_\beta^\dagger\right\}\rangle\Big] \tag{6.71}$$

The term $(*)$

To evaluate term $(*)$ from (6.50), namely

$$\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2} ds\, ds' \mathrm{Tr}\Big[\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\psi_\beta(s)\right)U_{\ell/2,-\ell/2} \\ \times(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\Big],$$

we proceed as in term $(**)$. We do not present the calculations, and state the result only. We find that term $(*)$ evaluates to

$$\ell\Big[\langle\left\{R_\alpha,R_\beta\right\}^\dagger R_\alpha|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)|R_\alpha\rho\, r_\alpha^{j\dagger}\rangle+\langle R_\alpha^\dagger r_\alpha^j|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)|\left\{R_\alpha,R_\beta\right\}\rho R_\alpha^\dagger\rangle \\ +\langle\mathbb{I}|\left\{R_\alpha,R_\beta\right\}\rho\, r_\alpha^{j\dagger}\rangle\Big]. \tag{6.72}$$

Final expression for $D^2+1\le j\le 2D^2$

Using equations (6.71) and (6.72) from the previous subsections and separating the vectors $|\rho\rangle$ and $\langle\mathbb{I}|$ using (4.29) we find that, for $D^2+1\le j\le 2D^2$,

$$\begin{aligned}\langle\partial_{\bar j}\Psi(\overline{z})|\hat V|\Psi(z)\rangle=\frac{\ell J}{\sqrt{2}}\Big[&\ell\langle\mathbb{I}|\left(R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha\right)|\rho\rangle\langle\mathbb{I}|\left(R_\alpha\otimes\overline{r}_\alpha^j\right)|\rho\rangle\\ &-\langle\mathbb{I}|\left(R_\alpha\otimes\overline{r}_\alpha^j\right)\frac{\mathbb{I}}{M}\left(R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha\right)|\rho\rangle\\ &-\langle\mathbb{I}|\left(R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha\right)\frac{\mathbb{I}}{M}\left(R_\alpha\otimes\overline{r}_\alpha^j\right)|\rho\rangle\\ &+\langle\mathbb{I}|R_\alpha\otimes\left\{\overline{R}_\beta,\overline{r}_\alpha^j\right\}|\rho\rangle+\langle\mathbb{I}|\left\{R_\alpha,R_\beta\right\}\otimes\overline{r}_\alpha^j|\rho\rangle\Big]\end{aligned} \tag{6.73}$$

We again note that the overall factor ℓ will not lead to a divergence in the limit $\ell\to\infty$ when considering the TDVP equation (6.16). Furthermore, the divergent terms in the first line of the right hand side will be removed when imposing the left gauge fixing requirement (6.47). This will become clear when considering the complete expression for L.

The case $1\le j\le D^2$

The calculations for $1\le j\le D^2$ are similar to the above, with the simplification that the tangent vector $\langle\partial_{\bar j}\Psi(\overline{z})|$ does not involve field operators $\psi^\dagger(s)$, see (6.23). This is evident

from the symmetry of both contributions in R_α and R_β. We find that in this case

$$\begin{aligned}\langle\partial_{\bar{j}}\Psi(\overline{z})|\hat{V}|\Psi(z)\rangle = \frac{\ell J}{\sqrt{2}}\Big[&\ell\langle\mathbb{I}|\left(\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha + R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}\right)|\rho\rangle\langle\mathbb{I}|\left(\mathbb{I}\otimes\overline{q}^j\right)|\rho\rangle \\ &-\langle\mathbb{I}|\left(R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha\right)\frac{\mathbb{I}}{M}\left(\mathbb{I}\otimes\overline{q}^j\right)|\rho\rangle \\ &-\langle\mathbb{I}|\left(\mathbb{I}\otimes\overline{q}^j\right)\frac{\mathbb{I}}{M}\left(R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha\right)|\rho\rangle\Big] \end{aligned} \tag{6.74}$$

The case $2D^2 \leq j \leq 3D^2$

The calculations for $2D^2 \leq j \leq 3D^2$ follow a similar pattern to that of $D^2+1 \leq j \leq 2D^2$. This is again evident when comparing the two final expressions, from the symmetry between R_α and R_β for $D^2+1 \leq j \leq 2D^2$ and $2D^2 \leq j \leq 3D^2$ respectively. We have

$$\begin{aligned}\langle\partial_{\bar{j}}\Psi(\overline{z})|\hat{V}|\Psi(z)\rangle = \frac{\ell J}{\sqrt{2}}\Big[&\ell\langle\mathbb{I}|\left(\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha + R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}\right)|\rho\rangle\langle\mathbb{I}|\left(R_\beta\otimes\overline{r}_\beta^j\right)|\rho\rangle \\ &-\langle\mathbb{I}|\left(R_\beta\otimes\overline{r}_\beta^j\right)\frac{\mathbb{I}}{M}\left(\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}\right)|\rho\rangle \\ &-\langle\mathbb{I}|\left(\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}\right)\frac{\mathbb{I}}{M}\left(R_\beta\otimes\overline{r}_\beta^j\right)|\rho\rangle \\ &+\langle\mathbb{I}|R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{r}_\beta^j\right\}|\rho\rangle\Big] \end{aligned} \tag{6.75}$$

Note that there is one term less than in the case $D^2+1 \leq j \leq 2D^2$. This is because the operator $\psi_\beta^\dagger(s)$ appears in $\langle\partial_{\bar{j}}\Psi(\overline{z})|$, rather than $\psi_\alpha^\dagger(s)$. Consequently, when shuffling the field operators around to reach the field vacuum via the introduction of commutation relations there is one less commutator of field operators of the same species, causing one less delta function contribution and thus one less term in the final expression.

6.2.7 Projection of the interaction term

The projection of the interaction term $\hat{W}$ of the Hamiltonian requires the evaluation of

$$\langle\partial_{\bar{j}}\Psi(\overline{z})|\hat{W}|\Psi(z)\rangle = \int_{-\ell/2}^{\ell/2} ds\ \langle\partial_{\bar{j}}\Psi(\overline{z})|\left(c\psi_\alpha^\dagger(s)\psi_\alpha^\dagger(s)\psi_\alpha(s)\psi_\alpha(s)\otimes\mathbb{I}\right)|\Psi(z)\rangle.$$

Using similar techniques to the above we find that

$$\begin{aligned}\langle\partial_{\bar{j}}\Psi(\overline{z})|\hat{W}|\Psi(z)\rangle = c\ell\Big[&4\ell\langle\mathbb{I}|\left(\mathbb{I}\otimes\overline{q}^j+R_\alpha\otimes\overline{r}_\alpha^j+R_\beta\otimes\overline{r}_\beta^j\right)|\rho\rangle\langle\mathbb{I}|\left(R_\alpha^2\otimes\overline{R}_\alpha^2\right)|\rho\rangle \\ &-4\langle\mathbb{I}|\left(\mathbb{I}\otimes\overline{q}^j+R_\alpha\otimes\overline{r}_\alpha^j+R_\beta\otimes\overline{r}_\beta^j\right)\frac{\mathbb{I}}{M}\left(R_\alpha^2\otimes\overline{R}_\alpha^2\right)|\rho\rangle \\ &-4\langle\mathbb{I}|\left(R_\alpha^2\otimes\overline{R}_\alpha^2\right)\frac{\mathbb{I}}{M}\left(\mathbb{I}\otimes\overline{q}^j+R_\alpha\otimes\overline{r}_\alpha^j+R_\beta\otimes\overline{r}_\beta^j\right)|\rho\rangle \\ &+2\langle\mathbb{I}|R_\alpha^2\otimes\left\{\overline{R}_\alpha,\overline{r}_\alpha^j\right\}|\rho\rangle\Big] \end{aligned} \tag{6.76}$$

6.2.8 Projection of the kinetic term

The projection of the kinetic term $\hat{T}$ of the Hamiltonian requires the evaluation of

$$\langle\partial_{\bar{j}}\Psi(\overline{z})|\,\hat{T}|\Psi(z)\rangle = \int_{-\ell/2}^{\ell/2} ds\ \langle\partial_{\bar{j}}\Psi(\overline{z})|\left(\frac{d\psi_\alpha^\dagger(x)}{dx}\frac{d\psi_\alpha(x)}{dx}\otimes\mathbb{I}\right)|\Psi(z)\rangle.$$

We find that

$$\begin{aligned}\langle\partial_{\bar{j}}\Psi(\overline{z})|\,\hat{T}|\Psi(z)\rangle = \ell\Big[&\langle\mathbb{I}|\,[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]|\rho\rangle\langle\mathbb{I}|\left(\mathbb{I}\otimes\overline{q}^j+R_\alpha\otimes\overline{r}_\alpha^j+R_\beta\otimes\overline{r}_\beta^j\right)|\rho\rangle\\ &-\langle\mathbb{I}|\,[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\frac{\mathbb{I}}{M}\left(\mathbb{I}\otimes\overline{q}^j+R_\alpha\otimes\overline{r}_\alpha^j+R_\beta\otimes\overline{r}_\beta^j\right)|\rho\rangle\\ &-\langle\mathbb{I}|\left(\mathbb{I}\otimes\overline{q}^j+R_\alpha\otimes\overline{r}_\alpha^j+R_\beta\otimes\overline{r}_\beta^j\right)\frac{\mathbb{I}}{M}\,[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]|\rho\rangle\\ &+\langle\mathbb{I}|\,[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{q}^j\right]|\rho\rangle+\langle\mathbb{I}|\,[R_\alpha,Q]\otimes\left[\overline{r}_\alpha^j,\overline{Q}\right]|\rho\rangle\Big]\end{aligned}\tag{6.77}$$

6.2.9 Final expression for L

Combining the projection of the density given by (6.73), (6.74) and (6.75), the projection of the interaction (6.76) and the projection of the kinetic term (6.77) we find that a general entry of L is given by

$$\begin{aligned}L_j = \ell\Big[&\ell\langle\mathbb{I}|\Big(\frac{J}{\sqrt{2}}\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+\frac{J}{\sqrt{2}}R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+4cR_\alpha^2\otimes\overline{R}_\alpha^2+[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\Big)|\rho\rangle\\ &\times\langle\mathbb{I}|\left(\mathbb{I}\otimes\overline{q}^j+R_\alpha\otimes\overline{r}_\alpha^j+R_\beta\otimes\overline{r}_\beta^j\right)|\rho\rangle\\ &-\langle\mathbb{I}|\Big(\frac{J}{\sqrt{2}}\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+\frac{J}{\sqrt{2}}R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+4cR_\alpha^2\otimes\overline{R}_\alpha^2+[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\Big)\frac{\mathbb{I}}{M}\\ &\times\left(\mathbb{I}\otimes\overline{q}^j+R_\alpha\otimes\overline{r}_\alpha^j+R_\beta\otimes\overline{r}_\beta^j\right)|\rho\rangle\\ &-\langle\mathbb{I}|\left(\mathbb{I}\otimes\overline{q}^j+R_\alpha\otimes\overline{r}_\alpha^j+R_\beta\otimes\overline{r}_\beta^j\right)\frac{\mathbb{I}}{M}\Big(\frac{J}{\sqrt{2}}\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+\frac{J}{\sqrt{2}}R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}\\ &+4cR_\alpha^2\otimes\overline{R}_\alpha^2+[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\Big)|\rho\rangle\\ &+\frac{J}{\sqrt{2}}\langle\mathbb{I}|R_\alpha\otimes\left\{\overline{R}_\beta,\overline{r}_\alpha^j\right\}|\rho\rangle+\frac{J}{\sqrt{2}}\langle\mathbb{I}|\left\{R_\alpha,R_\beta\right\}\otimes\overline{r}_\alpha^j|\rho\rangle+2c\langle\mathbb{I}|R_\alpha^2\otimes\left\{\overline{R}_\alpha,\overline{r}_\alpha^j\right\}|\rho\rangle\\ &+\langle\mathbb{I}|\,[R_\alpha,Q]\otimes\left[\overline{r}_\alpha^j,\overline{Q}\right]|\rho\rangle+\langle\mathbb{I}|\,[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{q}^j\right]|\rho\rangle+\frac{J}{\sqrt{2}}\langle\mathbb{I}|R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{r}_\beta^j\right\}|\rho\rangle\Big]\end{aligned}\tag{6.78}$$

As with the Gram matrix, the overall factor ℓ will not lead to a divergence in the limit $\ell\to\infty$ when substituting for L in the main TDVP equation (6.16). The divergent term inside the brackets can be removed by imposing orthogonality of the tangent vectors and states via the condition (6.47), as described in [Haegeman, 2011, Haegeman et al., 2011a]. In vector form we have

$$
L=\ell\left(\begin{array}{c}
\ell\langle\mathbb{I}|\Big(\frac{J}{\sqrt{2}}\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+\frac{J}{\sqrt{2}}R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+4cR_\alpha^2\otimes\overline{R}_\alpha^2+[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\Big)|\rho\rangle\langle\mathbb{I}|\left(\mathbb{I}\otimes\overline{q}^j\right)|\rho\rangle\\
-\langle\mathbb{I}|\Big(\frac{J}{\sqrt{2}}\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+\frac{J}{\sqrt{2}}R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+4cR_\alpha^2\otimes\overline{R}_\alpha^2+[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\Big)\frac{\mathbb{I}}{M}\left(\mathbb{I}\otimes\overline{q}^j\right)|\rho\rangle\\
-\langle\mathbb{I}|\left(\mathbb{I}\otimes\overline{q}^j\right)\frac{\mathbb{I}}{M}\Big(\frac{J}{\sqrt{2}}\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+\frac{J}{\sqrt{2}}R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+4cR_\alpha^2\otimes\overline{R}_\alpha^2+[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\Big)|\rho\rangle\\
+\langle\mathbb{I}|[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{q}^j\right]|\rho\rangle\\
\\
\ell\langle\mathbb{I}|\Big(\frac{J}{\sqrt{2}}\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+\frac{J}{\sqrt{2}}R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+4cR_\alpha^2\otimes\overline{R}_\alpha^2+[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\Big)|\rho\rangle\langle\mathbb{I}|\left(R_\alpha\otimes\overline{r}_\alpha^j\right)|\rho\rangle\\
-\langle\mathbb{I}|\Big(\frac{J}{\sqrt{2}}\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+\frac{J}{\sqrt{2}}R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+4cR_\alpha^2\otimes\overline{R}_\alpha^2+[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\Big)\frac{\mathbb{I}}{M}\left(R_\alpha\otimes\overline{r}_\alpha^j\right)|\rho\rangle\\
-\langle\mathbb{I}|\left(R_\alpha\otimes\overline{r}_\alpha^j\right)\frac{\mathbb{I}}{M}\Big(\frac{J}{\sqrt{2}}\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+\frac{J}{\sqrt{2}}R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+4cR_\alpha^2\otimes\overline{R}_\alpha^2+[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\Big)|\rho\rangle\\
+\frac{J}{\sqrt{2}}\langle\mathbb{I}|R_\alpha\otimes\left\{\overline{R}_\beta,\overline{r}_\alpha^j\right\}|\rho\rangle+\frac{J}{\sqrt{2}}\langle\mathbb{I}|\left\{R_\alpha,R_\beta\right\}\otimes\overline{r}_\alpha^j|\rho\rangle\\
+2c\langle\mathbb{I}|R_\alpha^2\otimes\left\{\overline{R}_\alpha,\overline{r}_\alpha^j\right\}|\rho\rangle+\langle\mathbb{I}|[R_\alpha,Q]\otimes\left[\overline{r}_\alpha^j,\overline{Q}\right]|\rho\rangle\\
\\
\ell\langle\mathbb{I}|\Big(\frac{J}{\sqrt{2}}\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+\frac{J}{\sqrt{2}}R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+4cR_\alpha^2\otimes\overline{R}_\alpha^2+[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\Big)|\rho\rangle\langle\mathbb{I}|\left(R_\beta\otimes\overline{r}_\beta^j\right)|\rho\rangle\\
-\langle\mathbb{I}|\Big(\frac{J}{\sqrt{2}}\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+\frac{J}{\sqrt{2}}R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+4cR_\alpha^2\otimes\overline{R}_\alpha^2+[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\Big)\frac{\mathbb{I}}{M}\left(R_\beta\otimes\overline{r}_\beta^j\right)|\rho\rangle\\
-\langle\mathbb{I}|\left(R_\beta\otimes\overline{r}_\beta^j\right)\frac{\mathbb{I}}{M}\Big(\frac{J}{\sqrt{2}}\left\{R_\alpha,R_\beta\right\}\otimes\overline{R}_\alpha+\frac{J}{\sqrt{2}}R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{R}_\beta\right\}+4cR_\alpha^2\otimes\overline{R}_\alpha^2+[R_\alpha,Q]\otimes\left[\overline{R}_\alpha,\overline{Q}\right]\Big)|\rho\rangle\\
+\frac{J}{\sqrt{2}}\langle\mathbb{I}|R_\alpha\otimes\left\{\overline{R}_\alpha,\overline{r}_\beta^j\right\}|\rho\rangle
\end{array}\right)
\tag{6.79}
$$

6.2.10 Analytical solution and implementation for $D=1$

We now consider analytically the calculations for approximating the time evolved state of the interacting field system according to $\tilde{H}_{\text{int}}$ in (6.20). Let the initial state $|\Psi(0)\rangle=|\psi(0)\rangle\otimes|\phi\rangle$, where $|\phi\rangle$ is a field coherent state, be the translation-invariant cMPS given by (6.21) with auxiliary system dimension $D=1$. The variational parameters thus comprise a set of $n=3$ complex numbers $\{Q,R_\alpha,R_\beta\}$. It was shown in [Brockt et al., 2012] that a cMPS with $D=1$ is a field coherent state. Furthermore, it can be shown that the field coherent states constitute a variational class for applications of the TDVP, which, when applied to the Lieb-Liniger model with external potential $V_{\text{ext}}(x)$, give the well known Gross-Pitaevskii equation (GPE)

$$
i\hbar\frac{\partial}{\partial t}\phi(x,t)=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V_{\text{ext}}(x)+g|\phi(x,t)|^2\right)\phi(x,t),
\tag{6.80}
$$

cf. Chapter 2, section 2.3.1. We therefore expect to obtain a GPE for the time evolution of our α field, that is in terms of the variational parameter $R_\alpha(t)$, which evolves according to the Lieb-Liniger model with an external potential given by the field position variable $\hat{z}(x)$.

We proceed with the implementation of the TDVP by introducing a time-dependent parameterisation of our variational parameters $\{Q(t), R_\alpha(t), R_\beta(t)\}$, where the optimum equations of motion satisfy

$$i\begin{pmatrix} dQ(t)/dt \\ dR_\alpha(t)/dt \\ dR_\beta(t)/dt \end{pmatrix} = G(Q,R_\alpha,R_\beta)^{-1}L(Q,R_\alpha,R_\beta) \tag{6.81}$$

where $G(Q,R_\alpha,R_\beta)$ and $L(Q,R_\alpha,R_\beta)$ are as defined in (6.48) and (6.79) respectively. In the case $D=1$ we find that the expressions for $G(Q,R_\alpha,R_\beta)$ and $L(Q,R_\alpha,R_\beta)$ are dramatically simplified. Recall that a typical entry of G is of the form

$$\ell\langle\mathbb{I}|\mathbb{I}\otimes\overline{q}^j|\rho\rangle\langle\mathbb{I}|r_\alpha^k\otimes\overline{R}_\alpha|\rho\rangle - \langle\mathbb{I}|\mathbb{I}\otimes\overline{q}^j\frac{\mathbb{I}}{M}r_\alpha^k\otimes\overline{R}_\alpha|\rho\rangle - \langle\mathbb{I}|r_\alpha^k\otimes\overline{R}_\alpha\frac{I}{M}\mathbb{I}\otimes\overline{q}^j|\rho\rangle.$$

In the case $D=1$ this simplifies as follows. The tensor products become numbers, for example $r_\alpha^k\otimes\overline{R}_\alpha = r_\alpha^k\overline{R}_\alpha$; similarly for the matrix M given in (6.29). In fact, using the decomposition of $Q=-iK-\frac{1}{2}R^\dagger R$, where K is an anti-hermitian matrix, as given in (4.13) and (4.51), we find that

$$\begin{aligned} M &= Q\otimes\mathbb{I}+\mathbb{I}\otimes\overline{Q}+R_\alpha\otimes\overline{R}_\alpha+R_\beta\otimes\overline{R}_\beta \\ &= -i(K\otimes\mathbb{I}-\mathbb{I}\otimes K^T)-\frac{1}{2}\sum_{j=\alpha,\beta}\left(R_j^\dagger R_j\otimes\mathbb{I}-2R_j\otimes\overline{R_j}+\mathbb{I}\otimes R_j^T\overline{R_j}\right)=0. \end{aligned} \tag{6.82}$$

The master equation (6.29) for $|\rho\rangle$ governed by M thus reduces to $\frac{d|\rho(t)\rangle}{dt}=0$. We can then arbitrarily take $|\rho\rangle=|\mathbb{I}\rangle$. Furthermore, since $\mathbb{I}/M$ is defined to be the pseudoinverse of M, where the diverging term in the spectral decomposition that would correspond to the reciprocal of the zero eigenvalue is taken to be zero, we have that $\mathbb{I}/M=0$. We therefore find that the $3D^2\times 3D^2 = 3\times 3$ matrix is

$$G(Q,R_\alpha,R_\beta)=\ell^2\begin{pmatrix} 1 & \overline{R_\alpha} & \overline{R_\beta} \\ R_\alpha & |R_\alpha|^2+1/\ell & R_\alpha\overline{R_\beta} \\ R_\beta & \overline{R_\alpha}R_\beta & |R_\beta|^2+1/\ell \end{pmatrix},$$

and the $3D^2\times 1 = 3\times 1$ vector $L(Q,R_\alpha,R_\beta)$ can be written

$$L(Q,R_\alpha,R_\beta)=\ell^2\begin{pmatrix} \sqrt{2}J|R_\alpha|^2\left(R_\beta+\overline{R_\beta}\right)+4c|R_\alpha|^4 \\ R_\alpha\left(\sqrt{2}J|R_\alpha|^2\left(R_\beta+\overline{R_\beta}\right)+4c|R_\alpha|^4+(\sqrt{2}J(R_\beta+\overline{R_\beta})+4c|R_\alpha|^2)/\ell\right) \\ R_\beta\left(\sqrt{2}J|R_\alpha|^2\left(R_\beta+\overline{R_\beta}\right)+4c|R_\alpha|^4\right)+\sqrt{2}|R_\alpha|^2/\ell \end{pmatrix}.$$

Substituting these expressions into the TDVP equation (6.81) results in the following equations of motion

$$i\begin{pmatrix} dQ(t)/dt \\ dR_\alpha(t)/dt \\ dR_\beta(t)/dt \end{pmatrix} = \begin{pmatrix} -\sqrt{2}|R_\alpha(t)|^2\overline{R_\beta(t)} \\ \left(2c|R_\alpha(t)|^2+\sqrt{2}J(R_\beta(t)+\overline{R_\beta(t)})\right)R_\alpha(t) \\ \sqrt{2}|R_\alpha(t)|^2 \end{pmatrix}.$$

We note that the application of gauge fixing conditions was unnecessary in this example, and the divergent terms involving ℓ cancelled. As expected, when compared to (6.80), we find that the equation of motion for $R_\alpha(t)$, describing the evolution of the primary quantum field system, is indeed a GPE, providing some verification of our TDVP calculations.

We now obtain solutions to this set of differential equations. We notice that the equation of motion for $Q(t)$ decouples and therefore proceed by considering the equations for $R_\alpha(t)$ and $R_\beta(t)$. For the initial conditions we take both $R_\alpha(t=0)$ and $R_\beta(t=0)$ to be real, in particular we choose

$$R_\alpha(0)=1, \qquad R_\beta(0)=0.$$

The initial condition for $R_\beta(t)$ corresponds to a zero mean for the β field position operator $\hat{z}(x)$ via

$$\langle\phi(x,t)|\hat{\psi}_\beta(x)+\hat{\psi}_\beta^\dagger(x)|\phi(x,t)\rangle \propto \mathrm{Re}\left(R_\beta\right),$$

where we use that, in the one-dimensional case, the R_β are the time-dependent eigenvalues of $\hat{\psi}_\beta(x)$ with respect to field coherent states $|\phi(x,t)\rangle$. In a similar manner, $R_\alpha(0)$ is chosen to correspond to fixed average particle density. The equation of motion for $R_\beta(t)$, namely

$$i\frac{dR_\beta(t)}{dt} = \sqrt{2}|R_\alpha(t)|^2,$$

can then be integrated, giving

$$R_\beta(t)-R_\beta(0) = -i\sqrt{2}\int_0^t |R_\alpha(t')|^2\,dt' = -i\sqrt{2}g(t),$$

where $g(t):\mathbb{R}_{>0}\to\mathbb{R}_{>0}$. Using that $R_\beta(0)=0$ thus implies

$$2\mathrm{Re}(R_\beta(t)) = (R_\beta(t)+\overline{R_\beta}(t)) = 0, \qquad \forall t.$$

We can therefore conclude that the disorder, with strength J, does not effect the dynamics of $R_\alpha(t)$. The obtained results could be due to the small dimension of the cMPS auxiliary system, which at this level cannot capture the relevant physical effects. Additionally, the symmetry of the randomness could have a strong effect. By choosing a Gaussian random

potential centred around zero the contributions of each realisation ultimately cancel, such that the overall effect is removed.

We now turn to solving for $R_\alpha(t)$. Since $R_\alpha(t):\mathbb{R}_{>0}\to\mathbb{C}$ we take $R_\alpha(t)=r_\alpha e^{i\phi(t)}$ as an ansatz and find that the equation of motion for $R_\alpha(t)$, namely

$$i\frac{dR_\alpha(t)}{dt}=2c|R_\alpha(t)|^2R_\alpha(t), \tag{6.83}$$

can be written

$$-r_\alpha\dot{\phi}(t)e^{i\phi(t)}=2c|r_\alpha|^2r_\alpha e^{i\phi(t)}. \tag{6.84}$$

Assuming $r_\alpha\neq 0$, we have that

$$\dot{\phi}(t)=-2c|r_\alpha|^2 \;\Rightarrow\; \phi(t)-\phi(0)=-2c|r_\alpha|^2t. \tag{6.85}$$

Since we chose $R_\alpha(0)=0$ to be real, we are free to set $\phi(0)=0$, leading to

$$\phi(t)=-2c|r_\alpha|^2t \;\Rightarrow\; R_\alpha(t)=r_\alpha e^{-2ic|r_\alpha|^2t}.$$

$R_\alpha(t)$ therefore circles the origin with frequency proportional to c.

We now consider different initial conditions for $R_\beta(0)$, where the Gaussian random potential is not symmetric about the origin. We assume that $R_\beta(0)\neq 0$ and instead, using that

$$R_\beta(t)=R_\beta(0)-\sqrt{2}i\int_0^t|R_\alpha(t')|^2dt'$$

we find that

$$i\frac{dR_\alpha(t)}{dt}=\left(2c|R_\alpha(t)|^2+2\sqrt{2}\mathrm{Re}\left(R_\beta(0)\right)\right)R_\alpha(t). \tag{6.86}$$

Applying the same ansatz $R_\alpha(t)=r_\alpha e^{i\phi(t)}$, we find that the equation of motion for $R_\alpha(t)$ can be written

$$-r_\alpha\dot{\phi}(t)e^{i\phi(t)}=2c|r_\alpha|^2r_\alpha e^{i\phi(t)}+2\sqrt{2}J\mathrm{Re}\left(R_\beta(0)\right)r_\alpha e^{i\phi(t)}, \tag{6.87}$$

which, again assuming that $\phi(0)=0$, gives

$$R_\alpha(t)=r_\alpha e^{i\left(-2c|r_\alpha|^2-2\sqrt{2}J\mathrm{Re}\left(R_\beta(0)\right)\right)t}.$$

We therefore find that $R_\alpha(t)$ circles the origin with frequency dependent on both c and J.

Having obtained the equations of motion for $Q(t)$, $R_\alpha(t)$ and $R_\beta(t)$ we have simulated the dynamics of the cMPS and in turn obtained an approximation for the time-evolved state

of the interacting field system. We can therefore determine the reduced density operator of the field α at time t after the evolution of the interacting system under $H_{\text{int}}(\hat{z}(x))$ given by (6.7), which according to the mapping (6.14) is equivalent to the density operator of the random system averaged over the disorder given by (6.6). With this identification at hand, we can use (6.7) to calculate expectation values of observables averaged over all possible realisations of the random potential.

In a next step it would be interesting to determine the dynamics of the system using cMPS with higher auxiliary system dimensions $D > 1$. The determination of G and L in these cases would ultimately require numerical methods to obtain quantities such as $\mathbb{I}/M$ and $|\rho\rangle$. Solving the corresponding equations of motion would also require a numerical treatment. By considering larger D we naturally obtain a better approximation to the actual evolved state, and in turn a better approximation to the exact dynamics of the random system.

6.3 Extensions and outlook

There are several natural extensions of our proposed method. For example, as in [Paredes et al., 2005], the scheme can also be used for the computation of higher moments of the distribution of physical observables. For example, the calculation of

$$\langle\langle \hat{O}^2\rangle - \langle\hat{O}\rangle^2\rangle = \operatorname{tr}\left[\hat{O}^2\rho(t)\right] - \operatorname{tr}\left[\hat{O}\rho(t)\right]\operatorname{tr}\left[\hat{O}\rho(t)\right] \tag{6.88}$$

is straightforward since our mapping from the cQRS to the interacting quantum system is on the level of $\rho(t)$. If performing an experimental implementation, we would require two independent copies of the system to obtain $\rho(t)$ twice, then in turn determine $\operatorname{tr}\left[\hat{O}^2\rho(t)\right]$ and $\operatorname{tr}\left[\hat{O}\rho(t)\right]$, squaring the latter. Similar expressions to (6.88) would give higher moments.

A generalisation of the TDVP equation presented here is also possible. The Lieb-Liniger model with two-particle delta potential $\delta(x-y)$ is a translationally invariant system. This makes the TDVP calculations using translationally invariant cMPS relatively straightforward. However, more general Hamiltonians for non-translationally invariant systems can also be accommodated by the TDVP by taking the cMPS in (6.21) to be position dependent via

$$Q \to Q(x), \qquad R_\alpha \to R_\alpha(x), \qquad R_\beta \to R_\beta(x).$$

This does result in some further complications to the calculations presented here, but is not problematic. The main differences arise in the presence of spatial derivatives of $dR_\alpha(x)/dx$, following from the spatial derivatives of $\hat{\psi}_\alpha(x)$, namely

$$\frac{d\psi_\alpha(x)}{dx}|\Psi(Q,\{R_\alpha\})\rangle = \langle\omega_R|U_{(\ell/2,x)}\left(-[Q(x),R_\alpha(x)] + \frac{dR_\alpha(x)}{dx}\right)U_{(x,-\ell/2)}|\omega_L\rangle|\Omega\rangle,$$

see (4.21) of Chapter 4, and the presence of path ordered integrals, involving the matrix

$$M \to M(x) = Q(x)\otimes\mathbb{I} + \mathbb{I}\otimes\overline{Q}(x) + R_\alpha(x)\otimes\overline{R}_\alpha(x) + R_\beta(x)\otimes\overline{R}_\beta(x),$$

first defined in this chapter in (6.29). For details of the TDVP for single component, non-translationally invariant systems we refer to [Haegeman, 2011, Haegeman et al., 2011a].

Finally, as with [Paredes et al., 2005], the scheme poses interesting experimental considerations, with the idea that the simulation of randomness in quantum fields can be achieved through interaction with an auxiliary quantum system, or conversely that existing experimental setups of interacting systems could be used as simulators for random systems.

6.4 Chapter summary

We have developed an algorithm that allows for the dynamical simulation of a cQRS. The randomness enters by means of an external potential governed by a continuous function of position, which is the limit of zero-mean Gaussian random potentials, under appropriate scaling, on a lattice. The simulation of such a system typically requires the evaluation of dynamics averaged over all realisations of the randomness, that is all sample paths of the underlying random process, such that the central object of study is the expectation value of the time-evolved states with respect to the random potentials. Since direct calculation of this object is impracticable, we have presented an algorithm that allows for this expectation value to be mapped to the expectation value in a corresponding system of interacting quantum fields. The algorithm thus converts the task of simulating a cQRS to that of simulating a non-random, interacting continuous quantum system.

Having established the equivalence of the aforementioned expectation values, we presented a method to solve the dynamics of the interacting quantum fields through an extension of the time-dependent variational principle for multi-component cMPS. The equations of motion determining the time evolution of the cMPS variational parameters were derived, and the method validated with the implementation of a simple analytical solution method. Considering the cMPS auxiliary system dimension D to be 1, so that the cMPS becomes a field coherent state, the equations of motion do indeed produce the anticipated Gross Pitaevski equation, providing encouraging support for the validity of our method at dimensions $D \geq 1$. Our approach thus allows for the simulation of randomness in continuous quantum systems to be performed within the framework of numerical methods that are able to efficiently simulate the corresponding interacting problem. We also discussed generalisations of the

method, including extensions for the calculation of higher moments and the simulation of non-translationally invariant systems, together with experimental implications.

Chapter 7

Summary and Conclusion

The understanding of quantum many-body systems, and subsequent engineering and exploiting of such systems for quantum information purposes and quantum simulations, continues to be a prime focus of modern physics. We are at a very interesting crossing point where different branches of physics, including quantum information theory and condensed matter physics, merge and incite fascinating insights. Furthermore, Feynman's vision of quantum simulation is starting to become a reality, since significant progress has been made in a number of experimental fields. Microscopic particles can now be isolated, manipulated and controlled, and detected with almost perfect fidelity. It is an exciting time, where the investigation of many-particle systems by means of classical or quantum simulation generates new proposals that improve the intuition and understanding of such systems. We have contributed to this area by developing two approaches for the simulation of continuous quantum systems in Chapters 5 and 6 by means of the application of variational methods, and in particular using the variational class of continuous matrix product states (cMPS). We now present a brief summary of our main results and a general outlook regarding future research.

Simulating Quantum Fields with Cavity QED

In Chapter 5 we presented an analogue algorithm for the quantum simulation of interacting quantum fields. The simulation was based on the observation that the continuous output of a cavity QED apparatus can be used as a continuous register recording a variational quantum state. We demonstrated that this interpretation allows for an analogue quantum simulation procedure of the interacting quantum field dynamics. Exploiting the fact that the stationary output of a cavity is of cMPS type, we performed a classical simulation using this variational class to validate the model. We were able to show that the proposed scheme is capable of simulating the paradigmatic Lieb-Liniger model with parameter ranges experimentally realisable with state of the art technology.

A discussion of extensions of the model was provided at the close of the chapter. For

example, we described the potential of the method for the simulation of multi-component fields. The setting of multi-component fields is of particular interest in the context of quantum simulation, since classical variational methods including calculations using cMPS soon fail due to the exponential scaling of the parameter space. This is arguably the precise purpose of quantum simulation - to solve complex problems involving many degrees of freedom and large scale entanglement that are inaccessible to classical computers - and this field certainly holds great promise for the future.

Our approach offered a new perspective for cavity QED systems, since such architectures could also be used to simulate interacting continuous quantum systems. It would be interesting to see what else could be simulated with existing devices, or to suggest new experiments based on theoretical insights. Along this line of thinking a recent body of work considers the link between matrix product states (MPS) and interferometry [Jaryzna and Demkowicz-Dobrzanski, 2013], where the optimal states in lossy quantum interferometry may be efficiently simulated using low rank MPS. In such a setting, it could be beneficial to consider rather cMPS. It would therefore be interesting to explore this idea further.

Simulating Continuous Quantum Random Systems

In Chapter 6 we developed an algorithm that allowed for the dynamical simulation of a continuous quantum random system (cQRS). The algorithm mapped the central quantity of interest when studying such systems, namely the expectation value of time evolved states with respect to the disorder, to the expectation value for a system comprising interacting quantum fields. Having established such an equivalence, we were able to design a method to solve the dynamics of the interacting fields by means of a novel extension of the time-dependent variational principle. Explicit equations of motion for the time evolved variational parameters were derived. Furthermore, by setting the cMPS auxiliary system dimension to $D = 1$ such that the cMPS becomes a field coherent state, the derived equations of motion produced the anticipated Gross Pitaevski equation.

The algorithm was a generalisation of the work presented in [Paredes et al., 2005], where the authors exploited quantum parallelism to simulate quantum random systems on a lattice. As an application, the dynamics of random spin chains were simulated using known numerical methods involving MPS. Indeed, much study of simulating dynamics of quantum many-body systems to date has focussed on lattice systems, using matrix product states and higher dimensional generalisations such as projected entangled pair states (PEPS). Considering

the correspondence between the well-studied MPS and their continuum analogies cMPS, we expect that the translation of many algorithms employing MPS to the continuum limit is possible, as demonstrated in this thesis. In addition, it would be interesting to see if we can further exploit the idea of mapping one problem that is difficult to solve to another problem, where known numerical methods can be applied or even where new methods can be designed.

A discussion of extensions of the model was provided at the close of the chapter. This included extensions to non-translationally invariant systems, via considering more general particle interactions and non-translationally invariant potentials, and to fermionic systems, for example to simulate disorder in a solid, such as semiconductors with impurities. We could also investigate whether instead of using the TDVP in conjunction with cMPS, one could envision a setup for the quantum simulation of the interacting quantum systems, similar to the proposal in Chapter 5, but in this case for the simulation of system dynamics. In principle this could require the preparation of the cavity system as described in Chapter 5, this time involving two output field modes, and an implementation of the interaction described in Chapter 6. After the required time-evolution one could discard the mode corresponding to the auxiliary field system via a suitable measurement and measure physical observables with respect to the remaining system of interest. Such a proposal certainly deserves further thought.

As a final remark, we wish to emphasise the importance of cMPS. The class of cMPS is still new and not well understood in the quantum information and condensed matter physics communities. However, as we have demonstrated in this thesis, they are a class of states with great potential and we expect they will become an essential tool in the study of continuous quantum systems, inspiring new methods and results. We hope that the work presented in this thesis motivates further studies in this direction.

Appendix A

Second Quantisation

Here we review the method of second quantisation, a procedure used to describe many-particle systems using a basis that describes the number of particles occupying each state in a complete set of single particle states. Second quantisation provides the framework of compactly treating many-particle systems with variable particle number, and lies at the foundation for the formulation of quantum field theory. Since in this thesis we consider interacting quantum fields, we review the motivation behind second quantisation in detail, followed by the introduction of a compact way of writing symmetrised wavefunctions and the concept of Fock space. Finally we recall how operators can be represented in terms of harmonic oscillator annihilation and creation operators, and in particular introduce a generic form of a field Hamiltonian, conveniently given in position representation, which we use throughout this thesis. In the following presentation we closely follow [Pickett, 2007].

A.1 Motivation: indistinguishable particles

Consider a system of N identical non-relativistic particles, where for simplicity we assume that the physical state of each particle $1 \leq j \leq N$ is described by its position x_j relative to some frame of reference. The wave function for such a system is denoted by $\Psi(x_1,\ldots,x_N)$. In quantum mechanics, particles do not have well defined trajectories: at some initial time t_0 the set of N particles maybe be localised at a set of well defined positions $x_1,\ldots,x_N$, but after evolution they will become delocalised. Therefore, since the particles are identical, the probability density $|\Psi(x_1,\ldots,x_N)|^2$ must remain unchanged under arbitrary exchanges of the identification labels, in this case x_j. Hence, permutations make up a symmetry of a many-body quantum mechanical system: identical particles are indistinguishable. We have that, for any operator P_{jk} that exchanges the labels of particles j and k, the wave function changes at most by a phase factor, that is

$$P_{jk}\Psi(x_1,\ldots,x_j,\ldots,x_k,\ldots x_N) = e^{i\phi}\Psi(x_1,\ldots,x_j,\ldots,x_k,\ldots x_N).$$

Under a second application of P_{jk} the particles return to their initial labelling and the original state is recovered. since $e^{i\phi}$ must not be an observable phase, this means that $\phi = 0, \pi$ [1]. Therefore Ψ is either even or odd under permutation. Systems of identical particles that are even under pairwise permutation of the particle labels are called bosons. Systems that are odd under pairwise permutation are called fermions. For example, the (normalised) two-particle wave functions for identical bosons and identical fermions are given by

$$\Psi_B(x_1, x_2) = \frac{1}{\sqrt{2}} \left(\psi_1(x_1)\psi_2(x_2) + \psi_2(x_1)\psi_1(x_2) \right)$$
$$\Psi_F(x_1, x_2) = \frac{1}{\sqrt{2}} \left(\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2) \right).$$

In the Dirac braket notation we can write

$$|\Psi_1, \Psi_2\rangle_B \equiv \frac{1}{\sqrt{2}} \left(|\psi_1\rangle \otimes |\psi_2\rangle + |\psi_2\rangle \otimes |\psi_1\rangle \right)$$
$$|\Psi_1, \Psi_2\rangle_F \equiv \frac{1}{\sqrt{2}} \left(|\psi_1\rangle \otimes |\psi_2\rangle - |\psi_2\rangle \otimes |\psi_1\rangle \right).$$

More generally, a symmetrised N-particle state for fermions ($\eta = -1$) or bosons ($\eta = 1$) must take the form

$$|\Psi_1, \ldots, \Psi_N\rangle = \frac{1}{\sqrt{N! n_1! n_2! \ldots n_N!}} \sum_{\mathcal{P}} \eta^{\mathcal{P}} |\Psi_{\mathcal{P}_1}\rangle \otimes |\Psi_{\mathcal{P}_2}\rangle \otimes \ldots \otimes |\Psi_{\mathcal{P}_N}\rangle,$$

where n_j is the total number of particles occupying state j (for fermions, Pauli exclusion enforces the constraint that $n_j \leq 1$). $\mathcal{P}$ denotes the parity, and is defined as the number of switches of two elements needed to bring the permutation $(\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_N)$ back to the ordered sequence $(1, 2, \ldots, N)$. The summation runs over all $N!$ permutations of the set of quantum numbers $\{1, 2, \ldots, N\}$. The pre-factor $\frac{1}{\sqrt{N! n_1! n_2! \ldots n_N!}}$ normalises the many-body wave function.

Whilst the above representation can be used to describe a many-body wave function, further thought shows that it is far from convenient. For example, performing computations within this formalism is cumbersome. To calculate the overlap of two wave functions one would need to form $(N!)^2$ different products. Also, we assume here that the total particle number N is fixed. Sometimes we require to work in a setting where N is allowed to vary. Or we might wish to use a representation where individual quasi-particles are fundamental, as opposed to the entangled set of quantum numbers of all constituents (i.e. when considering situations of particle creation followed by annihilation). The formalism of second quantisation affords the possibility to heavily condense the above representation and overcome the aforementioned disadvantages.

[1] Under certain conditions (e.g. in two dimensional systems) the phase factor can take different values to 0 and π. Such particles are called anyons.

A.2 Fock space

In the present notation introduced in A.1, quantum states are represented by tensor products with N components. Let us assume that the states are ordered by some convention[2], for position representation for example with increasing position from left to right, so that we can just label them by integer numbers, i.e. $\lambda_i = j$. The current notation therefore amounts to tensor products of numbers, for example $|1,1,1,2,2,3,4,4,\ldots\rangle$, where each particle and the state it occupies is specified. This representation contains much redundancy. A more efficient encoding of the state above would be to count the number of particles in a specific state, which in the previous example would result in $|3,2,1,2,\ldots\rangle$, where the i-th number denotes the number of particles occupying state i. This defines the occupation number representation, which is more compact and suffers no loss of information: the symmetrised state is completely characterised. In this alternate representation, a general basis state is given by $|n_1, n_2, \ldots\rangle$ where $\sum_i n_i = N$. We define $\mathcal{F}_N$ to be the linear span of all N-particle states $|n_1, n_2, \ldots\rangle$. Any state $|\Psi\rangle \in \mathcal{F}_N$ can be obtained by linear superposition $|\Psi\rangle = \sum_{n_1,n_2,\ldots} c_{n_1,n_2,\ldots} |n_1, n_2, \ldots\rangle$.

As mentioned above, we may also want to consider settings where we do not fix the particle number N. In this case, a Hilbert space that accommodates such a state with undetermined particle number is called the Fock space and is given by the direct sum

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{F}_N.$$

Note that the Fock space includes a contribution $\mathcal{F}_0$, the so-called vacuum space. This is a one dimensional Hilbert space that describes the case where no particles are present, and is spanned by the vector $|0\rangle$ called the vacuum state. To obtain the basis of $\mathcal{F}$ we simply take the totality of the previous basis states $|n_1, n_2, \ldots\rangle$ and drop the condition $\sum_i n_i = N$, i.e. now all sums over the different n_i run independently from 0 to ∞ without constraining each other. A general state of the Fock space is, therefore, a linear combination of states with any number of particles.

We now have a more compact representation, but are still faced with the formidable sums over the permutation group appearing in A.1. The second quantisation formalism removes the need to explicitly symmetrise the state, providing a comprehensive and highly efficient formulation of many-body quantum mechanics. To this end, we define creation operators $a_i^\dagger$

[2] we can always achieve this by the cost of at most of a minus sign in the case of fermions.

by its action on an arbitrary state in Fock space $\mathcal{F}$:

$$a_i^\dagger|n_1,\ldots,n_i,\ldots\rangle = (n_i+1)^{1/2}\,\eta^{s_i}|n_1,\ldots,n_i+1,\ldots\rangle, \tag{A.1}$$

where $s_i = \sum_{j=1}^{i-1} n_i$. Note that in the fermionic case, the occupation numbers are to be understood modulo 2, i.e. the application of $a_i^\dagger$ to a state with $n_i = 1$ annihilates this state.

By virtue of this definition, we are able to generate every basis state of $\mathcal{F}$ by repeated applications of $a_i^\dagger$ to the vacuum state $|0\rangle$, that is

$$|n_1, n_2, \ldots\rangle = \prod_i \frac{1}{(n_i!)^{1/2}} (a_i^\dagger)^{n_i}|0\rangle \tag{A.2}$$

Physically, an N-fold application of operators $a^\dagger$ to the empty vacuum state generates an N-particle state, which is why these operators are called creation operators. The introduction of creation operators merits some justification, for instance we must check the consistency with properties of Fock space. Consider two operators $a_i^\dagger$ and $a_j^\dagger$, $i \neq j$. From the definition (A.1) we see that

$$\left(a_i^\dagger a_j^\dagger - \eta a_j^\dagger a_i^\dagger\right)|n_1, n_2, \ldots\rangle = 0.$$

Since this must hold for every basis vector, this implies that

$$a_i^\dagger a_j^\dagger - \eta a_j^\dagger a_i^\dagger = [a_i^\dagger, a_j^\dagger]_\pm = 0.$$

Considering now $i = j$ we note that for bosonic systems $\left[a_i^\dagger, a_i^\dagger\right]_- = 0$, since identical operators commute, and for fermions $a_i^\dagger$ is nilpotent since the two-fold application of $a_i^\dagger$ to any state leads to its annihilation, which can be expressed as $\left[a_i^\dagger, a_i^\dagger\right]_+ = 0$. Therefore, we find that the creation operators obey the following canonical commutation relation $\forall i, j$

$$a_i^\dagger a_j^\dagger - \eta a_j^\dagger a_i^\dagger = [a_i^\dagger, a_j^\dagger]_\pm = 0. \tag{A.3}$$

The action of the hermitian conjugates $\left(a_i^\dagger\right)^\dagger = a_i$ of the creation operators is defined through

$$a_i|n_1,\ldots,n_i,\ldots\rangle = n_i^{1/2}\eta^{s_i}|n_1,\ldots,n_i-1,\ldots\rangle, \tag{A.4}$$

with s_i defined as above. This relation identifies a_i as an operator that annihilates particles. By taking the hermitian conjugate of (A.3) we obtain $\left[a_i, a_j\right] = 0$. In other words the operators $a_i^\dagger$ and a_i act in Fock space as $a_i^\dagger : \mathcal{F}_N \to \mathcal{F}_{N+1}$ and $a_i : \mathcal{F}_N \to \mathcal{F}_{N-1}$. From (A.1) and (A.4) we can infer that $[a_i, a_j^\dagger]_\pm = \mathbb{I}$ and therefore find that the operators $a_j, a_j^\dagger$ satisfy the following commutation relations

$$\left[a_i, a_j^\dagger\right] = \delta_{ij}, \quad \left[a_i, a_j\right] = 0, \quad \left[a_i^\dagger, a_j^\dagger\right] = 0, \tag{A.5}$$

where the minus sign applies in the case of bosonic systems and the plus sign in the case of fermionic systems.

A.3 Practical aspects

So far we have presented a compact and extremely efficient way to represent quantum many-particle systems, using annihilation and creation operators obeying simple commutation relations, which generate the full Fock space by acting on a single reference state, the vacuum. To turn these abstract definitions into a practical tool for performing computations we must put them into context with standard operations performed in quantum mechanics.

A.3.1 Change of basis

Suppose we wish to make a change of basis from one single particle basis $\{\lambda\}$ to another, say $\{\mu\}$. Using the completeness relation of the identity matrix $\mathbb{I} = \sum_\lambda |\lambda\rangle\langle\lambda|$ we can change basis via

$$|\mu\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\mu\rangle.$$

Following such a change of basis, we must specify transformation laws of the operators $\{a_\lambda\}$, where the operator $a_\lambda^\dagger$ creates a particle in state λ, in terms of the new basis to obtain $\{a_\mu\}$. Using the above relation, along with the definitions of the creation operators (see (A.2)), we find that the creation operator $a_\lambda^\dagger$ for a particle in state $|\lambda\rangle$ is related to the creation operator $a_\mu^\dagger$ for a particle in state $|\mu\rangle$ through

$$a_\mu^\dagger|0\rangle = |\mu\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\mu\rangle = \sum_\lambda \langle\lambda|\mu\rangle a_\lambda^\dagger|0\rangle$$

from which we infer

$$a_\mu^\dagger = \sum_\lambda \langle\lambda|\mu\rangle a_\lambda^\dagger. \tag{A.6}$$

A.3.2 Representation of one body and many particle operators

We first consider representations of standard operators of one-body systems in terms of the $\{a_\lambda\}$ and $\left\{a_\lambda^\dagger\right\}$. A convenient way to find the representation of a single particle operator $\hat{\mathcal{O}}_1$ acting in the N particle Hilbert space $\mathcal{F}_N$ in terms of a operators is to express $\hat{\mathcal{O}}_1$ in terms of a basis in which it is diagonal, then later transform to an arbitrary basis. For this purpose, we define the occupation number operator $\hat{n}_\lambda = a_\lambda^\dagger a_\lambda$ where

$$\hat{n}_\lambda \left(a_\lambda^\dagger\right)^n |0\rangle = n \left(a_\lambda^\dagger\right)^n |0\rangle$$

where n is the number of particles in state λ. Since $ABC-CAB=ABC+ACB-ACB-CAB$ the commutator of $\hat{n}_\lambda$ with $a^\dagger_{\lambda'}$ is

$$\begin{aligned}\left[\hat{n}_\lambda, a^\dagger_{\lambda'}\right] &= a^\dagger_\lambda \left\{a_\lambda, a^\dagger_{\lambda'}\right\} - \left\{a^\dagger_\lambda, a^\dagger_{\lambda'}\right\} a_\lambda \\ &= \delta\left(\lambda-\lambda'\right) a^\dagger_\lambda\end{aligned}$$

and so, from (A.2) we find that

$$\hat{n}_{\lambda_j}|n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle = n_{\lambda_j}|n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle,$$

that is $\hat{n}_{\lambda_j}$ simply counts the number of particles in state λ_j. Let us now consider a single particle operator $\hat{\mathcal{O}}_1$ that is diagonal in the basis $\{|\lambda\rangle\}$. Since such operators generally take the form $\hat{\mathcal{O}}_1 = \sum_{n=1}^{N} \hat{o}_n$, where $\hat{o}_n$ is an ordinary single particle operator acting on the n-th particle only, we have that

$$\hat{\mathcal{O}}_1 = \sum_i o_{\lambda_i} n_{\lambda_i} |\lambda_i\rangle\langle\lambda_i|$$

with $o_{\lambda_i} = \langle\lambda_i|\hat{o}|\lambda_i\rangle$ and $\sum_i n_{\lambda_i} = N$. Therefore one finds

$$\begin{aligned}\langle n'_{\lambda_1}, n'_{\lambda_2}, \ldots|\hat{\mathcal{O}}_1|n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle &= \sum_i o_{\lambda_i} n_{\lambda_i} \langle n'_{\lambda_1}, n'_{\lambda_2}, \ldots|n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle \\ &= \langle n'_{\lambda_1}, n'_{\lambda_2}, \ldots|\sum_i o_{\lambda_i} \hat{n}_{\lambda_i}|n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle.\end{aligned}$$

Since this equation holds for any set of states, we find that the second quantised representation of the operator $\hat{\mathcal{O}}_1$ is

$$\hat{\mathcal{O}}_1 = \sum_{\lambda=0}^{\infty} o_\lambda \hat{n}_\lambda = \sum_{\lambda=0}^{\infty} \langle\lambda|\hat{o}|\lambda\rangle a^\dagger_\lambda a_\lambda.$$

This equation tells us that a single particle operator engages a single particle at a time. In this diagonal representation, the number of particles in a state λ is counted and then multiplied by the corresponding eigenvalue of the one body operator. We can now use the transformation rule given in (A.6) to move from the diagonal representation to a general basis, and so we have that

$$\hat{\mathcal{O}}_1 = \sum_{\lambda,\mu} \langle\lambda|\hat{o}|\mu\rangle a^\dagger_\lambda a_\mu. \tag{A.7}$$

Furthermore, for two-particle operators, describing particle-particle interaction, it can be shown that

$$\hat{\mathcal{O}}_2 = \sum_{\lambda,\lambda',\mu,\mu'} \langle\lambda,\lambda'|\hat{\mathcal{O}}_2|\mu,\mu'\rangle a^\dagger_\lambda a^\dagger_{\lambda'} a_\mu a_{\mu'}. \tag{A.8}$$

The generalisation for many-particle operators of higher order is straightforward. Finally, we will give the explicit form of a Hamiltonian describing N particles interacting with each

other with respect to a delta- or contact-interaction and which are subject to an external potential $V_{ext}(\hat{x})$, given in position representation. More precisely the Hamiltonian consists of a kinetic term $\hat{T} = \hat{p}^2$ (where we set $\hbar = 2m = 1$), a potential term $\hat{V} = V_{ext}(\hat{x})$ and an interaction potential $\hat{W}$ describing contact interaction of strength c, which is modeled by a delta-distribution $c\delta(x - x')$ in position representation. Using the resolution of identity $\mathbb{I} = \int dx|x\rangle\langle x|$ in (A.7) and (A.8) we find that

$$\hat{H} = \int dx \psi^\dagger(x) \frac{\partial^2}{\partial x^2} \psi(x) + \int dx V_{ext}(x) \psi^\dagger(x)\psi(x) + c \int dx \psi^\dagger(x)\psi^\dagger(x)\psi(x)\psi(x) \quad \text{(A.9)}$$

where we defined the field creation and annihilation operators $\psi^\dagger(x) = \sum_i \phi_i^*(x) a_i^\dagger$ and $\psi(x) = \sum_i \phi_i(x) a_i$ respectively and $\phi_i(x) = \langle x|i\rangle$. Throughout this thesis we use Hamiltonians of this or similar form in position representation, where different expressions, for example in the case of finite range interactions, can be obtained in an analogous way.

Appendix B

Supplementary cMPS Calculations

B.1 Tangent vectors

Here we show how to calculate the tangent vector given by (4.7). Recall that a general tangent vector, which we will denote by $|\Phi(q,\{r_\alpha\};Q,\{R_\alpha\})\rangle$, is a linear combination of all $(N+1)D^2$ derivatives of the state with respect to each variational parameter, that is

$$|\Phi(q,\{r_\alpha\};Q,\{R_\alpha\})\rangle = \sum_{j,k=1}^{D^2} q_{jk}\partial[Q]_{jk}|\Psi(Q,\{R_\alpha\})\rangle + \sum_{j,k=D^2+1}^{2D^2}\sum_{\alpha=1}^{N}(r_\alpha)_{jk}\,\partial\,[R_\alpha]_{jk}\,|\Psi(Q,\{R_\alpha\})\rangle \tag{B.1}$$

where $\partial[Q]_{jk} = \partial/\partial[Q]_{jk}$, $\partial\,[R_\alpha]_{jk} = \partial/\partial\,[R_\alpha]_{jk}$ and $[Q]_{jk}$ and $[R_\alpha]_{jk}$ denote the jk-th entry of the matrices $Q(x)$ and $R_\alpha(x)$ respectively. To specify a general cMPS tangent vector we therefore must calculate

$$\begin{aligned}\partial[Q]_{jk}|\Psi(Q,\{R_\alpha\})\rangle &= \langle\omega_L|\partial[Q]_{jk}\left(U_{\ell/2,-\ell/2}\right)|\omega_R\rangle|\Omega\rangle \\ &= \langle\omega_L|\partial[Q]_{jk}\mathcal{P}\exp\left(\int_{-\ell/2}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(x)dx\right)|\omega_R\rangle|\Omega\rangle\end{aligned}$$

and

$$\begin{aligned}\partial[R_\alpha]_{jk}|\Psi(Q,\{R_\alpha\})\rangle &= \langle\omega_L|\partial\,[R_\alpha]_{jk}\left(U_{\ell/2,-\ell/2}\right)|\omega_R\rangle|\Omega\rangle \\ &= \langle\omega_L|\partial\,[R_\alpha]_{jk}\mathcal{P}\exp\left(\int_{-\ell/2}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(x)dx\right)|\omega_R\rangle|\Omega\rangle.\end{aligned}$$

with $\hat{H}_{\mathrm{cMPS}}(x) = Q(x)\otimes\mathbb{I} + \sum_{\alpha=1}^{N} R_\alpha(x)\otimes\psi_\alpha^\dagger(x)$. The path ordered exponential $\mathcal{P}\exp$ can be defined as the limit of the ordered product of infinitesimal exponentials

$$\mathcal{P}\exp\left(\int_{-\ell/2}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(x)dx\right) = \lim_{\epsilon\to 0}\left(e^{\int_{\ell/2-\epsilon}^{\ell/2}\hat{H}_{\mathrm{cMPS}}(x)dx}e^{\int_{\ell/2-2\epsilon}^{\ell/2-\epsilon}\hat{H}_{\mathrm{cMPS}}(x)dx}\ldots e^{\int_{-\ell/2}^{-\ell/2+\epsilon}\hat{H}_{\mathrm{cMPS}}(x)dx}\right).$$

Therefore, differentiating the path ordered exponential $U_{\ell/2,-\ell/2}$ with respect to $[Q]_{jk}$ is simply an application of the product rule. We find that

$$\begin{aligned}
&\partial [Q]_{jk} \mathcal{P} \exp\left(\int_{-\ell/2}^{\ell/2} \hat{H}_{\mathrm{cMPS}}(x) dx\right) \\
&= \lim_{\epsilon\to 0} \partial [Q]_{jk} \left(e^{\int_{\ell/2-\epsilon}^{\ell/2} \hat{H}_{\mathrm{cMPS}}(x)dx} e^{\int_{\ell/2-2\epsilon}^{\ell/2-\epsilon} \hat{H}_{\mathrm{cMPS}}(x)dx} \dots e^{\int_{-\ell/2}^{-\ell/2+\epsilon} \hat{H}_{\mathrm{cMPS}}(x)dx} \right) \\
&= \lim_{\epsilon\to 0} \sum_{i=0}^{L/\epsilon-1} \mathcal{P} \exp\left(\int_{\ell/2-i\epsilon}^{\ell/2} \hat{H}_{\mathrm{cMPS}}(x) dx\right) \partial [Q]_{jk} \exp\left(\int_{\ell/2-(i+1)\epsilon}^{\ell/2-i\epsilon} \hat{H}_{\mathrm{cMPS}}(x) dx\right) \\
&\qquad\qquad \times \mathcal{P} \exp\left(\int_{-\ell/2}^{\ell/2-(i+1)\epsilon} \hat{H}_{\mathrm{cMPS}}(x) dx\right).
\end{aligned}$$

In the limit $\epsilon \to 0$ we have that

$$\begin{aligned}
\partial [Q]_{jk} \exp\left(\int_{\ell/2-(i+1)\epsilon}^{\ell/2-i\epsilon} \hat{H}_{\mathrm{cMPS}}(x) dx\right) &= \partial [Q]_{jk} \exp\left(\epsilon \hat{H}_{\mathrm{cMPS}}(\ell/2 - i\epsilon)\right) \\
&= \partial [Q]_{jk} \left(\epsilon \hat{H}_{\mathrm{cMPS}}(\ell/2 - i\epsilon)\right) \exp\left(\epsilon \hat{H}_{\mathrm{cMPS}}(\ell/2 - i\epsilon)\right).
\end{aligned}$$

Since $\epsilon \partial [Q]_{jk} \hat{H}_{\mathrm{cMPS}}(\ell/2 - i\epsilon) = \epsilon \partial [Q]_{jk} (Q(\ell/2 - i\epsilon) \otimes \mathbb{I}) = \epsilon |j\rangle\langle k| \otimes \mathbb{I}$ where $|j\rangle\langle k|$ is simply a $D \times D$ matrix with a 1 in the jk-th entry, we find that

$$\begin{aligned}
&\partial [Q]_{jk} \mathcal{P} \exp\left(\int_{-\ell/2}^{\ell/2} \hat{H}_{\mathrm{cMPS}}(x) dx\right) \\
&= \lim_{\epsilon\to 0} \sum_{i=0}^{L/\epsilon-1} \epsilon \mathcal{P} \exp\left(\int_{\ell/2-i\epsilon}^{\ell/2} \hat{H}_{\mathrm{cMPS}}(x) dx\right) \left(|j\rangle\langle k| \otimes \mathbb{I}\right) \mathcal{P} \exp\left(\int_{-\ell/2}^{\ell/2-i\epsilon} \hat{H}_{\mathrm{cMPS}}(x) dx\right).
\end{aligned}$$

Taking the limit $\epsilon \to 0$ we can rewrite the summation as an integral to obtain

$$\begin{aligned}
&\partial [Q]_{jk} \mathcal{P} \exp\left(\int_{-\ell/2}^{\ell/2} \hat{H}_{\mathrm{cMPS}}(x) dx\right) \\
&= \int_{-\ell/2}^{\ell/2} ds \mathcal{P} \exp\left(\int_{s}^{\ell/2} \hat{H}_{\mathrm{cMPS}}(x) dx\right) \left(|j\rangle\langle k| \otimes \mathbb{I}\right) \mathcal{P} \exp\left(\int_{-\ell/2}^{s} \hat{H}_{\mathrm{cMPS}}(x) dx\right).
\end{aligned}$$

The same argument holds for differentiation of $U_{\ell/2,-\ell/2}$ with respect to $[R_\alpha]_{jk}$. A general tangent vector therefore takes the form of (4.7), namely

$$\begin{aligned}
|\Phi(q, \{r_\alpha\})\rangle &= \sum_{j,k=1}^{D^2} q_{jk} \langle \omega_L | \int_{-\ell/2}^{\ell/2} U_{\ell/2,x} \left(|j\rangle\langle k| \otimes \mathbb{I}\right) U_{x,-\ell/2} dx |\omega_R\rangle |\Omega\rangle \\
&\quad + \sum_{j,k=D^2+1}^{2D^2} \sum_{\alpha=1}^{N} [r_\alpha]_{jk} \langle \omega_L | \int_{-\ell/2}^{\ell/2} U_{\ell/2,x} \left(|j\rangle\langle k| \otimes \psi_\alpha^\dagger(x)\right) U_{x,-\ell/2} dx |\omega_R\rangle |\Omega\rangle \\
&= \int_{-\ell/2}^{\ell/2} \langle \omega_L | U_{\ell/2,x} \left(q(x) \otimes \mathbb{I} + \sum_{\alpha=1}^{N} r_\alpha(x) \otimes \psi_\alpha^\dagger(x)\right) U_{x,-\ell/2} |\omega_R\rangle |\Omega\rangle dx \qquad \text{(B.2)}
\end{aligned}$$

where we have defined $q(x)$ and $r_\alpha(x)$ as the matrices whose jk-th entries are the weightings q_{jk} and $(r_\alpha)_{jk}$ as given in equation (B.1).

B.2 Master Equation for $\rho(x)$

We now explicitly derive the master equation for $\rho(x)$ as given by (4.25). Recall that $\rho(x)$ is the reduced state of the auxiliary system after the unitary $U_{x,-\ell/2}$ has been applied to the composite system $|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|$, that is

$$\rho(x)=\mathrm{Tr}_{\mathcal{F}[-\ell/2,x])}\left(U_{x,-\ell/2}\left(|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|_{[-\ell/2,x]}\right)U^\dagger_{x,-\ell/2}\right) \tag{B.3}$$

where $\mathrm{Tr}_{\mathcal{F}[-\ell/2,x]}$ denotes the partial trace over the field from $-\ell/2$ to x. Similarly, we find that

$$\begin{aligned}\rho(x+\epsilon)&=\mathrm{Tr}_{\mathcal{F}[-\ell/2,x+\epsilon])}\left(U_{x+\epsilon,-\ell/2}\left(|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|_{[-\ell/2,x+\epsilon]}\right)U^\dagger_{x+\epsilon,-\ell/2}\right)\\&=\mathrm{Tr}_{\mathcal{F}[x,x+\epsilon])}\left(\mathrm{Tr}_{\mathcal{F}[-\ell/2,x])}\left(U_{x+\epsilon,x}U_{x,-\ell/2}\left(|\omega_R\rangle\langle\omega_R|\otimes|\Omega\rangle\langle\Omega|_{[-\ell/2,x+\epsilon]}\right)U^\dagger_{x,-\ell/2}U^\dagger_{x+\epsilon,x}\right)\right)\\&=\mathrm{Tr}_{\mathcal{F}[x,x+\epsilon])}\left(U_{x+\epsilon,x}\left(\rho(x)\otimes|\Omega\rangle\langle\Omega|_{[x,x+\epsilon]}\right)U^\dagger_{x+\epsilon,x}\right).\end{aligned} \tag{B.4}$$

We can expand $U_{x+\epsilon,x}$ as a Taylor series as follows

$$\begin{aligned}U_{x+\epsilon,x}&\simeq\mathcal{P}\exp\left(\int_x^{x+\epsilon}ds\;Q(s)\otimes\mathbb{I}+\sum_{\alpha=1}^N R_\alpha(s)\otimes\psi^\dagger_\alpha(s)+O(\epsilon^2)\right)\\&=\mathbb{I}+\epsilon\left(Q(x+\epsilon)\otimes\mathbb{I}+\sum_{\alpha=1}^N R_\alpha(x+\epsilon)\otimes\psi^\dagger_\alpha(x+\epsilon)\right)\\&\quad+\frac{\epsilon^2}{2}\left(Q(x+\epsilon)\otimes\mathbb{I}+\sum_{\alpha=1}^N R_\alpha(x+\epsilon)\otimes\psi^\dagger_\alpha(x+\epsilon)\right)^2+\ldots\end{aligned}$$

where in the first line we have removed the need of the path ordering since this infinitesimal section is assumed to be ordered correctly, i.e. with the arguments increasing from left to right. It is now useful to recall that a continuous matrix product state can be constructed by taking the continuum limit of a subclass of matrix product states (see section (4.2)). We now revert this method of construction and discretise our system: we approximate the continuum by a lattice $\mathcal{L}$ with lattice spacing ϵ and $n=L/\epsilon$ sites, taking $\epsilon\to 0$. On every site of the lattice j we can annihilate and create particles by acting with the annihilation and creation operators a_j and $a_j^\dagger$ respectively. We identify $\psi(x)=\psi(j\epsilon)=\frac{a_j}{\sqrt{\epsilon}}$ and $|\Omega\rangle_{[x,x+\epsilon]}=|0\rangle_{j+1}$, giving

$$U_{x+\epsilon,x}=\mathbb{I}+\epsilon\left(Q\otimes\mathbb{I}+\sum_{\alpha=1}^N R_\alpha\otimes\frac{(a_\alpha)^\dagger_{j+1}}{\sqrt{\epsilon}}\right)+\frac{\epsilon^2}{2}\left(Q\otimes\mathbb{I}+\sum_{\alpha=1}^N R_\alpha\otimes\frac{(a_\alpha)^\dagger_{j+1}}{\sqrt{\epsilon}}\right)^2+\ldots$$

Substitution into (B.4) gives

$$
\begin{aligned}
&\rho(j\epsilon+\epsilon)\\
&=\mathrm{Tr}_{j+1}\left[\left(\mathbb{I}+\epsilon\left(Q\otimes\mathbb{I}+\sum_{\alpha=1}^{N}R_\alpha\otimes\frac{(a_\alpha)_{j+1}^\dagger}{\sqrt{\epsilon}}\right)+\frac{\epsilon^2}{2}\left(Q\otimes\mathbb{I}+\sum_{\alpha=1}^{N}R_\alpha\otimes\frac{(a_\alpha)j+1^\dagger}{\sqrt{\epsilon}}\right)^2+\ldots\right)\right.\\
&\qquad\times\rho(j\epsilon)\otimes|0\rangle\langle 0|_{j+1}\\
&\qquad\left.\times\left(\mathbb{I}+\epsilon\left(Q\otimes\mathbb{I}+\sum_{\alpha=1}^{N}R_\alpha\otimes\frac{(a_\alpha)_{j+1}^\dagger}{\sqrt{\epsilon}}\right)+\frac{\epsilon^2}{2}\left(Q\otimes\mathbb{I}+\sum_{\alpha=1}^{N}R_\alpha\otimes\frac{(a_\alpha)_{j+1}^\dagger}{\sqrt{\epsilon}}\right)^2+\ldots\right)^\dagger\right].
\end{aligned}
$$

We now collect and evaluate the terms of order $\mathcal{O}(1)$, $\mathcal{O}(\sqrt{\epsilon})$ and $\mathcal{O}(\epsilon\sqrt{\epsilon})$ within the trace. To $\mathcal{O}(1)$ we have

$$\mathrm{Tr}_{j+1}\left[\rho(j\epsilon)\otimes|0\rangle\langle 0|_{j+1}\right]=\rho(j\epsilon).$$

To $\mathcal{O}(\sqrt{\epsilon})$ we apply the cyclic rule of trace to annihilate the vacuum state, that is we use that $(a_\alpha)_{j+1}|0\rangle_{j+1}=0$, to obtain

$$\mathrm{Tr}_{j+1}\left[\rho(j\epsilon)\sum_{\alpha=1}^{N}R_\alpha^\dagger\otimes|0\rangle\langle 0|_{j+1}(a_\alpha)_{j+1}+R_\alpha\rho(j\epsilon)\otimes(a_\alpha)_{j+1}^\dagger|0\rangle\langle 0|_{j+1}\right]=0.$$

To $\mathcal{O}(\epsilon)$ we collect more terms, namely

$$
\begin{aligned}
&\mathrm{Tr}_{j+1}\left[\sum_{\alpha=1}^{N}\rho(j\epsilon)Q^\dagger\otimes|0\rangle\langle 0|+Q\rho(j\epsilon)\otimes|0\rangle\langle 0|+R_\alpha\rho(j\epsilon)R_\alpha^\dagger\otimes(a_\alpha)_{j+1}^\dagger|0\rangle\langle 0|(a_\alpha)_{j+1}\right]\\
&+\mathrm{Tr}_{j+1}\left[\sum_{\alpha=1}^{N}R_\alpha^2\rho(j\epsilon)\otimes(a_\alpha)_{j+1}^\dagger(a_\alpha)_{j+1}^\dagger|0\rangle\langle 0|_{j+1}+\rho(j\epsilon)R_\alpha^\dagger R_\alpha^\dagger\otimes|0\rangle\langle 0|_{j+1}(a_\alpha)_{j+1}(a_\alpha)_{j+1}\right]\\
&=\rho(j\epsilon)Q^\dagger+Q\rho(j\epsilon)+\sum_{\alpha=1}^{N}R_\alpha\rho(j\epsilon)R_\alpha^\dagger.
\end{aligned}
$$

where the second term does not contribute due to the annihilation of the vacuum state. Combining these terms and excluding terms of higher order (since we take the limit $\epsilon\to 0$), we find that

$$\rho(j\epsilon+\epsilon)=\rho(j\epsilon)+\epsilon\left(\rho(j\epsilon)Q^\dagger+Q\rho(j\epsilon)+R\rho(j\epsilon)R^\dagger\right)+\mathcal{O}(\epsilon\sqrt{\epsilon}).$$

To obtain the Lindblad equation given in (4.25) we undo the discretisation and let $\epsilon\to 0$ to give

$$\frac{d\rho(x)}{dx}=\left(\rho(x)Q^\dagger+Q\rho(x)+R\rho(x)R^\dagger\right).$$

Appendix C

Gram Matrix Calculations

Here we present more information on how to completely specify the gram matrix as given by equation (6.46) in section 6.2.4. The techniques used are almost identical to that given in the main body of the thesis, but the approach for each block differs slightly dependent on whether multiple, single or no field operators are present. We study the jk-th entry of the gram matrix, as given by

$$G_{jk} = \langle \partial_{\bar{j}} \Psi | \partial_k \Psi \rangle = \mathrm{Tr}\left[|\partial_k \Psi\rangle\langle \partial_{\bar{j}} \Psi| \right]$$

where $|\Psi\rangle$ is the multi-component cMPS $|\Psi\rangle = |\Psi(Q, R_\alpha, R_\beta)\rangle$ and

$$|\partial_j \Psi\rangle = \begin{cases} \int ds \langle \omega_L | U_{\ell/2,s} (q^j \otimes \mathbb{I} \otimes \mathbb{I}) U_{s,-\ell/2} | \omega_R \rangle |\Omega\rangle_{\alpha,\beta} & \text{if } 1 \leq j \leq D^2; \\ \int ds \langle \omega_L | U_{\ell/2,s} (r^j_\alpha \otimes \psi^\dagger_\alpha(s) \otimes \mathbb{I}) U_{s,-\ell/2} | \omega_R \rangle |\Omega\rangle_{\alpha,\beta} & \text{if } D^2+1 \leq j \leq 2D^2; \\ \int ds \langle \omega_L | U_{\ell/2,s} (r^j_\beta \otimes \mathbb{I} \otimes \psi^\dagger_\beta(s)) U_{s,-\ell/2} | \omega_R \rangle |\Omega\rangle_{\alpha,\beta} & \text{if } 2D^2+1 \leq j \leq 3D^2 \end{cases}$$

with $q_j = \partial_j Q$, $r^j_\alpha = \partial_j R_\alpha$ and $r^j_\beta = \partial_j R_\beta$. To specify the matrix in full there are 9 different cases dependent on where j, k are in $\left[1, 3D^2\right]$. Since the gram matrix is hermitian we need only consider the block entries on the main diagonal and either the remaining upper or lower triangle. We already gave a detailed description on how to calculate block five in Chapter 6. The calculations for block nine are entirely identical except for the presence of r^j_β matrices instead of r^j_α. We therefore first present some guidelines for calculating block one. Following this we consider block two. The procedure for block three is identical to that of block two, with the exception that the matrices r^j_β appear instead of r^j_α, and so we do not present the calculations for this case. Finally, we review block six. In all following calculations we use the shortened notation $\omega_R \equiv |\omega_R\rangle\langle\omega_R|$, $\Omega \equiv |\Omega\rangle\langle\Omega|_{a,b}$ and $q^k \equiv q^k \otimes \mathbb{I} \otimes \mathbb{I}$ etc. to keep expressions succinct.

C.1 Block 1 of G

This is the most straightforward of the 9 blocks, due to the absence of both field operators $\hat{\psi}_\alpha(x)$ and $\hat{\psi}_\beta(x)$. We have $1 \leq j \leq D^2, 1 \leq k \leq D^2$ and so must evaluate

$$\begin{aligned}&\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right]\\&=\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2} ds\,ds'\,\mathrm{Tr}\Big[\langle\omega_L|U_{\ell/2,s}q^k U_{s,-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}(q^j)^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\Big].\end{aligned}$$

The first step will always be to break up the integral over s and s' into two integrals via

$$\int_{-\ell/2}^{\ell/2} ds\int_{-\ell/2}^{\ell/2} ds' = \int_{-\ell/2}^{\ell/2} ds\int_{-\ell/2}^{s} ds' + \int_{-\ell/2}^{\ell/2} ds'\int_{-\ell/2}^{s'} ds$$

and consider each term separately. For $s < s'$ we have that

$$\begin{aligned}&\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right]\\&=\int_{-\ell/2}^{\ell/2} ds'\int_{-\ell/2}^{s'} ds\,\mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s}q^k U_{s,-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{s,-\ell/2}U^\dagger_{s',s}(q^j)^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\right].\end{aligned}$$

This expression has the same form as (6.28) in section 6.2.3, and we proceed accordingly. We use results from Chapter 4 regarding the auxiliary system associated to the cMPS representation in which the matrices Q, R_α and R_β act. We find that

$$\begin{aligned}&\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right]\\&=\int_{-\ell/2}^{\ell/2} ds'\int_{-\ell/2}^{s'} ds\,\mathrm{Tr}_{s,\ell/2}\left[\langle\omega_L|U_{\ell/2,s}(q^k\rho\otimes\Omega_{s,\ell/2})U^\dagger_{s',s}(q^j)^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\right]\end{aligned}$$

where ρ is the right density matrix defined in (4.23). We then trace over the field in $[s, s']$ to obtain

$$\mathrm{Tr}_{s',\ell/2}\left[\int_{-\ell/2}^{\ell/2} ds'\int_{-\ell/2}^{s'} ds\,\langle\omega_L|U_{\ell/2,s'}\tau(s)\otimes\Omega_{s',\ell/2}(q^j)^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\right]$$

where, similarly to before (see section (6.2.3)), $|\tau(s)\rangle = e^{(s'-s)M}|q^k\rho\rangle$. We then rewrite the equation in terms of a trace over the auxiliary system and fully perform the trace over the field. Inserting the full expression for $|\tau(s)\rangle$ and solving the integral identical to that in section (6.2.3), namely $\int_{-\ell/2}^{\ell/2} ds'\int_{-\ell/2}^{s'} e^{(s'-s)M}ds = L\left(\frac{L}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)$ we find that

$$\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right] = L\langle q^j|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|q^k\rho\rangle.$$

We use an identical method to evaluate the integral for $s > s'$. We obtain a contribution of

$$L\langle(q^k)^\dagger|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|\rho(q^j)^\dagger\rangle$$

such that the total block entry of the gram matrix in this case is given by

$$\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right] = L\left[\langle q^j|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|q^k\rho\rangle + \langle(q^k)^\dagger|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|\rho(q^j)^\dagger\rangle\right].$$

We note that, as in the main text, the overall factor L will not lead to a divergence in the limit $\ell \to \infty$ when using the expression in the TDVP equation (6.16). In addition, the diverging terms in the above expression will be removed when applying the left gauge fixing requirement (6.47), as explained in Chapter 6.

C.2 Block 2 of G

We now evaluate the block matrix entry of G obtained when $1 \leq j \leq D^2$ and $D^2+1 \leq k \leq 2D^2$, namely

$$\begin{aligned}&\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right]\\ &= \int_{-\ell/2}^{\ell/2} ds \int_{-\ell/2}^{\ell/2} ds' \mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s}(r_\alpha^k \otimes \hat{\psi}_\alpha^\dagger(s)\otimes\mathbb{I})U_{s,-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}(q^j)^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\right]\end{aligned}$$

We break the integral up into pieces for $s \leq s'$ and $s > s'$ and first consider $s \leq s'$. Unlike the previous calculation, we now have an expression where the field operator $\hat{\psi}_\alpha^\dagger(s)$ is present. We eliminate the operator using the same method as in section (6.2.3), namely via the insertion and subsequent evaluation of commutators. We replace the product

$$\begin{aligned}&U^\dagger_{s',-\ell/2}(q^j)^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(\mathbb{I}\otimes\hat{\psi}_\alpha^\dagger(s)\otimes\mathbb{I})\\ &\to \left[U^\dagger_{s',-\ell/2}(q^j)^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}\ ,\ (\mathbb{I}\otimes\hat{\psi}_\alpha^\dagger(s)\otimes\mathbb{I})\right]\\ &= U^\dagger_{s,-\ell/2}R^\dagger_\alpha U^\dagger_{s',s}(q^j)^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}\end{aligned} \tag{C.1}$$

where in the last line we have used the relation given in (4.16). We therefore evaluate

$$\int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} ds \mathrm{Tr}\left[\langle\omega_L|U_{\ell/2,s}r_\alpha^k U_{s,-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{s,-\ell/2}R^\dagger_\alpha U^\dagger_{s',s}(q^j)^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\right]$$

Now that the field operator has been removed we have an expression of the form (6.28) in section 6.2.3, and we proceed as before, tracing over the field from $[-\ell/2, s]$ followed by $[s, s']$. We then have that

$$\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right] = \int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} ds \mathrm{Tr}_{s',\ell/2}\left[\langle\omega_L|U_{\ell/2,s'}(\tau(s')\otimes\Omega_{s',\ell/2})(q^j)^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\right]$$

where $|\tau(s')\rangle = e^{(s'-s)M}|r_\alpha^k\rho R_\alpha^\dagger\rangle$. We then rewrite the equation in terms of a trace over the auxiliary system and fully perform the trace over the field. Inserting the full expression for $|\tau(s')\rangle$ and solving the integral identical to that in section (6.2.3), namely

$\int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} e^{(s'-s)M} ds = L\left(\frac{L}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)$ we find that

$$\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right] = L\langle q^j|\left(\frac{L}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|r_\alpha^k \rho R_\alpha^\dagger\rangle$$

We use a similar method to evaluate the integral for $s' < s$, the difference arising in the simplification of the commutator (C.1). We obtain a contribution of

$$\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right] = L\langle(r_\alpha^k)^\dagger R_\alpha|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|\rho(q^j)^\dagger\rangle.$$

Combining both integrals for $s \leq s'$ and $s' < s$ we find that the block entry of the gram matrix in this case is given by

$$\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right] = L\left[\langle q^j|\left(\frac{L}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|r_\alpha^k\rho R_\alpha^\dagger\rangle + \langle(r_\alpha^k)^\dagger R_\alpha|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|\rho(q^j)^\dagger\rangle\right].$$

C.3 Block 6 of G

We now evaluate the block matrix entry of G obtained when $D^2+1 \leq j \leq D^2$ and $2D^2+1 \leq k \leq 3D^2$, namely

$$\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right] = \int_{-\ell/2}^{\ell/2} ds \int_{-\ell/2}^{\ell/2} ds' \mathrm{Tr}\Big[\langle\omega_L|U_{\ell/2,s}(r_\beta^k\otimes\mathbb{I}\otimes\hat{\psi}_\beta^\dagger(s))U_{s,-\ell/2}(\omega_R\otimes\Omega) \times U_{s',-\ell/2}^\dagger(r_\alpha^j\otimes\hat{\psi}_\alpha^\dagger(s')\otimes\mathbb{I})^\dagger U_{\ell/2,s'}^\dagger|\omega_L\rangle\Big].$$

We break the integral up into pieces for $s \leq s'$ and $s > s'$ and first consider $s \leq s'$. The first step is to remove the field operators $\hat{\psi}_\beta^\dagger(s)$ and $\hat{\psi}_\alpha^\dagger(s')$ using the same method as in section 6.2.3, that is we replace the product

$$\begin{aligned}
&U_{s',-\ell/2}^\dagger(r_\alpha^j\otimes\hat{\psi}_\alpha^\dagger(s')\otimes\mathbb{I})^\dagger U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(\mathbb{I}\otimes\mathbb{I}\otimes\hat{\psi}_\beta^\dagger(s)) \\
&\to\left[U_{s',-\ell/2}^\dagger(r_\alpha^j\otimes\hat{\psi}_\alpha^\dagger(s')\otimes\mathbb{I})^\dagger U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}\ ,\ (\mathbb{I}\otimes\mathbb{I}\otimes\hat{\psi}_\beta^\dagger(s))\right] \\
&= U_{s,-\ell/2}^\dagger R_\beta^\dagger U_{s',s}^\dagger(r_\alpha^j\otimes\hat{\psi}_\alpha^\dagger(s')\otimes\mathbb{I})^\dagger U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}
\end{aligned} \tag{C.2}$$

where in the last line we have used the relation given in (4.16). To remove the second field operator we then make the replacement

$$\begin{aligned}
&(\mathbb{I}\otimes\hat{\psi}_\alpha(s')\otimes\mathbb{I})U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(r_\beta^k\otimes\mathbb{I}\otimes\mathbb{I})U_{s,-\ell/2} \\
&\to\left[(\mathbb{I}\otimes\hat{\psi}_\alpha(s')\otimes\mathbb{I})\ ,\ U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}(r_\beta^k\otimes\mathbb{I}\otimes\mathbb{I})U_{s,-\ell/2}\right] \\
&= U_{\ell/2,s'}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s'}R_\alpha U_{s',s}(r_\beta^k\otimes\mathbb{I}\otimes\mathbb{I})U_{s,-\ell/2}
\end{aligned} \tag{C.3}$$

such that we evaluate

$$\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right] = \int_{-\ell/2}^{\ell/2} ds \int_{-\ell/2}^{\ell/2} ds' \mathrm{Tr}\Big[\langle\omega_L|U_{\ell/2,s'}R_\alpha U_{s',s} r_\beta^k U_{s,-\ell/2}(\omega_R\otimes\Omega) \\ \times U^\dagger_{s,-\ell/2} R^\dagger_\beta U^\dagger_{s',s}(r^j_\alpha)^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\Big].$$

Now that the field operator has been removed we have an expression of the form (6.28) in section 6.2.3, and we proceed as before, tracing over the field from $[-\ell/2, s]$ followed by $[s, s']$. We then have that

$$\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right] = \int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} ds \mathrm{Tr}_{s',\ell/2}\left[\langle\omega_L|U_{\ell/2,s'}R_\alpha(\tau(s')\otimes\Omega_{s',\ell/2})(r^j_\alpha)^\dagger U^\dagger_{\ell/2,s'}|\omega_L\rangle\right]$$

where $|\tau(s')\rangle = e^{(s'-s)M}|r^k_\beta \rho R^\dagger_\beta\rangle$. We then rewrite the equation in terms of a trace over the auxiliary system and fully perform the trace over the field. Inserting the full expression for $|\tau(s')\rangle$ and solving the integral identical to that in section (6.2.3), namely $\int_{-\ell/2}^{\ell/2} ds' \int_{-\ell/2}^{s'} e^{(s'-s)M} ds = L\left(\frac{L}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)$ we find that

$$\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right] = L\langle R^\dagger_\alpha r^j_\alpha|\left(\frac{L}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|r^k_\beta\rho R^\dagger_\beta\rangle.$$

We use a similar method to evaluate the integral for $s' < s$, the difference arising in the simplification of the commutator (C.2), and following this the commutator (C.3). We obtain a contribution of

$$\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right] = L\langle(r^k_\beta)^\dagger R_\beta|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|R_\alpha\rho(r^j_\alpha)^\dagger\rangle.$$

Combining both integrals for $s \le s'$ and $s' < s$ we find that the block entry of the gram matrix in this case is given by

$$\begin{aligned}&\mathrm{Tr}\left[|\partial_k\Psi\rangle\langle\partial_{\bar{j}}\Psi|\right] \\ =&L\left[\langle R^\dagger_\alpha r^j_\alpha|\left(\frac{L}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|r^k_\beta\rho R^\dagger_\beta\rangle + \langle(r^k_\beta)^\dagger R_\beta|\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M}\right)|R_\alpha\rho(r^j_\alpha)^\dagger\rangle\right].\end{aligned}$$

As mentioned in the beginning of the section, the calculations for other blocks are analogous to the ones presented here, and we do not detail them here. The complete expression for the gram matrix can be found in (6.46).

Appendix D

Projection Matrix Calculations

Here we present more information on how to completely specify the projection matrix as given by (6.78) in Section 6.2.9. We study the j-th row element of the projection matrix, as given by

$$L_j = \langle \partial_{\bar{j}} \Psi | \hat{H} | \Psi \rangle = \langle \partial_{\bar{j}} \Psi | \left(\hat{T} + \hat{W} + \hat{V} \right) | \Psi \rangle = \mathrm{Tr} \left[\left(\hat{T} + \hat{W} + \hat{V} \right) | \Psi \rangle \langle \partial_{\bar{j}} \Psi | \right]$$

where $|\Psi\rangle$ is the multi-component cMPS $|\Psi\rangle = |\Psi(Q, R_\alpha, R_\beta)\rangle$, the Hamiltonian $\hat{H} = \left(\hat{T} + \hat{W} + \hat{V} \right)$ is given by

$$\begin{aligned}
\hat{T} &= \int_{-\ell/2}^{\ell/2} dx \left(\frac{d\psi_\alpha^\dagger(x)}{dx} \frac{d\psi_\alpha(x)}{dx} \otimes \mathbb{I} \right) \\
\hat{W} &= \int_{-\ell/2}^{\ell/2} dx \left(c \psi_\alpha^\dagger(x) \psi_\alpha^\dagger(x) \psi_\alpha(x) \psi_\alpha(x) \otimes \mathbb{I} \right) \\
\hat{V} &= \int_{-\ell/2}^{\ell/2} dx 1\sqrt{2} \left(\psi_\alpha^\dagger(x) \psi_\alpha(x) \otimes \left(\hat{\psi}_\beta(x) + \psi_\beta^\dagger(x) \right) \right)
\end{aligned}$$

and

$$|\partial_j \Psi\rangle = \begin{cases}
\int ds \langle \omega_L | U_{\ell/2,s} (q^j \otimes \mathbb{I} \otimes \mathbb{I}) U_{s,-\ell/2} | \omega_R \rangle | \Omega \rangle_{\alpha,\beta} & \text{if } 1 \le j \le D^2; \\
\int ds \langle \omega_L | U_{\ell/2,s} (r_\alpha^j \otimes \psi_\alpha^\dagger(s) \otimes \mathbb{I}) U_{s,-\ell/2} | \omega_R \rangle | \Omega \rangle_{\alpha,\beta} & \text{if } D^2 + 1 \le j \le 2D^2; \\
\int ds \langle \omega_L | U_{\ell/2,s} (r_\beta^j \otimes \mathbb{I} \otimes \psi_\beta^\dagger(s)) U_{s,-\ell/2} | \omega_R \rangle | \Omega \rangle_{\alpha,\beta} & \text{if } 2D^2 + 1 \le j \le 3D^2
\end{cases}$$

with $q_j = \partial_j Q$, $r_\alpha^j = \partial_j R_\alpha$ and $r_\beta^j = \partial_j R_\beta$. In the main body of the thesis we presented the derivations for the projection of the density term $\hat{V}$. Here we present the derivations for the projection of the interaction and kinetic energy terms $\hat{W}$ and $\hat{T}$. The techniques used are almost identical to that given in the main body of the thesis, but the approach differs slightly dependent on whether multiple, single or derivatives of field operators are present. As before, in all following calculations we use the shortened notation $\omega_R \equiv |\omega_R\rangle\langle\omega_R|$, $\Omega \equiv |\Omega\rangle\langle\Omega|_{a,b}$ and $q^k \equiv q^k \otimes \mathbb{I} \otimes \mathbb{I}$ etc. to keep expressions succinct.

D.1 Projection of the interaction energy term

The projection of the interaction term of the Hamiltonian $\hat{W}$ requires the evaluation of

$$\langle\partial_{\bar{j}}\Psi(\overline{z})|\hat{W}|\Psi(z)\rangle = c\int_{-\ell/2}^{\ell/2} ds\ \langle\partial_{\bar{j}}\Psi|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\psi_\alpha^\dagger(s)\psi_\alpha(s)\psi_\alpha(s)\otimes\mathbb{I}\right)|\Psi\rangle$$

for the different cases $1\le j\le D^2$, $D^2+1\le j\le 2D^2$, and $2D^2+1\le j\le 3D^2$. As in the main body of the thesis we will detail only one of these cases, a pattern for calculating the different cases is soon established. We choose $D^2+1\le j\le 2D^2$, since this case has the additional complexity of a field operator of the same type appearing in the derivative of the tangent vector

$$|\partial_j\Psi\rangle = \int_{-\ell/2}^{\ell/2} ds\langle\omega_L|U_{\ell/2,s}(r_\alpha^j\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I})U_{s,-\ell/2}|\omega_R\rangle|\Omega\rangle_{\alpha,\beta},\qquad D^2+1\le j\le 2D^2.$$

Derivations for $\mathbf{D^2+1\le j\le 2D^2}$

We evaluate

$$\begin{aligned}
&\langle\partial_{\bar{j}}\Psi(\overline{z})|\hat{W}|\Psi(z)\rangle = \mathrm{Tr}\left[\hat{W}|\Psi(z)\rangle\langle\partial_{\bar{j}}\Psi(\overline{z})|\right]\\
&=\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2} ds\,ds'\mathrm{Tr}\Big[\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\psi_\alpha^\dagger(s)\psi_\alpha(s)\psi_\alpha(s)\otimes\mathbb{I}\right)U_{\ell/2,-\ell/2}\\
&\qquad\qquad\times(\omega_R\otimes\Omega)U_{s',-\ell/2}^\dagger\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U_{\ell/2,s'}^\dagger|\omega_L\rangle\Big].
\end{aligned}$$

To eliminate the field operators $\hat{\psi}_\alpha(s)$ we use that $\hat{\psi}_\alpha(s)|\Omega\rangle_\alpha = 0$ to replace the product

$$\left(\mathbb{I}\otimes\psi_\alpha(s)\psi_\alpha(s)\otimes\mathbb{I}\right)U_{\ell/2,-\ell/2}(\omega_R\otimes\Omega) = \left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}\right)\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}\right)U_{\ell/2,-\ell/2}(\omega_R\otimes\Omega)$$

with the commutator

$$\begin{aligned}
&\Big[\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}\right)\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}\right)\ ,\ U_{\ell/2,-\ell/2}\Big](\omega_R\otimes\Omega)\\
&=\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}\right)\Big[\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}\right)\ ,\ U_{\ell/2,-\ell/2}\Big](\omega_R\otimes\Omega)\\
&=\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}\right)U_{\ell/2,s}(R_\alpha\otimes\mathbb{I}\otimes\mathbb{I})U_{s,-\ell/2}(\omega_R\otimes\Omega).
\end{aligned}$$

where in the last line we have used the relation given in (4.16). We substitute this expression back into the main equation and repeat the procedure this time replacing

$$\begin{aligned}
&\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}\right)U_{\ell/2,s}(R_\alpha\otimes\mathbb{I}\otimes\mathbb{I})U_{s,-\ell/2}(\omega_R\otimes\Omega)\\
\to&\Big[\left(\mathbb{I}\otimes\psi_\alpha(s)\otimes\mathbb{I}\right)\ ,\ U_{\ell/2,s}(R_\alpha\otimes\mathbb{I}\otimes\mathbb{I})U_{s,-\ell/2}\Big](\omega_R\otimes\Omega)\\
=&2U_{\ell/2,s}(R_\alpha^2\otimes\mathbb{I}\otimes\mathbb{I})U_{s,-\ell/2}(\omega_R\otimes\Omega).
\end{aligned}$$

We therefore evaluate

$$\begin{aligned}
&\mathrm{Tr}\left[\hat{W}|\Psi(z)\rangle\langle\partial_{\bar{j}}\Psi(\bar{z})|\right] \\
&=2\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2} ds\, ds'\mathrm{Tr}\Big[\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)U_{\ell/2,s}(R_\alpha^2\otimes\mathbb{I}\otimes\mathbb{I})U_{s,-\ell/2} \\
&\qquad\qquad\times(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\Big].
\end{aligned}$$

To eliminate the remaining field operators we use that $\langle\Omega|_\alpha\psi_\alpha^\dagger(s)=0$ and apply the same method. We replace the product

$$(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)$$

with the commutator

$$\begin{aligned}
&(\omega_R\otimes\Omega)\Big[U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\,,\,\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\Big] \\
=&(\omega_R\otimes\Omega)\Big[U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\,,\,\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\Big]\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)
\end{aligned}$$

which can be expanded as follows

$$\begin{aligned}
&(\omega_R\otimes\Omega)\Big[U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\,,\,\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\Big]\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right) \\
&=(\omega_R\otimes\Omega)\Big[U^\dagger_{s',-\ell/2}\,,\,\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\Big]\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right) \\
&+(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)\Big[U^\dagger_{\ell/2,s'}\,,\,\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\Big]|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right) \\
&+(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}\Big[\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)\,,\,\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\Big]U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right).
\end{aligned}$$

Using (4.16) this simplifies to

$$\Theta(s-s')(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{s,s'}R_\alpha^\dagger U^\dagger_{s,\ell/2}|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right) \tag{D.1}$$

$$+\Theta(s'-s)(\omega_R\otimes\Omega)U^\dagger_{s,-\ell/2}R_\alpha^\dagger U^\dagger_{s',s}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right) \tag{D.2}$$

$$+(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\delta(s'-s)\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right). \tag{D.3}$$

where Θ is the heaviside step function as defined in (6.56). It is then convenient to consider substituting each of these expressions back into the main calculation separately. For (D.1) we are required to evaluate

$$\begin{aligned}
2\int_{-\ell/2}^{\ell/2}ds'\int_{-\ell/2}^{s'}ds\,\mathrm{Tr}\Big[&\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)U_{\ell/2,s}(R_\alpha^2\otimes\mathbb{I}\otimes\mathbb{I})U_{s,-\ell/2}(\omega_R\otimes\Omega) \\
&\times U^\dagger_{s',-\ell/2}\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U^\dagger_{s,s'}R_\alpha^\dagger U^\dagger_{s,\ell/2}|\omega_L\rangle\Big].
\end{aligned}$$

We eliminate the field operator $\psi_\alpha^\dagger(s)$ by making the replacement

$$\begin{aligned}
&(\omega_R\otimes\Omega)U_{s',-\ell/2}^\dagger\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U_{s,s'}^\dagger R_\alpha^\dagger U_{s,\ell/2}^\dagger|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\\
\rightarrow&(\omega_R\otimes\Omega)\Big[U_{s',-\ell/2}^\dagger\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U_{s,s'}^\dagger R_\alpha^\dagger U_{s,\ell/2}^\dagger|\omega_L\rangle\langle\omega_L|\ ,\ \left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)\Big]\\
=&2(\omega_R\otimes\Omega)U_{s',-\ell/2}^\dagger\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U_{s,s'}^\dagger(R_\alpha^2)^\dagger U_{s,\ell/2}^\dagger|\omega_L\rangle\langle\omega_L|
\end{aligned}$$

such that we evaluate

$$\begin{aligned}
4\int_{-\ell/2}^{\ell/2}ds'\int_{-\ell/2}^{s'}ds\,\mathrm{Tr}\Big[&\langle\omega_L|U_{\ell/2,s}R_\alpha^2U_{s,-\ell/2}(\omega_R\otimes\Omega)U_{s',-\ell/2}^\dagger\\
&\times\left(r_\alpha^{j\dagger}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U_{s,s'}^\dagger(R_\alpha^2)^\dagger U_{s,\ell/2}^\dagger|\omega_L\rangle\Big].
\end{aligned}$$

The final step is to replace

$$\begin{aligned}
&\left(\mathbb{I}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)U_{s,s'}^\dagger(R_\alpha^2)^\dagger U_{s,\ell/2}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}R_\alpha^2U_{s,-\ell/2}(\omega_R\otimes\Omega)\\
\rightarrow&\Big[\left(\mathbb{I}\otimes\psi_\alpha(s')\otimes\mathbb{I}\right)\ ,\ U_{s,s'}^\dagger(R_\alpha^2)^\dagger U_{s,\ell/2}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}R_\alpha^2U_{s,-\ell/2}\Big](\omega_R\otimes\Omega)\\
=&U_{s,s'}^\dagger(R_\alpha^2)^\dagger U_{s,\ell/2}^\dagger|\omega_L\rangle\langle\omega_L|U_{\ell/2,s}R_\alpha^2U_{s,s'}R_\alpha U_{s',-\ell/2}(\omega_R\otimes\Omega)
\end{aligned}$$

such that the final, field operator free expression is given by

$$\begin{aligned}
4\int_{-\ell/2}^{\ell/2}ds'\int_{-\ell/2}^{s'}ds\,\mathrm{Tr}\Big[&\langle\omega_L|U_{\ell/2,s}R_\alpha^2U_{s,s'}R_\alpha U_{s',-\ell/2}(\omega_R\otimes\Omega)\\
&\times U_{s',-\ell/2}^\dagger r_\alpha^{j\dagger}U_{s,s'}^\dagger(R_\alpha^2)^\dagger U_{s,\ell/2}^\dagger|\omega_L\rangle\Big].
\end{aligned}$$

The integrand in this equation is of the form (6.28), and so to continue our evaluation we follow an identical procedure to the evaluation of (6.28), see (6.28) through (6.37). We find that we have a contribution towards the final expression of the projection of the interaction term for $D^2+1\leq j\leq 2D^2$ of

$$4L\langle\mathbb{I}|(R_\alpha\otimes\overline{R}_\alpha)^2\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)R_\alpha\otimes\overline{r}_\alpha|\rho\rangle.$$

The evaluation of (D.3) follows an analogous process, and we find that we have a contribution towards the final expression of the projection of the interaction term for $D^2+1\leq j\leq 2D^2$ of

$$4L\langle\mathbb{I}|R_\alpha\otimes\overline{r}_\alpha\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)(R_\alpha\otimes\overline{R}_\alpha)^2|\rho\rangle.$$

Finally we consider (D.2). We evaluate

$$\begin{aligned}
2\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2}ds\,ds'\mathrm{Tr}\Big[&\langle\omega_L|\left(\mathbb{I}\otimes\psi_\alpha^\dagger(s)\otimes\mathbb{I}\right)U_{\ell/2,s}(R_\alpha^2\otimes\mathbb{I}\otimes\mathbb{I})U_{s,-\ell/2}\\
&\times(\omega_R\otimes\Omega)U_{s',-\ell/2}^\dagger\left(r_\alpha^{j\dagger}\otimes\delta(s'-s)\otimes\mathbb{I}\right)U_{\ell/2,s'}^\dagger|\omega_L\rangle\Big].
\end{aligned}$$

We integrate out the delta function, then replace the product

$$(\omega_R \otimes \Omega) U^\dagger_{s,-\ell/2} \left(r^{j\dagger}_\alpha \otimes \mathbb{I} \otimes \mathbb{I} \right) U^\dagger_{\ell/2,s} |\omega_L\rangle\langle\omega_L| \left(\mathbb{I} \otimes \psi^\dagger_\alpha(s) \otimes \mathbb{I} \right)$$

with the commutator

$$(\omega_R \otimes \Omega) \Big[U^\dagger_{s,-\ell/2} \left(r^{j\dagger}_\alpha \otimes \mathbb{I} \otimes \mathbb{I} \right) U^\dagger_{\ell/2,s} |\omega_L\rangle\langle\omega_L| \, , \, \left(\mathbb{I} \otimes \psi^\dagger_\alpha(s) \otimes \mathbb{I} \right) \Big]$$

which simplifies to

$$(\omega_R \otimes \Omega) U^\dagger_{s,-\ell/2} \left\{ R^\dagger_\alpha, r^{j\dagger}_\alpha \right\} U^\dagger_{\ell/2,s} |\omega_L\rangle\langle\omega_L|.$$

We then can apply the same techniques used to evaluate (6.28) and obtain a contribution of

$$2L\langle\mathbb{I}|R^2_\alpha \otimes \left\{ \overline{R_\alpha, r^j_\alpha} \right\} |\rho\rangle$$

such that combining the separate results we find the complete expression for $D^2+1 \leq j \leq 2D^2$ is given by

$$2L \Big[2\langle\mathbb{I}|(R_\alpha \otimes \overline{R}_\alpha)^2 \left(\frac{\ell}{2} |\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M} \right) R_\alpha \otimes \overline{r}_\alpha |\rho\rangle + \langle\mathbb{I}|R^2_\alpha \otimes \left\{ \overline{R_\alpha, r^j_\alpha} \right\} |\rho\rangle$$
$$+ 2\langle\mathbb{I}|R_\alpha \otimes \overline{r}_\alpha \left(\frac{\ell}{2} |\rho\rangle\langle\mathbb{I}| - \frac{\mathbb{I}}{M} \right) (R_\alpha \otimes \overline{R}_\alpha)^2 |\rho\rangle \Big].$$

We note that, as in the main text, the overall factor L will not lead to a divergence in the limit $\ell \to \infty$ when using the expression in the TDVP equation (6.16). In addition, the diverging terms in the above expression will be removed when applying the left gauge fixing requirement (6.47), as explained in Chapter 6.

The calculations for $1 \leq j \leq D^2$ and $2D^2+1 \leq j \leq 3D^2$ follow a similar pattern, the main difference being that the second term in the above equation does not appear due to the absence of the field operator $\hat{\psi}^\dagger_\alpha$ in the tangent vector $\langle\partial_j\Psi|$. We do not present these derivations, and the complete expression for the projection of the interaction term can be found in (6.76).

D.2 Projection of the kinetic energy term

The projection of the kinetic term of the Hamiltonian $\hat{T}$ requires the evaluation of

$$\langle\partial_{\bar{j}}\Psi(\overline{z})|\hat{T}|\Psi(z)\rangle = \int_{-\ell/2}^{\ell/2} ds \; \langle\partial_{\bar{j}}\Psi| \left(\mathbb{I} \otimes \frac{d\psi^\dagger_\alpha(x)}{dx} \frac{d\psi_\alpha(x)}{dx} \otimes \mathbb{I} \right) |\Psi\rangle$$

for the different cases $1 \leq j \leq D^2$, $D^2+1 \leq j \leq 2D^2$, and $2D^2+1 \leq j \leq 3D^2$. As in the main body of the thesis we will detail only one of these cases, a pattern for calculating the different cases is soon established. We choose $1 \leq j \leq D^2$.

Derivations for $1 \leq j \leq D^2$

We evaluate

$$\begin{aligned}
&\langle \partial_{\bar{j}} \Psi(\overline{z}) | \hat{T} | \Psi(z) \rangle = \mathrm{Tr}\left[\hat{T} | \Psi(z) \rangle \langle \partial_{\bar{j}} \Psi(\overline{z}) | \right] \\
&= \int_{-\ell/2}^{\ell/2} \int_{-\ell/2}^{\ell/2} ds\, ds' \mathrm{Tr}\Big[\langle \omega_L | \left(\mathbb{I} \otimes \frac{d\psi_\alpha^\dagger(x)}{dx} \frac{d\psi_\alpha(x)}{dx} \otimes \mathbb{I} \right) U_{\ell/2,-\ell/2} \\
&\qquad \times (\omega_R \otimes \Omega) U_{s',-\ell/2}^\dagger \left(q^{j\dagger} \otimes \mathbb{I} \otimes \mathbb{I} \right) U_{\ell/2,s'}^\dagger | \omega_L \rangle \Big].
\end{aligned}$$

We begin by treating the $d\hat{\psi}_\alpha(x)/dx$ term. Since $\hat{\psi}_\alpha(x)$ annihilates the field vacuum $|\Omega\rangle_\alpha$ we have that $\frac{d\hat{\psi}_\alpha(x)}{dx}|\Omega\rangle_\alpha = \frac{d}{dx}(\hat{\psi}_\alpha(x)|\Omega\rangle_\alpha) = 0$. We therefore replace the product

$$\left(\mathbb{I} \otimes \frac{d\psi_\alpha(x)}{dx} \otimes \mathbb{I} \right) U_{\ell/2,-\ell/2} (\omega_R \otimes \Omega)$$

with the commutator

$$\left[\left(\mathbb{I} \otimes \frac{d\psi_\alpha(x)}{dx} \otimes \mathbb{I} \right) \, , \, U_{\ell/2,-\ell/2} \right] (\omega_R \otimes \Omega).$$

Since the operator $U_{\ell/2,-\ell/2}$ does not directly depend on x, we can simplify this commutator by pulling the derivative outside of the commutator and using (4.16). We find that

$$\begin{aligned}
\left[\left(\mathbb{I} \otimes \frac{d\psi_\alpha(x)}{dx} \otimes \mathbb{I} \right) \, , \, U_{\ell/2,-\ell/2} \right] &= \frac{d}{dx} \left[\left(\mathbb{I} \otimes \psi_\alpha(x) \otimes \mathbb{I} \right) \, , \, U_{\ell/2,-\ell/2} \right] \\
&= \frac{d}{dx} \left(U_{\ell/2,x} (R_\alpha \otimes \mathbb{I} \otimes \mathbb{I}) U_{x,-\ell/2} \right) \\
&= \Big(\frac{dU_{\ell/2,x}}{dx} (R_\alpha \otimes \mathbb{I} \otimes \mathbb{I}) U_{x,-\ell/2} + U_{\ell/2,x} (R_\alpha \otimes \mathbb{I} \otimes \mathbb{I}) \frac{dU_{\ell/2,x}}{dx} \Big) \\
&= U_{\ell/2,x} \left[(R_\alpha \otimes \mathbb{I} \otimes \mathbb{I}) \, , \, \hat{H}_{\mathrm{cMPS}}(x) \right] U_{x,-\ell/2}
\end{aligned}$$

where we have used the relations (4.19) and (4.20) to evaluate the derivatives of the operators $U_{\ell/2,x}$ and $U_{x,-\ell/2}$. To simplify further we have that

$$\begin{aligned}
\left[(R_\alpha \otimes \mathbb{I} \otimes \mathbb{I}) \, , \, \hat{H}_{\mathrm{cMPS}}(x) \right] &= \left[(R_\alpha \otimes \mathbb{I} \otimes \mathbb{I}) \, , \, Q \otimes \mathbb{I} + \sum_{\alpha=1}^{N} R_\alpha \otimes \psi_\alpha^\dagger(x) \right] \\
&= [R_\alpha, Q] \otimes \mathbb{I} \otimes \mathbb{I}
\end{aligned}$$

where we have used (4.22), that is $\left[R_\alpha, R_\beta\right] = 0$. We have thus eliminated $d\hat{\psi}_\alpha(x)/dx$ and are now required to evaluate

$$\begin{aligned}
&\mathrm{Tr}\left[\hat{T} | \Psi(z) \rangle \langle \partial_{\bar{j}} \Psi(\overline{z}) | \right] \\
&= \int_{-\ell/2}^{\ell/2} \int_{-\ell/2}^{\ell/2} ds\, ds' \mathrm{Tr}\Big[\langle \omega_L | \left(\mathbb{I} \otimes \frac{d\psi_\alpha^\dagger(x)}{dx} \otimes \mathbb{I} \right) ([R_\alpha, Q] \otimes \mathbb{I} \otimes \mathbb{I}) U_{\ell/2,-\ell/2} \\
&\qquad \times (\omega_R \otimes \Omega) U_{s',-\ell/2}^\dagger \left(q^{j\dagger} \otimes \mathbb{I} \otimes \mathbb{I} \right) U_{\ell/2,s'}^\dagger | \omega_L \rangle \Big].
\end{aligned}$$

The elimination of the $d\hat{\psi}^\dagger_\alpha(x)/dx$ term is slightly more complicated. As before we first make the replacement

$$
\begin{aligned}
&(\omega_R\otimes\Omega)U^\dagger_{s',-\ell/2}\left(q^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\left(\mathbb{I}\otimes\frac{d\psi^\dagger_\alpha(x)}{dx}\otimes\mathbb{I}\right)\\
&\to(\omega_R\otimes\Omega)\Big[U^\dagger_{s',-\ell/2}\left(q^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\,,\,\left(\mathbb{I}\otimes\frac{d\psi^\dagger_\alpha(x)}{dx}\otimes\mathbb{I}\right)\Big]\\
&=\Theta(s'-x)(\omega_R\otimes\Omega)\Big[U^\dagger_{s',-\ell/2}\,,\,\left(\mathbb{I}\otimes\frac{d\psi^\dagger_\alpha(x)}{dx}\otimes\mathbb{I}\right)\Big]\left(q^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\\
&+\Theta(x-s')(\omega_R\otimes\Omega)\Big[U^\dagger_{s',-\ell/2}\left(q^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)\Big[U^\dagger_{\ell/2,s'}\,,\,\left(\mathbb{I}\otimes\frac{d\psi^\dagger_\alpha(x)}{dx}\otimes\mathbb{I}\right)\Big]|\omega_L\rangle\langle\omega_L|. \qquad \text{(D.4)}
\end{aligned}
$$

We proceed in the usual manner. When $s'>x$ the second term is zero, and we consider

$$
\begin{aligned}
&(\omega_R\otimes\Omega)\Big[U^\dagger_{s',-\ell/2}\,,\,\left(\mathbb{I}\otimes\frac{d\psi^\dagger_\alpha(x)}{dx}\otimes\mathbb{I}\right)\Big]\left(q^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\\
&=(\omega_R\otimes\Omega)\frac{d}{dx}\Big[U^\dagger_{s',-\ell/2}\,,\,\left(\mathbb{I}\otimes\psi^\dagger_\alpha(x)\otimes\mathbb{I}\right)\Big]\left(q^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\\
&=(\omega_R\otimes\Omega)\frac{d}{dx}\left(U^\dagger_{x,-\ell/2}R^\dagger_\alpha U_{s',x}\right)\left(q^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|\\
&=(\omega_R\otimes\Omega)U^\dagger_{x,-\ell/2}\left(\left[R^\dagger_\alpha\,,\,Q^\dagger\right]\otimes\mathbb{I}\otimes\mathbb{I}\right)U_{s',x}\left(q^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|
\end{aligned}
$$

such that substitution into the main equation gives

$$
\begin{aligned}
&\mathrm{Tr}\left[\hat{T}|\Psi(z)\rangle\langle\partial_{\bar{j}}\Psi(\bar{z})|\right] \qquad \text{(D.5)}\\
&=\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2}ds\,ds'\mathrm{Tr}\Big[\langle\omega_L|([R_\alpha,Q]\otimes\mathbb{I}\otimes\mathbb{I})U_{\ell/2,-\ell/2}(\omega_R\otimes\Omega)U^\dagger_{x,-\ell/2}\\
&\qquad\qquad\times\left(\left[R^\dagger_\alpha\,,\,Q^\dagger\right]\otimes\mathbb{I}\otimes\mathbb{I}\right)U_{s',x}\left(q^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\Big].
\end{aligned}
$$

Since this expression is now free from field operators we can proceed as when treating (6.28). We find that we obtain a contribution of

$$
L\langle\mathbb{I}|\mathbb{I}\otimes\overline{q}^j\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)[R_\alpha,Q]\otimes\left[\overline{R_\alpha,Q}\right]|\rho\rangle.
$$

For $x>s'$ the calculations are analogous and we obtain a contribution of

$$
L\langle\mathbb{I}|[R_\alpha,Q]\otimes\left[\overline{R_\alpha,Q}\right]\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)\mathbb{I}\otimes\overline{q}^j|\rho\rangle.
$$

We must now consider the case $x = s$. Evaluation of (D.4) is then more complicated, since we cannot pull the differential operator out of the commutator. Instead we have that

$$\begin{aligned}
\left[U^\dagger_{x,-\ell/2}\,,\,\frac{d\psi^\dagger_\alpha(x)}{dx}\right] &= \frac{d}{dx}\left[U^\dagger_{x,-\ell/2}\,,\,\psi^\dagger_\alpha(x)\right] - \left[\frac{dU^\dagger_{x,-\ell/2}}{dx}\,,\,\psi^\dagger_\alpha(x)\right] \\
&= \frac{d}{dx}\left(U^\dagger_{x,-\ell/2}R^\dagger_\alpha\right) - \left[U^\dagger_{x,-\ell/2}\hat{H}^\dagger_{\text{cMPS}}(x)\,,\,\psi^\dagger_\alpha(x)\right] \\
&= \frac{d}{dx}\left(U^\dagger_{x,-\ell/2}R^\dagger_\alpha\right) - \left[U^\dagger_{x,-\ell/2}\,,\,\psi^\dagger_\alpha(x)\right]\hat{H}^\dagger_{\text{cMPS}}(x) - U^\dagger_{x,-\ell/2}\left[\hat{H}^\dagger_{\text{cMPS}}(x)\,,\,\psi^\dagger_\alpha(x)\right] \\
&= \frac{dU^\dagger_{x,-\ell/2}}{dx}R^\dagger_\alpha - \left[U^\dagger_{x,-\ell/2}\,,\,\psi^\dagger_\alpha(x)\right]\hat{H}^\dagger_{\text{cMPS}}(x) - U^\dagger_{x,-\ell/2}R^\dagger_\alpha \\
&= U^\dagger_{x,-\ell/2}\left[\hat{H}^\dagger_{\text{cMPS}}(x)\,,\,R^\dagger_\alpha\right] - U^\dagger_{x,-\ell/2}R^\dagger_\alpha \\
&= U^\dagger_{x,-\ell/2}\left[Q^\dagger\,,\,R^\dagger_\alpha\right] - U^\dagger_{x,-\ell/2}R^\dagger_\alpha.
\end{aligned}$$

Similarly we find that

$$\begin{aligned}
\left[U^\dagger_{\ell/2,x}\,,\,\frac{d\psi^\dagger_\alpha(x)}{dx}\right] &= \frac{d}{dx}\left[U^\dagger_{\ell/2,x}\,,\,\psi^\dagger_\alpha(x)\right] - \left[\frac{dU^\dagger_{\ell/2,x}}{dx}\,,\,\psi^\dagger_\alpha(x)\right] \\
&= \left[Q^\dagger\,,\,R^\dagger_\alpha\right]U^\dagger_{\ell/2,x} + R^\dagger_\alpha U^\dagger_{\ell/2,x}
\end{aligned}$$

The first two terms involving the commutator $\left[Q^\dagger\,,\,R^\dagger_\alpha\right]$ have already contributed to the final term in the evaluation of (D.4). This can be seen by equating $x = s$ in (D.5). We therefore include the second terms involving R_α only. Substituting into (D.4) gives

$$\begin{aligned}
&(\omega_R\otimes\Omega)\left[U^\dagger_{s',-\ell/2}\,,\,\left(\mathbb{I}\otimes\frac{d\psi^\dagger_\alpha(x)}{dx}\otimes\mathbb{I}\right)\right]\left(q^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L| \\
&+(\omega_R\otimes\Omega)\left[U^\dagger_{s',-\ell/2}\left(q^{j\dagger}\otimes\mathbb{I}\otimes\mathbb{I}\right)\left[U^\dagger_{\ell/2,s'}\,,\,\left(\mathbb{I}\otimes\frac{d\psi^\dagger_\alpha(x)}{dx}\otimes\mathbb{I}\right)\right]|\omega_L\rangle\langle\omega_L| \\
&=(\omega_R\otimes\Omega)U^\dagger_{x,-\ell/2}\left(\left[q^{j\dagger},R^\dagger_\alpha\right]\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\langle\omega_L|.
\end{aligned}$$

Substituting into the main expression means we evaluate

$$\begin{aligned}
&\text{Tr}\left[\hat{T}|\Psi(z)\rangle\langle\partial_{\overline{j}}\Psi(\overline{z})|\right] \\
&=\int_{-\ell/2}^{\ell/2}\int_{-\ell/2}^{\ell/2}ds\,ds'\text{Tr}\Big[\langle\omega_L|([R_\alpha,Q]\otimes\mathbb{I}\otimes\mathbb{I})U_{\ell/2,-\ell/2}(\omega_R\otimes\Omega) \\
&\qquad\qquad\times U^\dagger_{x,-\ell/2}\left(\left[q^{j\dagger},R^\dagger_\alpha\right]\otimes\mathbb{I}\otimes\mathbb{I}\right)U^\dagger_{\ell/2,s'}|\omega_L\rangle\Big],
\end{aligned}$$

resulting in a contribution to the final term of

$$\langle\mathbb{I}|\,[R_\alpha,Q]\otimes\left[\overline{R_\alpha,q^j}\right]|\rho\rangle.$$

We therefore find that, for $1 \leq j \leq D^2$, we obtain a contribution towards the projection of the kinetic energy term of

$$\begin{aligned} & L\Big[\langle \mathbb{I}|\mathbb{I}\otimes\overline{q}^j\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)[R_\alpha,Q]\otimes\left[\overline{R_\alpha,Q}\right]|\rho\rangle \\ & + L\langle\mathbb{I}|[R_\alpha,Q]\otimes\left[\overline{R_\alpha,Q}\right]\left(\frac{\ell}{2}|\rho\rangle\langle\mathbb{I}|-\frac{\mathbb{I}}{M}\right)\mathbb{I}\otimes\overline{q}^j|\rho\rangle \\ & + \langle\mathbb{I}|[R_\alpha,Q]\otimes\left[\overline{R_\alpha,q^j}\right]|\rho\rangle\Big]. \end{aligned}$$

The calculations for $D^2+1 \leq j \leq 2D^2$ and $2D^2+1 \leq j \leq 3D^2$ follow a similar pattern, with the inclusion of an extra step due to the presence of the field operators in the tangent vector. We do not present these derivations, and the complete expression for the projection of the interaction term can be found in (6.77).

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