Interacting many-particle systems on general compact quantum graphs

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Declaration of authorship

I, Joachim Friedrich Kerner, 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.

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Abstract

In this thesis, we discuss many-particle systems on general compact quantum graphs. The results cover systems of distinguishable particles as well as systems of bosons or fermions. The main focus lies on the introduction of many-particle interactions in order to establish a useful model regarding many-particle quantum chaos and one-dimensional Bose-Einstein condensation (BEC). Using suitable quadratic forms, we will characterise self-adjoint realisations of the two- and many-particle Laplacian which incorporate two different types of interactions, i.e. singular interactions localised at the vertices of the graph and contact interactions which are also present along the edges. In that context, we will establish regularity results in order to characterise the domains of the self-adjoint realisations explicitly. We will also discuss spectral properties of the constructed operators by establishing discreteness of their spectra and Weyl laws for the corresponding eigenvalue counts. Finally, based on the introduced models of interacting particles, we discuss Bose-Einstein condensation on general quantum graphs. We will distinguish between systems of bosons for which BEC occurs and such for which no BEC is present at any finite temperature. As a final result, we prove that no Bose-Einstein condensation occurs (in the sense of phase transitions) in a system of bosons interacting via repulsive hard-core interactions.

CONTENTS

1. INTRODUCTION

This thesis is concerned with the description of (interacting) many-particle systems on general compact quantum graphs. Originally, quantum graphs were introduced in the 1950s to model the spectrum of free electrons in organic molecules [RS53]. Since then, quantum graphs have found application in various interesting areas of physics such as nanotechnology and condensed matter physics. In the latter, they served as a model to investigate Anderson localisation [SS00] as well as the quantum Hall effect [GG08]. Furthermore, in a paper by Kottos and Smilansky [KS97b], quantum graphs were introduced into the field of quantum chaos by showing that their quantum mechanical spectra exhibit the same correlations as the spectra of random Hermitian matrices. On the other hand, a famous conjecture in quantum chaos states that such correlations are expected in all systems with chaotic classical counterparts [BGS84]. For this reason, one can regard quantum graphs as simple quantum mechanical systems whose underlying dynamics are chaotic and hence they provide the playground for a better understanding of quantum chaos. In general, to understand the origin of chaos in a given system can be quite difficult and this is true, in particular, for interacting many-particle systems [VSCdL01, JS97]. Accordingly, there are many open questions in the field of many-particle quantum chaos [GKK$^+$11]. One aim of this thesis is, therefore, by discussing interacting many-particle systems on quantum graphs, to contribute to a better understanding of many-particle quantum chaos.

Also, it is another aim of this thesis to discuss Bose-Einstein condensation (BEC) on general compact quantum graphs. In a gas of non-interacting bosons in three dimensions, condensation was predicted by Einstein almost ninety years ago [Ein25]. He showed that, below some critical temperature, the particles start to condense into the one-particle ground state. In other words, the one-particle ground state becomes macroscopically occupied. In a system of interacting bosons, on the other hand, it is in general very difficult to establish condensation [LSSY05]. Indeed, already the definition of Bose-Einstein condensation in such a system is not

straightforward [PO56, Mic07]. Therefore, using the introduced models of interacting particles, we want to elucidate the role of interactions in the context of Bose-Einstein condensation.

A graph $\Gamma = \Gamma(\mathcal{V}, \mathcal{E})$ consists of a finite number of vertices $\mathcal{V} = \{1, ..., V\}$ which are connected by a finite number of edges $\mathcal{E} = \{1, ..., E\}$. To each edge $e \in \mathcal{E}$, we associate an interval $(0, l_e) \subset \mathbb{R}^+$ with $l_e \in \mathbb{R}^+ \cup \{\infty\}$ being the length of the edge. Whenever all lengths are finite, we call the graph *compact*. Accordingly, the (one-particle) Hilbert space on a graph is defined by

$$L^2(\Gamma) = \bigoplus_{e=1}^{E} L^2(0, l_e), \tag{1.0.1}$$

implying that a one-particle wave function $\Psi \in L^2(\Gamma)$ is a vector of scalar-valued functions, i.e.

$$\Psi = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_E \end{pmatrix}. \tag{1.0.2}$$

If one introduces Schrödinger type operators on the Hilbert space (1.0.1), we call the graph a *quantum graph*. A prominent example of such an operator, which in fact will serve as the one-particle Hamiltonian, is the Laplacian $-\Delta_1$ which acts on $F \in C^\infty(\Gamma)$ via

$$(-\Delta_1 F)_e = -\frac{\mathrm{d}^2}{\mathrm{d}x_e^2} f_e, \quad \forall e \in \mathcal{E}. \tag{1.0.3}$$

In quantum mechanics, one usually requires the Hamiltonian to be self-adjoint [JBE08]. For the Laplacian $-\Delta_1$, each self-adjoint realisation is characterised by a domain $\mathcal{D}_1(A, B) \subset L^2(\Gamma)$ such that each function $F \in \mathcal{D}_1(A, B)$ fulfils the boundary conditions

$$A \begin{pmatrix} f_1(0) \\ \vdots \\ f_E(0) \\ f_1(l_1) \\ \vdots \\ f_E(l_E) \end{pmatrix} + B \begin{pmatrix} f_1'(0) \\ \vdots \\ f_E'(0) \\ -f_1'(l_1) \\ \vdots \\ -f_E'(l_E) \end{pmatrix} = 0, \tag{1.0.4}$$

where $A, B \in \mathbb{C}^{2E\times 2E}$ are such that $\operatorname{rank}(A, B) = 2E$ and AB^* is self-adjoint [KS99]. Note that the boundary conditions (1.0.4) can be interpreted as the result of external potentials localised at the vertices of the graph.
In quantum chaos, it is generally believed that the presence of chaos in a classical system manifests itself in the spectrum of the corresponding quantum system [BGS84, Haa91]. An important quantity in that context is the nearest-neighbour level spacings distribution

$$P(s) = \lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{N} \delta\left(s - (E_{n+1} - E_n)\right), \tag{1.0.5}$$

where δ is the standard Dirac delta function and $\{E_n\}_{n\in\mathbb{N}_0}$ the rescaled eigenvalues of the system, i.e. they are rescaled such that the mean level spacing is one [Haa91]. According to the Berry-Tabor conjecture [BT77], one expects a Poissonian behaviour of (1.0.5) for a classically integrable (non-chaotic) system, i.e.

$$P(s) = e^{-s}. \tag{1.0.6}$$

Hence, the eigenvalues tend to cluster and one observes a level attraction. On the other hand, in the case of quantum systems whose classical counterparts are chaotic, the distribution $P(s)$ is expected to be determined by the eigenvalue statistics of random Hermitian matrices and is such that larger distances of neighbouring eigenvalues are preferred, i.e. one observes level repulsion.
In the early days of quantum theory, energy spectra where described in terms of Bohr-Sommerfeld quantisation rules [Gut90] and Einstein observed that this is possible for integrable systems only [Ein17]. After full quantum mechanics had been established by Heisenberg, Schrödinger and Dirac, however, reference to classical properties seemed to be obsolete. Interestingly enough, using a semiclassical approximation, Gutzwiller [Gut71] derived a formula that allowed to calculate the spectral density

$$d(E) = \sum_{n=0}^{\infty} \delta\left(E - E_n\right) \tag{1.0.7}$$

for chaotic systems using classical quantities only (we shall assume that the periodic orbits are isolated and unstable). Although this so-called *trace formula* suffers in general from serious problems related to convergence [BK90, SS90], it

nevertheless establishes an interesting connection between the quantum mechanical spectrum of a system and the (periodic) orbits of its classical counterpart. Most interestingly, it was possible to establish an equivalent trace formula for the spectrum of the operator $-\Delta_1$ on general quantum graphs [KS97b, BE09]. Also, in contrast to the result of Gutzwiller, the trace formula on graphs is not restricted to a semi-classical limit. Noting that the trace formula on graphs takes into account only non-negative eigenvalues $\{k_n^2 \geq 0\}_{n\in\mathbb{N}_0}$, it reads

$$\begin{aligned}\sum_{n=0}^{\infty} h(k_n) =& \mathcal{L}\hat{h}(0) + \gamma h(0) - \frac{1}{4\pi}\int_{-\infty}^{\infty} h(k)\frac{\operatorname{Im}\operatorname{Tr} S(k)}{k}\,\mathrm{d}k \\ &+ \sum_{po}\left[\left(\hat{h} * \hat{A}_{po}\right)(l_{po}) + \left(\hat{h} * \hat{\overline{A}}_{po}\right)(l_{po})\right],\end{aligned} \tag{1.0.8}$$

where $\mathcal{L} = \sum_{e=1}^{E} l_e$ is the total length of the graph, γ a constant related to the multiplicity of the eigenvalue zero and $*$ a convolution defined in [BE09]. Furthermore, the function $h : \mathbb{C} \to \mathbb{C}$ is a suitable test function with corresponding Fourier transform $\hat{h}$. Also, $\hat{A}_{po}$ is the Fourier transform of an amplitude $A_{po}(k)$ which is associated with any periodic orbit *po* of length l_{po}. Note that the boundary conditions (1.0.4) are implicitly contained in the so-called *scattering matrix* $S(k)$. As an important consequence, the trace formula (1.0.8) establishes a close connection between the quantum mechanical spectrum of the system and the periodic orbits of its classical counterpart.

We have already mentioned that it is one aim of this thesis to contribute to a better understanding of many-particle quantum chaos by developing models of interacting many-particle systems on general compact quantum graphs. Indeed, the presented models incorporate two different types of two-particle interactions. In a first step, we will introduce *singular* two-particle interactions that are localised at the vertices of the graph. This means that two particles interact only whenever at least one particle is located at a vertex. As shown in [KS97b], the chaotic behaviour of a one-particle system on a quantum graph originates in the scattering of the particle in the vertices. Therefore, by implementing singular two-particle interactions localised at the vertices, the scattering is altered involving two-particle effects which then provides an opportunity to investigate many-particle quantum chaos. Note that Melnikov and Pavlov [MP95] introduced singular interactions on a tree-like graph, i.e. a graph with three edges of infinite length joined at one

common vertex, in order to investigate the effect of short range two-particle interactions as present, for example, between electrons in a solid. To illustrate our approach which leads to the implementation of singular two-particle interactions, consider the simplest compact graph, i.e. an interval of length l. In this case, the configuration space of two particles is the square $D = (0, l) \times (0, l)$ and the two-particle Hilbert space (for two distinguishable particles) is given by $L^2(D)$. As a two-particle Hamiltonian, we consider the two-dimensional Laplacian

$$-\Delta_2 = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \,, \tag{1.0.9}$$

which, defined on the set of all functions in $C_0^\infty(D)$, is a symmetric and densely defined operator. The idea is then to characterise suitable self-adjoint extensions of $(-\Delta_2, C_0^\infty(D))$ which incorporate singular interactions. Indeed, these self-adjoint extenstions will be obtained via the construction of suitable quadratic forms. It is interesting to note that the domains of the corresponding self-adjoint operators can be characterised in a way very similar to (1.0.4), i.e. each function $f \in H^2(D)$ in such a domain fulfils the two-particle boundary conditions

$$A(y) \begin{pmatrix} f(0,y) \\ f(l,y) \\ f(y,0) \\ f(y,l) \end{pmatrix} + B(y) \begin{pmatrix} f_x(0,y) \\ -f_x(l,y) \\ f_y(y,0) \\ -f_y(y,l) \end{pmatrix} = 0, \quad y \in [0,l]. \tag{1.0.10}$$

Here the maps $A(y), B(y) \in \mathbb{C}^{4\times 4}$ are required to fulfil, for each value $y \in [0, l]$, the same properties as corresponding one-particles maps [KS99]. In order to elucidate the two-particle interactions which are induced by the boundary conditions (1.0.10), consider the (non-compact) graph that is obtained by replacing the origin of the real line by a vertex. Indeed, if the maps $A(y)$ and $B(y)$ are chosen appropriately, the boundary conditions at this vertex effectively describe a two-particle system on the real line with (formal) Hamiltonian

$$\hat{H} = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \alpha(x, y) \left[\delta(x) + \delta(y)\right], \tag{1.0.11}$$

where α is a variable interaction strength [BK13b]. One can see that the δ-functions lead to strongly localised two-particle interactions at the vertex of the

graph. Furthermore, if we choose the function α with support close to the origin, the interactions are present only whenever both particles are close to the vertex. In this way, we can relate our model to the model considered by Melnikov and Pavlov in which both particles interact only in the vertex.
Subsequently we will introduce, in addition to singular interactions located at the vertices, *contact* interactions which are also present along the edges of the graph, i.e. whenever two particles are located at the same position. The introduction of such contact interactions is again interesting from the point of view of many-particle quantum chaos. In a one-particle system, the motion of the particle along the edges is simple since scattering takes place at the vertices only. However, in a many-particle system with contact interactions, the particles also scatter in the interior of an edge whenever at least two particles hit each other. Due to this additional source of scattering, the dynamics of the system becomes more involved. More precisely, the interactions we want to implement are point-like contact interactions and, most prominently, δ-interactions. Such interactions are, for a system of N particles moving on the real line, described by the (formal) Hamiltonian

$$\hat{H}_N = -\sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + \alpha \sum_{i>j} \delta(x_i - x_j), \tag{1.0.12}$$

where $\alpha \in \mathbb{R}$ is the interaction strength. Note that the limit $\alpha \to \infty$ corresponds to (repulsive) hard-core interactions. In fact, it will be our goal to give a rigorous realisation of the Hamiltonian (1.0.12) on general compact quantum graphs. Note that a Hamiltonian of the form (1.0.12) is considered, for example, in the Lieb-Liniger model [LL63] which plays an important role in one-dimensional Bose-Einstein condensation [CCG$^+$11] and our results will indeed provide a generalisation of the Lieb-Liniger model to general compact quantum graphs.
Finally, we will use the models of interacting particles introduced to discuss Bose-Einstein condensation (BEC) in the context of quantum graphs. In contrast to a free Bose gas in three dimensions, no Bose-Einstein condensation occurs at any finite temperature ($T > 0$) in a free one-dimensional Bose gas [DGPS99]. However, if a gas of bosons in one dimension is trapped and hence not free, Bose-Einstein condensation might nevertheless occur [BK91]. Also, condensation was proved in [IRH76] for a one-dimensional Bose gas on the real line with one-particle Hamil-

tonian

$$\hat{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \alpha\delta(x), \tag{1.0.13}$$

where $\alpha > 0$ is the interaction strength. Accordingly, even a small and strongly localised interaction can lead to Bose-Einstein condensation and, indeed, in one of the main results we will establish condensation in a large class of many-particle systems on quantum graphs. More precisely, given a system without particle-particle interactions, BEC is shown to occur if and only if the interactions with external potentials, as induced by the boundary conditions (1.0.4), are not fully repulsive. Subsequently, we will extend the discussion to include systems of interacting bosons, i.e. the particles shall be interacting via singular interactions as well as contact interactions. Since it is, as mentioned above, in general very difficult to prove condensation in a system of interacting particles [LSSY05], we approach the problem indirectly by taking into account the connection of Bose-Einstein condensation and phase transitions. As a final result, we will show that (in the sense of phase transitions) no Bose-Einstein condensation occurs in a system of bosons interacting via repulsive hard-core interactions. Most importantly, this result holds *independently* of the singular interactions in the vertices of the graph.

2. MATHEMATICAL BACKGROUND

In this chapter, we present the necessary mathematical theorems and techniques in order to establish the results of the thesis. Most of the mathematical repertoire we use originates in the theory of functional analysis as well as the theory of partial differential equations. Quantum mechanics, as the fundamental theory to describe the physics of the microscopic world, makes extensive use of operator theory and, in particular, self-adjoint and symmetric operators on some appropriate Hilbert space [RS72, JBE08, Tak08].

2.1 Basics in operator theory

The material presented in this section can be found in [Kat66, RS72, RS78, BB93, RR04]. In the following, $\mathcal{H}$ will denote a separable, complex Hilbert space with scalar product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$.

Definition 2.1.1. A linear operator $\hat{A}$ on a Hilbert space $\mathcal{H}$ is a linear map from a linear subspace $\mathcal{D}(\hat{A})$ into $\mathcal{H}$. Furthermore, a linear operator $\hat{A}$ is called *densely defined* if $\mathcal{D}(\hat{A})$ is dense in $\mathcal{H}$.

Note that we will, in the following, consider linear and densely defined operators only.

Definition 2.1.2. An operator $\hat{A}$ is *bounded* if there exists a constant $c \in \mathbb{R}$ such that

$$\|\hat{A}\varphi\|_{\mathcal{H}} \leq c\|\varphi\|_{\mathcal{H}}, \quad \forall \varphi \in \mathcal{D}(\hat{A}). \tag{2.1.1}$$

Otherwise, the operator is called *unbounded*.

Note that a bounded operator can always be defined on the whole Hilbert space $\mathcal{H}$.

Definition 2.1.3. The norm of a bounded operator is given by

$$\|\hat{A}\|_{op} = \sup_{\varphi\in\mathcal{D}(\hat{A});\|\varphi\|_{\mathcal{H}}\neq 0} \frac{\|\hat{A}\varphi\|_{\mathcal{H}}}{\|\varphi\|_{\mathcal{H}}} \,. \tag{2.1.2}$$

Often it is interesting to identify extensions of an operator. In particular, it will be important in later chapters to identify self-adjoint extensions of symmetric operators.

Definition 2.1.4. An operator $\big(\hat{B}, \mathcal{D}(\hat{B})\big)$ is called an *extension* of some operator $\big(\hat{A}, \mathcal{D}(\hat{A})\big)$, denoted as $\hat{A} \subseteq \hat{B}$, if $\mathcal{D}(\hat{A}) \subseteq \mathcal{D}(\hat{B})$ and

$$\hat{A}\varphi = \hat{B}\varphi, \quad \forall\varphi \in \mathcal{D}(\hat{A}). \tag{2.1.3}$$

As a next step we define closed operators.

Definition 2.1.5. An operator $\hat{A}$ is called *closed* if for every sequence $\{\varphi_n\}_{n\in\mathbb{N}} \in \mathcal{D}(\hat{A})$ converging to $\varphi \in \mathcal{H}$ and $\hat{A}\varphi_n \underset{n\to\infty}{\longrightarrow} \psi \in \mathcal{H}$, we have

$$\varphi \in \mathcal{D}(\hat{A}) \;\text{ and }\; \psi = \hat{A}\varphi. \tag{2.1.4}$$

Definition 2.1.6. An operator $\hat{A}$ is called *closable* if it has a closed extension.

Note that the smallest closed extension of an operator is called its closure.

Definition 2.1.7. A bounded operator $\hat{A}$ is called *compact* if for every bounded sequence $\{\varphi_n\}_{n\in\mathbb{N}}$ the sequence $\{\hat{A}\varphi_n\}_{n\in\mathbb{N}}$ contains a convergent subsequence.

The most prominent operators in physics are self-adjoint operators. Most importantly, the Hamiltonian of a system is in general required to be self-adjoint.

Definition 2.1.8. An operator $\hat{A}$ is called *symmetric* if

$$\langle\hat{A}\psi, \varphi\rangle_{\mathcal{H}} = \langle\psi, \hat{A}\varphi\rangle_{\mathcal{H}}, \quad \forall\psi, \varphi \in \mathcal{D}(\hat{A}). \tag{2.1.5}$$

It is important to note that every symmetric operator is closable [JBE08].

Definition 2.1.9. A symmetric operator $\hat{A}$ is bounded from below if

$$\langle\psi, \hat{A}\psi\rangle_{\mathcal{H}} \geq -\lambda\|\psi\|^2_{\mathcal{H}}, \quad \forall\psi \in \mathcal{D}(\hat{A}), \tag{2.1.6}$$

for some number $\lambda \geq 0$. If an operator is bounded from below we call it *semi-bounded*. Furthermore, if $\lambda = 0$ we call it *positive*.

Definition 2.1.10. Let $\hat{A}$ be an operator on a Hilbert space $\mathcal{H}$. Define $\mathcal{D}(\hat{A}^*)$ to be the set of $\psi \in \mathcal{H}$ for which there is an $\chi \in \mathcal{H}$ such that

$$\langle \hat{A}\varphi, \psi \rangle_{\mathcal{H}} = \langle \varphi, \chi \rangle_{\mathcal{H}}, \quad \forall \varphi \in \mathcal{D}(\hat{A}). \tag{2.1.7}$$

For each such $\psi \in \mathcal{D}(\hat{A}^*)$, one sets $\hat{A}^*\psi = \chi$. Then the operator $(\hat{A}^*, \mathcal{D}(\hat{A}^*))$ is called the *adjoint* of $\hat{A}$.

Definition 2.1.11. An operator $\hat{A}$ is *self-adjoint* if $\hat{A} = \hat{A}^*$, i.e. if $\mathcal{D}(\hat{A}) = \mathcal{D}(\hat{A}^*)$ and

$$\hat{A}\varphi = \hat{A}^*\varphi, \quad \forall \varphi \in \mathcal{D}(\hat{A}). \tag{2.1.8}$$

Definition 2.1.12. Let $\hat{A}$ be a closed, symmetric operator. Its *deficiency indices* are defined as

$$\begin{aligned} n_+ &= \dim \ker (\hat{A}^* - i), \\ n_- &= \dim \ker (\hat{A}^* + i). \end{aligned} \tag{2.1.9}$$

Lemma 2.1.13. *A closed, symmetric operator is self-adjoint if and only if* $n_\pm = 0$.

Sometimes it is difficult to determine the closure of a given symmetric operator. For this reason, one would like to define a weaker form of self-adjointness which does not require the operator to be closed.

Definition 2.1.14. A symmetric operator $\hat{A}$ is said to be *essentially self-adjoint* if its closure is self-adjoint.

For an operator $\hat{A}$, we define the set $C^\infty(\hat{A}) := \bigcap_{n=1}^\infty \mathcal{D}(\hat{A}^n)$. A vector $\varphi \in C^\infty(\hat{A})$ is called an *analytic vector* if the power series

$$\sum_{n=0}^{\infty} \|\hat{A}^n\varphi\|_{\mathcal{H}} \frac{z^n}{n!} \tag{2.1.10}$$

has a non-zero convergence radius [JBE08]. Based on this, we can state the important theorem of Nelson that allows to establish essential self-adjointness of an operator. For this, note that a subset $X \subset \mathcal{H}$ of a Hilbert space is called total if $\overline{\text{span}(X)} = \mathcal{H}$.

Theorem 2.1.15 (Nelson)**.** *Let $\hat{A}$ be a symmetric operator whose analytic vectors form a total set. Then $\hat{A}$ is essentially self-adjoint.*

Before we move on to characterise the spectrum of an operator, we mention an important subclass of compact operators which are also very important in physics. For this we note that one can define the "square root" of a bounded, positive operator $\hat{A}$, i.e. there exists a bounded, positive operator $\sqrt{\hat{A}}$ such that $(\sqrt{\hat{A}})^2 = \hat{A}$ [JBE08].

Definition 2.1.16. A bounded operator $\hat{A}$ is said to be of *trace-class* if

$$\operatorname{Tr}|\hat{A}| := \sum_{n=1}^{\infty} \langle e_n, |\hat{A}| e_n \rangle_{\mathcal{H}} < \infty \,, \tag{2.1.11}$$

where $|\hat{A}| := \sqrt{A^* A}$ and $\{e_n\}_{n\in\mathbb{N}}$ is some orthonormal basis of $\mathcal{H}$. Note that $\operatorname{Tr}|\hat{A}|$, i.e. the trace of $|\hat{A}|$, can shown to be independent of the basis chosen [JBE08].

Theorem 2.1.17. *Let $\hat{A}$ be a trace-class operator. Then*

$$\operatorname{Tr}\hat{A} := \sum_{n=1}^{\infty} \langle e_n, \hat{A} e_n \rangle_{\mathcal{H}} \tag{2.1.12}$$

is well defined, i.e. the sum on the right-hand side converges absolutely and is independent of the basis $\{e_n\}_{n\in\mathbb{N}}$.

Now we want to give basic definitions regarding the spectrum of an operator. In contrast to the finite-dimensional case, where the spectrum of a matrix consists of finitely many eigenvalues, the spectrum of operators on infinite-dimensional Hilbert spaces is more complex since it may not be purely discrete.

Definition 2.1.18. Let $\hat{A}$ be a closed operator on a Hilbert space $\mathcal{H}$. Let $\lambda \in \mathbb{C}$ be a complex number and consider the operator $(\hat{A} - \lambda \mathrm{I}, \mathcal{D}(\hat{A}))$. If this operator has dense range, is bijective and has bounded inverse, we say that λ is in the resolvent set $\rho(\hat{A})$. Furthermore,

$$R_\lambda(\hat{A}) = (\hat{A} - \lambda \mathrm{I})^{-1} \tag{2.1.13}$$

is called the *resolvent* of $\hat{A}$ at λ. If $\lambda \notin \rho(\hat{A})$, then λ is in the *spectrum* $\sigma(\hat{A})$ of $\hat{A}$.

The spectrum $\sigma(\hat{A})$ of a closed operator $\hat{A}$ can be decomposed into three (disjoint) subsets, i.e. the point spectrum, the continuous spectrum and the residual spectrum.

Definition 2.1.19. The *point spectrum* is the set of all values $\lambda \in \mathbb{C}$ for which $\hat{A} - \lambda \mathrm{I}$ is not bijective, i.e.

$$\sigma_p(\hat{A}) = \{\lambda \in \sigma(\hat{A}) |\ R_\lambda(\hat{A}) \text{ doesn't exist}\}. \tag{2.1.14}$$

Definition 2.1.20. The *continuous spectrum* is the set

$$\sigma_c(\hat{A}) = \{\lambda \in \sigma(\hat{A}) |\ \mathrm{ran}(\hat{A} - \lambda \mathrm{I}) \text{ is dense};\ R_\lambda(\hat{A}) \text{ exists but is unbounded}\}. \tag{2.1.15}$$

Definition 2.1.21. The *residual spectrum* is the set

$$\sigma_r(\hat{A}) = \{\lambda \in \sigma(\hat{A}) |\ R_\lambda(\hat{A}) \text{ exists};\ \mathrm{ran}\,(\hat{A} - \lambda \mathrm{I}) \text{ is not dense}\}. \tag{2.1.16}$$

One reason why self-adjoint operators are important in physics is due to the fact that their spectrum is purely real.

Lemma 2.1.22. *Let $\hat{A}$ be a self-adjoint operator. Then its spectrum is purely real, i.e.*

$$\sigma(\hat{A}) \subseteq \mathbb{R}. \tag{2.1.17}$$

An important subset of the point spectrum is the discrete spectrum which consists of all isolated eigenvalues with finite multiplicity.

Definition 2.1.23. The *discrete spectrum* of an operator $\hat{A}$ consists of all elements $\lambda \in \sigma_p(\hat{A})$ for which

1. $\dim \ker (\hat{A} - \lambda) < \infty$,
2. λ is an isolated value in the point spectrum.

In physics, there are numerous examples of operators with purely discrete spectrum, e.g. the Hamiltonian of the harmonic oscillator. However, as for the Hamiltonian of the hydrogen atom, the spectrum may not always be purely discrete.

Theorem 2.1.24. *[RS78] Let $\hat{A}$ be a semi-bounded, self-adjoint operator. Then $\hat{A}$ has purely discrete spectrum if and only if its resolvent is a compact operator.*

Proving that a given symmetric operator is self-adjoint is often difficult. One suitable way to identify self-adjoint operators is through the construction of suitable quadratic forms.

Definition 2.1.25. A sesquilinear form Q, defined on a linear subspace $\mathcal{D}_Q \subset \mathcal{H}$, is a map

$$S : \mathcal{D}_Q \times \mathcal{D}_Q \mapsto \mathbb{C}, \tag{2.1.18}$$

that is anti-linear in the first and linear in the second argument. The form is called *symmetric* if

$$Q[\psi, \varphi] = \overline{Q[\varphi, \psi]}, \tag{2.1.19}$$

and it is called *densely defined* if its domain $\mathcal{D}_Q$ is dense in $\mathcal{H}$. Furthermore, a quadratic form $Q[\psi] := Q[\psi, \psi]$ is called *bounded from below* if there exists a $\lambda \geq 0$ such that

$$Q[\psi] \geq -\lambda \|\psi\|^2_{\mathcal{H}}, \quad \forall \psi \in \mathcal{D}_Q. \tag{2.1.20}$$

A quadratic form is called *closed* if $\mathcal{D}_Q$ is complete with respect to the norm

$$\|\cdot\|^2_Q = Q[\cdot] + (\lambda + 1)\|\cdot\|^2_{\mathcal{H}}. \tag{2.1.21}$$

Note that, since there is a one-to-one correspondence between sesquilinear and quadratic forms [JBE08], we will also refer to both briefly as a form.

Theorem 2.1.26 (representation theorem)**.** *Let $Q : \mathcal{D}_Q \times \mathcal{D}_Q \to \mathcal{H}$ be a densely defined form which is closed, symmetric and bounded from below. Then there exists a unique, semi-bounded and self-adjoint operator $\hat{A}$ on $\mathcal{H}$ such that $\mathcal{D}(\hat{A}) \subset \mathcal{D}_Q$ and*

$$\langle \psi, \hat{A}\varphi \rangle_{\mathcal{H}} = Q[\psi, \varphi], \quad \forall \psi \in \mathcal{D}_Q, \varphi \in \mathcal{D}(\hat{A}). \tag{2.1.22}$$

Let $\hat{A}$ be a self-adjoint operator with purely discrete spectrum and eigenvalues (counted with multiplicity) $\{\lambda_n\}_{n \in \mathbb{N}_0}$. Then we define the counting function of $\hat{A}$ by

$$N_{\hat{A}}(\lambda) = \#\{n \in \mathbb{N}_0 |\ \lambda_n \leq \lambda\}, \tag{2.1.23}$$

where $\lambda \in \mathbb{R}$ is some real number. Using the representation theorem, it is possible to compare the counting functions of two operators. More precisely, let $\hat{A}$ and $\hat{B}$ be self-adjoint operators with corresponding forms $Q_{\hat{A}}$ and $Q_{\hat{B}}$ as characterised in Theorem 2.1.26. Suppose that both operators have compact resolvent. Then, if

$\mathcal{D}_{Q_{\hat{A}}} \subseteq \mathcal{D}_{Q_{\hat{B}}}$ and $Q_{\hat{A}}[\psi] \geq Q_{\hat{B}}[\psi]$ for all $\psi \in \mathcal{D}_{Q_{\hat{A}}}$, one has

$$N_{\hat{A}}(\lambda) \leq N_{\hat{B}}(\lambda), \quad \forall \lambda \in \mathbb{R}. \tag{2.1.24}$$

Note that the inequality (2.1.24) follows from the min-max principle (see Theorem XIII.2 [RS78]). In order to formulate it, we use the shorthand notation $[\varphi_1, \ldots, \varphi_m]^\perp$ for $\{\psi |\ \langle \psi, \varphi_j \rangle_{\mathcal{H}} = 0,\ j = 1, ..., m\}$ [RS78].

Theorem 2.1.27 (min-max principle)**.** *Let $\hat{A}$ be self-adjoint and bounded from below with corresponding quadratic form $Q_{\hat{A}}$ as described in Theorem 2.1.26. We then define the number*

$$\mu_n(\hat{A}) = \sup_{\varphi_1,\ldots,\varphi_{n-1} \in \mathcal{H}} \inf_{\substack{\psi \in [\varphi_1,\ldots,\varphi_{n-1}]^\perp \\ \psi \in \mathcal{D}_{Q_{\hat{A}}}, \|\psi\|=1}} \langle \psi, \hat{A}\psi \rangle_{\mathcal{H}} \ . \tag{2.1.25}$$

In particular, if $\hat{A}$ has compact resolvent, $\mu_n(\hat{A})$ is the n-th eigenvalue counting multiplicity.

2.2 Sobolev spaces and Lipschitz domains

In this section, we introduce the concept of Sobolev spaces since they are suitable spaces for the discussion of partial differential operators. We also introduce Lipschitz domains and provide important properties of Sobolev spaces on Lipschitz domains. Note that all results stated in this section can be found in [Dob05] unless otherwise stated. For a more detailed analysis of Sobolev spaces and properties of Sobolev functions on general domains see [Ada75, MP01].
In the following, $\Omega \subset \mathbb{R}^N$ shall always denote an open, bounded domain, i.e. Ω is connected. A multi-index α is a vector $\alpha = (\alpha_1, ..., \alpha_N) \in \mathbb{N}_0^N$ with

$$|\alpha| = \alpha_1 + ... + \alpha_N, \tag{2.2.1}$$

as well as

$$D^\alpha = \partial_{x_1}^{\alpha_1} ... \partial_{x_N}^{\alpha_N}. \tag{2.2.2}$$

Definition 2.2.1. Let $\psi \in L^2(\Omega)$ be a function. The function $\chi \in L^2(\Omega)$ is a

weak derivative of order α of ψ, if

$$\langle \psi, D^\alpha \varphi \rangle_{L^2(\Omega)} = (-1)^{|\alpha|} \langle \chi, \varphi \rangle_{L^2(\Omega)}, \quad \forall \varphi \in C_0^\infty(\Omega). \tag{2.2.3}$$

A function $\psi \in L^2(\Omega)$ is called m-times weakly differentiable if it is weakly differentiable of all orders α with $|\alpha| \leq m$.

Remark 2.2.2. Note that, for each $j = 1, ..., N$, the weak derivative with respect to x_j will also be denoted by ∂_j.

Definition 2.2.3. Let $m \in \mathbb{N}_0$. The m-th Sobolev space $H^m(\Omega)$ consists of all functions $\psi \in L^2(\Omega)$ that are m-times weakly differentiable. Then

$$\|\psi\|_{H^m(\Omega)} = \left(\sum_{|\alpha| \leq m} \|D^\alpha \psi\|^2_{L^2(\Omega)} \right)^{\frac{1}{2}} \tag{2.2.4}$$

is a norm on $H^m(\Omega)$.

Remark 2.2.4. It follows that $H^0(\Omega) = L^2(\Omega)$.

Lemma 2.2.5. *The space $H^m(\Omega)$ is a Hilbert space with scalar product*

$$\langle \psi, \varphi \rangle_{H^m(\Omega)} = \sum_{0 \leq |\alpha| \leq m} \int_\Omega \overline{(D^\alpha \psi)} D^\alpha \varphi \, \mathrm{d}x. \tag{2.2.5}$$

A very important class of (bounded) domains Ω are Lipschitz domains. Loosely speaking, Lipschitz domains are domains that allow for corners. Due to this, they are very important in applied mathematics since domains with corners appear naturally, e.g. in the area of fluid dynamics or electrodynamics.

Definition 2.2.6. The space $C^0(\overline{\Omega})$ consists of all bounded and uniformly continuous functions on Ω. Furthermore, the space $C^m(\overline{\Omega})$ is the subset of $C^m(\Omega)$ which consists of all functions that have bounded and uniformly continuous derivatives up to order $|\alpha| \leq m$.

Definition 2.2.7. The space $C^{0,1}(\overline{\Omega})$ consists of all functions $\varphi \in C^0(\overline{\Omega})$ that are Lipschitz continuous.

Now, in order to introduce Lipschitz domains as well as smooth domains more precisely, let $h^r_\eta : B^{N-1}_\eta(0) \to \mathbb{R}$ be a function such that $h^r_\eta \in C^m(\overline{B^{N-1}_\eta(0)})$ or

$h_\eta^r \in C^{0,1}(\overline{B_\eta^{N-1}(0)})$ with $\eta, r > 0$ some constants and where $B_\eta^{N-1}(0)$ is the open ball of radius $\eta \in \mathbb{R}$ around the origin $0 \in \mathbb{R}^{N-1}$. Note that, in the following, we use the convention $x = (x', x_N)^T \in \mathbb{R}^N$ where $x' \in \mathbb{R}^{N-1}$ and $x_N \in \mathbb{R}$.

Definition 2.2.8. Let $m \in \mathbb{N}$ or $m = 0$ with $\alpha = 1$. A domain Ω is said to be of class C^m (or of class $C^{0,1}$) if, for every boundary point $x_0 \in \partial\Omega$, we can translate and rotate the coordinate system such that a neighbourhood U of x_0 can be parametrized as

$$x' = y', \quad x_N = h_\eta^r(y') + y_N, \quad y' \in B_\eta^{N-1}(0), \quad |y_N| < r, \tag{2.2.6}$$

where $h_\eta^r \in C^m(\overline{B_\eta^{N-1}(0)})$ (or $h_\eta^r \in C^{0,1}(\overline{B_\eta^{N-1}(0)})$) with $y_N > 0$ for all points $U \cap \Omega$, $y_N = 0$ for all points $U \cap \partial\Omega$ and $y_N < 0$ for all points $U \cap \Omega^c$. Furthermore, a domain of class $C^{0,1}$ is called *Lipschitz domain*.

Using the characterisation of the boundary as established in the previous definition together with a partition of unity argument, it is possible to define an L^2-space on the boundary of a Lipschitz domain:

Definition 2.2.9. Let $\Omega \subset \mathbb{R}^N$ be a Lipschitz domain and $U = \bigcup_{j=1}^J U_j$ a finite open cover of the boundary with $\sum_{j=1}^J \phi_j(x) = 1$ in U, $\phi_j \in C_0^\infty(U_j)$. For each open domain $U_j \subset \mathbb{R}^N$, let $h_{\eta_j}^{r_j}$ denote the function characterising the boundary as introduced above. Then, if $\psi : \partial\Omega \to \mathbb{C}$ is a function on the boundary, consider the restrictions $\psi_j(y') = (\phi_j\psi)(y', h_{\eta_j}^{r_j}(y'))$ with $y' \in B_{\eta_j}^{N-1}(0)$. We say that ψ is measurable on $\partial\Omega$ whenever all ψ_j are measurable in $B_{\eta_j}^{N-1}(0)$. Also, ψ is called integrable on $\partial\Omega$ if the integrals

$$\int_{\partial\Omega} \psi_j \, \mathrm{d}\sigma := \int_{B_{\eta_j}^{N-1}(0)} \psi_j \sqrt{1 + |\nabla h_{\eta_j}^{r_j}|^2} \, \mathrm{d}y' \tag{2.2.7}$$

exist in the sense of Lebesgue for all $j \in \{1, ..., J\}$. Furthermore, the integral

$$\int_{\partial\Omega} \psi \, \mathrm{d}\sigma := \sum_{j=1}^J \int_{\partial\Omega} \psi_j \, \mathrm{d}\sigma \tag{2.2.8}$$

is called the boundary integral of ψ. Defining the norm $\|\psi\|_{L^2(\partial\Omega)} = \left(\int_{\partial\Omega} |\psi|^2 \mathrm{d}\sigma\right)^{\frac{1}{2}}$, the space $L^2(\partial\Omega)$ consists of all measurable functions $\psi : \partial\Omega \to \mathbb{C}$ with finite $L^2(\partial\Omega)$-norm.

Theorem 2.2.10. *Let $\Omega \subset \mathbb{R}^N$ be a Lipschitz domain. Then, the set of all restrictions of functions in $C_0^\infty(\mathbb{R}^N)$ to Ω is dense in $H^m(\Omega)$.*

A fundamental property of Lipschitz domains is that one is able to assign boundary values to a Sobolev function. Note that this is not straightforward since the boundary is a set of (Lebesgue) measure zero.

Theorem 2.2.11. *Let $\Omega \subset \mathbb{R}^N$ be a Lipschitz domain. Then there exists a unique, continuous linear operator $\gamma : H^1(\Omega) \to L^2(\partial\Omega)$ such that*

$$\gamma\psi = \psi|_{\partial\Omega} \tag{2.2.9}$$

for $\psi \in C^\infty(\overline{\Omega})$. Moreover, there exists $c > 0$ such that

$$\|\gamma\psi\|_{L^2(\partial\Omega)} \leq c\|\psi\|_{H^1(\Omega)}. \tag{2.2.10}$$

The constant $c > 0$ is called the trace constant.

Remark 2.2.12. The Sobolev spaces $H_0^m(\Omega)$ consist of all functions $\varphi \in H^m(\Omega)$ such that $\gamma\left(D^\alpha\varphi\right) = 0$ for $|\alpha| \leq m-1$.

Note that a generalisation of the trace theorem (on Lipschitz domains) can be found in [Din96]. Indeed, one can show that the traces of functions in $H^1(\Omega)$ are elements of the fractional Sobolev space $H^{\frac{1}{2}}(\partial\Omega)$ [Dob05, RR04]. Also, it is possible to estimate the boundary integral more precisely than provided by (2.2.10).

Theorem 2.2.13. *[Gri11] Let $\Omega \subset \mathbb{R}^N$ be a Lipschitz domain. Then there exists a constant $K > 0$ such that*

$$\int_{\partial\Omega} |\gamma\varphi|^2 \, \mathrm{d}\sigma \leq K\left(\delta \int_\Omega |\nabla\varphi|^2 \, \mathrm{d}x + \frac{1}{\delta}\int_\Omega |\varphi|^2 \, \mathrm{d}x\right) \tag{2.2.11}$$

for all $\varphi \in H^1(\Omega)$ and $\delta \in (0,1)$. Furthermore, the constant K depends only the the domain Ω and its boundary.

Finally, we want to state an important result concerning *convex* domains.

Definition 2.2.14. Let $\Omega \subset \mathbb{R}^N$ be a domain. If for every two points $x, y \in \Omega$, the point $tx + (1-t)y$ is in Ω for all values $t \in [0,1]$, we call the domain convex.

Theorem 2.2.15. *[Gri11] Let $\Omega \subset \mathbb{R}^N$ be a convex domain. Then Ω has a Lipschitz boundary.*

Note that all domains considered in this thesis will be convex.

2.3 Boundary value problems

Let $\Omega \subset \mathbb{R}^N$ be an open, bounded Lipschitz domain and consider the classical boundary value problem: Given $f \in L^2(\Omega)$ and $\lambda \geq 0$, find a function $\psi \in C^2(\Omega) \cap C^1(\overline{\Omega})$ such that

$$(-\Delta + \lambda)\psi = f, \quad \forall x \in \Omega, \tag{2.3.1}$$

and

$$\frac{\partial \psi}{\partial \vec{n}} + \alpha\psi = 0, \quad \forall x \in \partial\Omega, \tag{2.3.2}$$

with some constant $\alpha \in \mathbb{R}$ or

$$\psi = 0, \quad \forall x \in \partial\Omega. \tag{2.3.3}$$

The boundary conditions (2.3.2) are so called Robin conditions, where $c \equiv 0$ corresponds to Neumann conditions. Furthermore, (2.3.3) are Dirichlet boundary conditions. Now, one would like to prove existence as well as uniqueness of a classical solution $\psi \in C^2(\Omega) \cap C^1(\overline{\Omega})$. However, it was soon realised that one cannot expect a classical solution to exist for arbitrary data $f \in L^2(\Omega)$ and independent of the domain considered [RR04, Dob05]. Therefore, the concept of a *weak solution* was introduced into the modern theory of partial differential equations. To illustrate this concept, let $\mathcal{H}$ be a Hilbert space, $a(\cdot,\cdot)$ a sesquilinear form

$$a : \mathcal{H} \times \mathcal{H} \mapsto \mathbb{C}, \tag{2.3.4}$$

and $f(\cdot)$ a linear and continuous functional on $\mathcal{H}$. Then we can formulate the abstract boundary value problem: Find $\psi \in \mathcal{H}$ such that

$$a(\psi, \varphi) = f(\varphi), \quad \forall \varphi \in \mathcal{H}. \tag{2.3.5}$$

Definition 2.3.1. If $\psi \in \mathcal{H}$ is a solution of the abstract boundary value problem

(2.3.5), we call it a weak solution.

In order to relate the abstract boundary value problem (2.3.5) to the classical boundary value problem above, we associate with the Laplacian a suitable sesquilinear form and define this form on a suitable Hilbert space $\mathcal{H}$. In the case of the Robin boundary value problem (2.3.2), we introduce the form

$$a_R(\psi,\varphi) = \int_\Omega \nabla\bar{\psi}\nabla\varphi \,\mathrm{d}x + \lambda\int_\Omega \bar{\psi}\varphi \,\mathrm{d}x + \alpha\int_{\partial\Omega} \bar{\psi}\varphi \,\mathrm{d}\sigma \tag{2.3.6}$$

and define it on the Hilbert space $\mathcal{H} = H^1(\Omega)$. The variational version of the boundary value problem (2.3.2) then reads: Find a function $\psi \in H^1(\Omega)$ such that

$$a_R(\psi,\varphi) = \langle f,\varphi\rangle_{\mathcal{H}}, \quad \forall\varphi \in H^1(\Omega). \tag{2.3.7}$$

Furthermore, the variational version of the Dirichlet problem (2.3.3) is obtained by defining the form

$$a_D(\psi,\varphi) = \int_\Omega \nabla\bar{\psi}\nabla\varphi \,\mathrm{d}x + \lambda\int_\Omega \bar{\psi}\varphi \,\mathrm{d}x \tag{2.3.8}$$

on the Hilbert space $\mathcal{H} = H_0^1(\Omega)$. The boundary value problem then reads: Find a function $\psi \in H_0^1(\Omega)$ such that

$$a_D(\psi,\varphi) = \langle f,\varphi\rangle_{\mathcal{H}}, \quad \forall\varphi \in H_0^1(\Omega). \tag{2.3.9}$$

To show the existence of a unique weak solution, one applies the theorem of Lax-Milgram [Gri11, Dob05, RR04].

Theorem 2.3.2. *Let $a(\cdot,\cdot) : \mathcal{H}\times\mathcal{H} \mapsto \mathbb{C}$ a sesquilinear form on $\mathcal{H}$. Suppose there exist two constants $c_1, c_2 > 0$ such that*

$$|a(\psi,\varphi)| \le c_1\|\psi\|_{\mathcal{H}}\|\varphi\|_{\mathcal{H}}, \quad \forall\psi,\varphi \in \mathcal{H} \tag{2.3.10}$$

and

$$a(\varphi,\varphi) \ge c_2\|\varphi\|_{\mathcal{H}}^2, \quad \forall\varphi \in \mathcal{H}. \tag{2.3.11}$$

Then, for every continuous and linear functional $f(\cdot)$, there exists a unique $\psi \in \mathcal{H}$ such that

$$a(\psi,\varphi) = f(\varphi), \quad \forall\varphi \in \mathcal{H}. \tag{2.3.12}$$

Theorem 2.3.3. *[Gri11] Let $\Omega \subset \mathbb{R}^N$ be an open bounded convex domain. Then, for each function $f \in L^2(\Omega)$, the boundary value problems* (2.3.9) *with $\lambda \geq 0$ and* (2.3.7) *with $\lambda > 0$ and $\alpha \geq 0$ have a unique weak solution $\psi \in H^2(\Omega)$.*

The most important conclusion from Theorem 2.3.3 is not that there exists a unique weak solution $\psi \in H^1(\Omega)$ but that this solution actually belongs to a Sobolev space of higher order. In general, if a weak solution $\psi \in H^1(\Omega)$ is such that $\psi \in H^2(\Omega)$, we call it H^2-regular or regular for short. As it turns out, however, there is no general criterion which allows one to conclude that a weak solution of an arbitrary boundary value problem is regular. Instead, the regularity of a weak solution strongly depends on the domain $\Omega \subset \mathbb{R}^N$, its boundary $\partial\Omega$ and the boundary conditions imposed [Neč67, Dau88, Gri11, Dob05]. Also, it is particularly difficult to establish regularity on domains with corners since the standard technique that works for smooth boundaries usually cannot be applied. A standard technique to establish regularity is the *difference quotient technique* introduced by Nirenberg [Nir59, RR04, Dob05]. Since we will use this technique in the proof of a regularity theorem given in part B of the appendix, we here provide the necessary technical prerequisites.

Definition 2.3.4. Let e_n be the unit vector in the direction of the n-th coordinate. For given $h > 0$ and given function $\psi : \mathbb{R}^N \to \mathbb{C}$, we define the two difference quotients

$$\begin{aligned} \left(D_n^{+h}\psi\right)(x) &= \frac{\psi(x + he_n) - \psi(x)}{h} \,, \\ \left(D_n^{-h}\psi\right)(x) &= \frac{\psi(x) - \psi(x - he_n)}{h} \,. \end{aligned} \tag{2.3.13}$$

Note that the difference quotients are usually not defined for all $x \in \Omega$.

Lemma 2.3.5. *Let $\psi, \varphi \in L^2_{loc}(\Omega)$ be two functions with one function having compact support in Ω. Then, for h small enough, we have the partial summation rule*

$$\langle \psi, D_n^{+h}\varphi\rangle_{\mathcal{H}} = -\langle D_n^{-h}\psi, \varphi\rangle_{\mathcal{H}}. \tag{2.3.14}$$

Theorem 2.3.6. *Let $\Omega_0 \Subset \Omega$ be an open subset which is compactly contained in Ω. Then there exists $h_0(\Omega_0) > 0$, depending on the set Ω_0, such that for $0 \leq h \leq$*

$h_0(\Omega_0)$ we have

$$\|D_n^{+h}\psi\|_{L^2(\Omega_0)} \leq \|\partial_n\psi\|_{L^2(\Omega)}, \quad \forall\psi \in H^1(\Omega). \tag{2.3.15}$$

Furthermore, let $\psi \in L^2(\Omega)$ be such that $\|D_n^{+h}\psi\|_{L^2(\Omega_0)} \leq K$ for all $\Omega_0 \Subset \Omega$ and all $0 \leq h \leq h_0(\Omega_0)$, then ψ is weakly differentiable with respect to x_n and we have

$$\|\partial_n\psi\|_{L^2(\Omega)} \leq K. \tag{2.3.16}$$

3. FUNDAMENTALS OF ONE-PARTICLE QUANTUM GRAPHS AND (QUANTUM) CHAOS

In this chapter, we briefly describe the basic features of one-particle quantum graphs as well as (quantum) chaos. The classical configuration space of a quantum graph is a compact metric graph, i.e. a finite graph $\Gamma = (\mathcal{V}, \mathcal{E})$ with vertices $\mathcal{V} = \{1, ..., V\}$ and edges $\mathcal{E} = \{1, ..., E\}$. To each edge $e \in \mathcal{E}$, we associate an interval $(0, l_e)$ and a corresponding coordinate $x_e \in (0, l_e)$. Accordingly, functions on the graph are collections of functions on the edges, i.e.

$$F = (f_1, \ldots, f_E) \quad \text{with} \quad f_e : (0, l_e) \to \mathbb{C}, \tag{3.0.1}$$

so that spaces of functions on Γ are (finite) direct sums of the respective spaces of functions on the edges. For example, the one-particle Hilbert space is defined by

$$\mathcal{H}_1 = L^2(\Gamma) = \bigoplus_{e=1}^{E} L^2(0, l_e), \tag{3.0.2}$$

and, in the same way, Sobolev spaces of order $m \in \mathbb{N}$ are given by

$$H^m(\Gamma) = \bigoplus_{e=1}^{E} H^m(0, l_e). \tag{3.0.3}$$

As it is standard in quantum mechanics, one now introduces a Hamiltonian on the Hilbert space. On quantum graphs, the most prominent Hamiltonian is the one-particle Laplacian $-\Delta_1$. This operator acts on $F \in C^\infty(\Gamma)$ via

$$-\Delta_1 F = (-f_1'', \ldots, -f_E'') \tag{3.0.4}$$

and hence acts as the standard one-dimensional Laplacian on each component of the wave function. We here use the index 1 to indicate that this is a one-

particle Laplacian in order to distinguish it, later on, from the two- or many-particle Laplacian. Note that, although the operator (3.0.4) is the most prominent Hamiltonian on one-particle quantum graphs, one could also add an additional interaction term $\hat{V}$ to (3.0.4) in order to account for external potentials along the edges. In this case, the associated Hamiltonian $\hat{H}$ is

$$\hat{H} = -\Delta_1 + \hat{V}. \tag{3.0.5}$$

For example, if $\hat{V}$ is a diagonal and bounded multiplication operator, one has

$$(\hat{H}F)_e = -f_e'' + V_e f_e, \quad \forall e \in \mathcal{E}, \tag{3.0.6}$$

for functions $F \in C^\infty(\Gamma)$. Note that Hamiltonians of the form (3.0.5), introducing electric or magnetic potentials along the edges, are also frequently considered [GS06]. For theoretical reasons, the introduction of magnetic potentials is interesting since they can generate a breaking of the time-reversal symmetry [Sch97]. Such symmetries are important, for example, in the field of quantum chaos since they determine to which ensemble of random matrices the system can be associated [Haa91].

3.1 Self-adjoint realisations of the one-particle Laplacian

As mentioned before, in quantum mechanics one usually requires the Hamiltonian to be self-adjoint. In order to characterise self-adjoint realisations of the one-particle Laplacian $-\Delta_1$, we begin by considering it on the set of all infinitely differentiable functions with compact support.

Lemma 3.1.1. *The operator* $(-\Delta_1, C_0^\infty(\Gamma))$ *is densely defined and symmetric.*

Proof. Let $I = (a, b)$ be an open interval. A standard result in integration theory then states that $C_0^\infty(I) \subset L^2(I)$ is dense [Dob05]. Since $L^2(\Gamma)$ is a direct sum of L^2-spaces over intervals, density follows directly. For two functions $\Psi, \Phi \in C_0^\infty(\Gamma)$,

we calculate

$$\begin{aligned}\langle \Phi, -\Delta_1 \Psi \rangle_{L^2(\Gamma)} &= -\sum_{e=1}^{E} \int_0^{l_e} \bar{\varphi}(x_e)\psi''(x_e)\, \mathrm{d}x_e \\ &= -\sum_{e=1}^{E} \big(\bar{\varphi}(x_e)\psi'(x_e) - \bar{\varphi}'(x_e)\psi(x_e)\big)_0^{l_e} + \langle -\Delta_1 \Phi, \Psi \rangle_{L^2(\Gamma)} \\ &= \langle -\Delta_1 \Phi, \Psi \rangle_{L^2(\Gamma)}.\end{aligned} \tag{3.1.1}$$

Since the functions are in $C_0^\infty(\Gamma)$, we could integrate by parts and since they have compact support, the term containing the boundary values vanishes. Hence, the operator is symmetric. □

However, the operator $(-\Delta_1, C_0^\infty(\Gamma))$ is *not* self-adjoint. The idea is now to look for (symmetric) extensions of this operator in order to enlarge its domain in such a way that it finally becomes self-adjoint. The basic theorem, on which this idea is based, is a standard result in operator theory.

Theorem 3.1.2. *[BB93] Let $\mathcal{H}$ be a Hilbert space and $\hat{A}, \hat{B}$ two densely defined and symmetric operators such that*

$$\hat{A} \subseteq \hat{B}. \tag{3.1.2}$$

Denoting the corresponding adjoint operators as $\hat{A}^*$ and $\hat{B}^*$, we have the inclusion

$$\hat{B}^* \subseteq \hat{A}^*. \tag{3.1.3}$$

Hence, by enlarging the domain of a densely defined and symmetric operator $\hat{A}$, the domain of its adjoint $\hat{A}^*$ becomes smaller. Since one always has the inclusion $\hat{A} \subset \hat{A}^*$, one hopes to enlarge the domain of $\hat{A}$ such that it finally becomes self-adjoint. Now, let

$$F_{bv} = \big(f_1(0), \ldots, f_E(0), f_1(l_1), \ldots, f_E(l_E)\big)^T \in \mathbb{C}^{2E} \tag{3.1.4}$$

be a vector that contains the boundary values of a function $F \in H^1(\Gamma)$ and

$$F'_{bv} = \big(f'_1(0), \ldots, f'_E(0), -f'_1(l_1), \ldots, -f'_E(l_E)\big)^T \in \mathbb{C}^{2E} \tag{3.1.5}$$

an additional vector for functions $F \in H^2(\Gamma)$ that contains the boundary values of its derivative. Then, using this notation and based on the idea introduced above, Kostrykin and Schrader characterised all self-adjoint realisations of the one-particle Laplacian $-\Delta_1$.

Theorem 3.1.3. *[KS99] Any self-adjoint realisation of the Laplacian on a compact, metric graph has a domain of the form*

$$\mathcal{D}_1(A,B) = \{F \in H^2(\Gamma);\ AF_{bv} + BF'_{bv} = 0\}, \tag{3.1.6}$$

where $A, B \in \mathrm{M}(2E, \mathbb{C})$ *are such that* $\mathrm{rank}(A,B) = 2E$ *and* AB^* *is self-adjoint.*

Moreover, two such realisations with domains $\mathcal{D}(A,B)$ *and* $\mathcal{D}(A',B')$ *are equivalent, iff there exists* $C \in \mathrm{GL}(2E,\mathbb{C})$ *such that* $A' = CA$ *and* $B' = CB$.

Remark 3.1.4. In order to clarify the notation, we consider an example which will also be of interest in the last chapter of the thesis when we discuss Bose-Einstein condensation. To this end, let Γ be a graph with two edges $\mathcal{E} = \{e_1, e_2\}$, each of length l, and three vertices $\mathcal{V} = \{v_1, v_2, v_3\}$. Intuitively, one should think of the interval $(-l, +l)$ with an additional vertex placed at the origin. Furthermore, we choose the boundary conditions

$$AF_{bv} + BF'_{bv} = 0 \tag{3.1.7}$$

with maps

$$A = \begin{pmatrix} 1 & -1 & 0 & 0 \\ -\alpha & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{3.1.8}$$

where $\alpha > 0$ is some constant. The interesting property of this example is that the boundary conditions (3.1.7) are the same as the boundary conditions (at $x = 0$) in a one-particle system moving on the interval $(-l, +l)$ and whose (formal) Hamiltonian is given by

$$\hat{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \alpha\delta(x). \tag{3.1.9}$$

Indeed, it is well known that a delta potential leads (at $x = 0$) to the conditions

$$\begin{aligned} \psi(0^+) &= \psi(0^-), \\ \psi'(0^+) - \psi'(0^-) &= \alpha\psi(0^+), \end{aligned} \tag{3.1.10}$$

where $\psi \in H^2((-l, 0) \cup (0, +l))$ is some function. Now, it is straightforward to check that the boundary conditions (3.1.10) equal, at the origin, the conditions (3.1.7) with maps (3.1.8).

Remark 3.1.5. As established in the previous example, boundary conditions on a one-particle quantum graph can be regarded as the result of external potentials, localised at the vertices of the graph.

Besides the approach of Kostrykin and Schrader, there exists another approach to characterise self-adjoint realisations of the one-particle Laplacian $-\Delta_1$ which is due to Kuchment [Kuc04]. Indeed, it is this approach that will provide us with the starting point to characterise self-adjoint realisations of the two- and many-particle Laplacian in later chapters. To introduce this approach, let $P \in \mathrm{M}(2E, \mathbb{C})$ and $L \in \mathrm{M}(2E, \mathbb{C})$ be two matrices such that

1. P is an orthogonal projection;
2. L is a self-adjoint endomorphism on $\ker P \subset \mathbb{C}^{2E}$.

Moreover, we set $Q = \mathbb{1}_{2E} - P$. Note that the second condition implies that Q commutes with L when acting on elements in the kernel of P. Indeed, since L is a self-adjoint endomorphism one concludes that $PL = LP$ on $\ker P$ from which one immediately gets $QL = LQ$ on $\ker P$. Now, one can define the quadratic form

$$Q^{(1)}_{P,L}[F] = \sum_{e=1}^{E} \int_0^{l_e} |f_e'(x)|^2 \, \mathrm{d}x - \langle F_{bv}, LF_{bv} \rangle_{\mathbb{C}^{2E}} \tag{3.1.11}$$

with domain

$$\mathcal{D}_{Q^{(1)}} = \{F \in H^1(\Gamma);\ PF_{bv} = 0\}. \tag{3.1.12}$$

Lemma 3.1.6. *[Kuc04] The quadratic form $Q^{(1)}_{P,L}$ is symmetric, closed and bounded from below.*

Proof. Let $\Psi, \Phi \in \mathcal{D}_{Q^{(1)}}$ be two functions. Taking the self-adjointness of L into account, we have

$$\begin{aligned} Q^{(1)}_{P,L}[\Psi,\Phi] &= \sum_{e=1}^{E} \int_0^{l_e} \bar{\psi}'(x_e)\varphi'(x_e)\, \mathrm{d}x_e - \langle \Psi_{bv}, L\Phi_{bv}\rangle_{\mathbb{C}^{2E}} \\ &= \overline{Q^{(1)}_{P,L}[\Phi,\Psi]}, \end{aligned} \tag{3.1.13}$$

and hence $Q^{(1)}_{P,L}$ is symmetric. Furthermore,

$$Q^{(1)}_{P,L}[\Psi] \geq \|\Psi'\|^2_{L^2(\Gamma)} - L_{\max}\|\Psi_{bv}\|^2_{\mathbb{C}^{2E}}, \tag{3.1.14}$$

where $L_{\max}$ is the largest eigenvalue of the matrix L. Using the estimate

$$\|\Psi_{bv}\|^2_{\mathbb{C}^{2E}} \leq \delta\|\Psi'\|^2_{L^2(\Gamma)} + \frac{2}{\delta}\|\Psi\|^2_{L^2(\Gamma)}, \quad \forall \delta \leq l_{\min}, \tag{3.1.15}$$

as established in [Kuc04], we arrive at

$$\begin{aligned} Q^{(1)}_{P,L}[\Psi] &\geq (1 - L_{\max}\delta)\|\Psi'\|^2_{L^2(\Gamma)} - \frac{2L_{\max}}{\delta}\|\Psi\|^2_{L^2(\Gamma)} \\ &\geq -\frac{2L_{\max}}{\delta}\|\Psi\|^2_{L^2(\Gamma)}, \end{aligned} \tag{3.1.16}$$

for δ small enough. Hence, the form is bounded from below. Finally, consider the form norm

$$\|\cdot\|^2_{Q^{(1)}_{P,L}} = Q^{(1)}_{P,L}[\Psi] + (\lambda_{\max}+1)\|\Psi\|^2_{L^2(\Gamma)}, \tag{3.1.17}$$

where we have set $\lambda_{\max} = \frac{2L_{\max}}{\delta}$.

Proposition 3.1.7. *On $H^1(\Gamma)$, the form norm $\|\cdot\|_{Q^{(1)}_{P,L}}$ is equivalent to the H^1-norm $\|\cdot\|_{H^1(\Gamma)}$.*

Proof. Let $\Psi \in H^1(\Gamma)$ be some function. Using (3.1.15) we have

$$\begin{aligned} \|\Psi\|^2_{Q^{(1)}_{P,L}} &= Q^{(1)}_{P,L}[\Psi] + (\lambda_{\max}+1)\|\Psi\|^2_{L^2(\Gamma)} \\ &\leq (1+\delta L_{\max})\|\Psi'\|^2_{L^2(\Gamma)} + (2\lambda_{\max}+1)\,\|\Psi\|^2_{L^2(\Gamma)} \\ &\leq c_1\|\Psi\|^2_{H^1(\Gamma)} \end{aligned} \tag{3.1.18}$$

for some $\delta \leq l_{\min}$ and $c_1 > 0$ some constant. Furthermore, using (3.1.16) we

directly obtain

$$\begin{aligned} \|\Psi\|^2_{Q^{(1)}_{P,L}} &= Q^{(1)}_{P,L}[\Psi] + (\lambda_{\max}+1)\|\Psi\|^2_{L^2(\Gamma)} \\ &\geq (1-\delta L_{\max})\,\|\Psi'\|^2_{L^2(\Gamma)} + \|\Psi\|^2_{L^2(\Gamma)} \\ &\geq c_2\|\Psi\|^2_{H^1(\Gamma)}, \end{aligned} \tag{3.1.19}$$

for δ small and $c_2 > 0$ some constant. □

Now, let $\{\Psi_n\}_{n\in\mathbb{N}} \in \mathcal{D}_{Q^{(1)}}$ be a Cauchy sequence with respect to the form norm. Since it is equivalent to the H^1-norm, we immediately conclude that $\{\Psi_n\}_{n\in\mathbb{N}}$ is a Cauchy-Sequence in $H^1(\Gamma)$. By the completeness of $H^1(\Gamma)$, there exists a function $\Psi \in H^1(\Gamma)$ such that

$$\|\Psi - \Psi_n\|^2_{Q^{(1)}_{P,L}} \leq \epsilon, \tag{3.1.20}$$

for all $n \geq n_0$ and arbitrary small ϵ. Furthermore,

$$\begin{aligned} \|P\Psi_{bv}\|^2_{\mathbb{C}^{2E}} &\leq \|P\|_{op}\|\Psi_{bv} - \Psi_{n;bv}\|^2_{\mathbb{C}^{2E}} \\ &\leq \|P\|_{op}\left(\delta\|\Psi' - \Psi'_n\|^2_{L^2(\Gamma)} + \frac{2}{\delta}\|\Psi - \Psi_n\|^2_{L^2(\Gamma)}\right) \\ &\leq \epsilon, \end{aligned} \tag{3.1.21}$$

for $\delta \leq l_{\min}$ and $\|P\|_{op}$ the operator norm of P. Hence, we conclude that $P\Psi_{bv} = 0$ and $\Psi \in \mathcal{D}_{Q^{(1)}}$ which implies that the form $Q^{(1)}_{P,L}$ is closed. □

Now, by the standard representation theorem of quadratic forms [Kat66], there exists a unique self-adjoint operator associated with each form (3.1.11). In fact, as shown in the next theorem, this operator is the one-particle Laplacian $-\Delta_1$ with a suitable domain.

Theorem 3.1.8. *[Kuc04] The unique, self-adjoint and semi-bounded operator associated with the quadratic form* (3.1.11) *is the one-particle Laplacian* $-\Delta_1$ *with domain*

$$\mathcal{D}_1(P,L) = \{F \in H^2(\Gamma);\ PF_{bv} = 0 \text{ and } QF'_{bv} + LQF_{bv} = 0\}. \tag{3.1.22}$$

Proof. The starting point is the quadratic form (3.1.11). We denote the associated self-adjoint operator by $(\hat{\mathcal{H}}, \mathcal{D}(\hat{\mathcal{H}}))$. According to [Kat66], the domain $\mathcal{D}(\hat{\mathcal{H}})$

consists of all $\Phi \in \mathcal{D}_{Q^{(1)}}$ for which there exists a $\Lambda \in L^2(\Gamma)$ such that the relation

$$Q^{(1)}_{P,L}[\Psi, \Phi] = \langle \Psi, \Lambda \rangle_{L^2(\Gamma)} \tag{3.1.23}$$

holds for all $\Psi \in \mathcal{D}_{Q^{(1)}}$. Note that the action of $\hat{\mathcal{H}}$ is then given by $\hat{\mathcal{H}}\Phi = \Lambda$. Now, choosing $\Psi \in C_0^\infty(\Gamma)$, we calculate

$$\begin{aligned} Q^{(1)}_{P,L}[\Psi, \Phi] &= \sum_{e=1}^{E} \int_0^{l_e} \bar{\psi}'(x_e)\varphi'(x_e)\, \mathrm{d}x_e \\ &= -\sum_{e=1}^{E} \int_0^{l_e} \bar{\psi}''(x_e)\varphi(x_e)\, \mathrm{d}x_e = \langle \Psi, \Lambda \rangle_{L^2(\Gamma)}. \end{aligned} \tag{3.1.24}$$

Comparing the last line of (3.1.24) with Definition 2.2.1 of the second weak derivative implies that $\Phi \in H^2(\Gamma)$. Furthermore, using the fundamental lemma of variational calculus [Dob05], we conclude that the operator $\hat{\mathcal{H}}$ acts as the negative second derivative, i.e. the Laplacian in one dimension.
Now, let $\Psi \in \mathcal{D}_{Q^{(1)}}$ and calculate

$$\begin{aligned} Q^{(1)}_{P,L}[\Psi, \Phi] &= \sum_{e=1}^{E} \int_0^{l_e} \bar{\psi}'(x_e)\varphi'(x_e)\, \mathrm{d}x_e - \langle \Psi_{bv}, L\Phi_{bv} \rangle_{\mathbb{C}^{2E}} \\ &= -\sum_{e=1}^{E} \int_0^{l_e} \bar{\psi}(x_e)\varphi''(x_e)\, \mathrm{d}x_e - \langle \Psi_{bv}, \Phi'_{bv} + L\Phi_{bv} \rangle_{\mathbb{C}^{2E}}. \end{aligned} \tag{3.1.25}$$

Since the operator $\hat{\mathcal{H}}$ is the one-dimensional Laplacian, the second term on the right-hand side must vanish. Furthermore, since $P\Psi_{bv} = 0$ and P is a projection, we conclude that $Q\Phi'_{bv} + QL\Phi_{bv} = 0$. Finally, we take into account that by definition L and Q commute when acting on elements in $\ker P$. □

Remark 3.1.9. [Kuc04] Above we characterised all self-adjoint realisations of the one-particle Laplacian in two different ways. However, these two approaches are connected as follows: P is the orthogonal projection onto $\ker B \subset \mathbb{C}^{2E}$ and L is the self-adjoint endomorphism $L = (B|_{\operatorname{ran} B^*})^{-1} AQ$ of $\mathbb{C}^{2E}$ (see [Kuc04] for a detailed construction). Note that $(B|_{\operatorname{ran} B^*})^{-1}$ is the inverse of the map $Q_1 BQ : \operatorname{ran} B^* \to \operatorname{ran} B$, $Q_1 = \mathbb{1} - P_1$ and P_1 the projection on $\ker B^*$.

Finally, we want to distinguish between *local* and *non-local* boundary condi-

tions. Local boundary conditions respect the graph structure, i.e. the boundary conditions are called local whenever all matrices $M \in \{A, B; P, L\}$ have the block structure

$$M = \bigoplus_{v=1}^{V} M_v. \tag{3.1.26}$$

Here M_v, corresponding to the vertex v, connects only such components of F_{bv} and F'_{bv} that end or start in the vertex v. For instance, the boundary conditions of Example (3.1.8) are local boundary conditions. For physical reasons, non-local boundary conditions are often discarded [BE09].

3.2 The spectrum of the one-particle Laplacian

In this section, we discuss spectral properties of the Laplacian $(-\Delta_1, \mathcal{D}_1(A, B))$ or, equivalently, $(-\Delta_1, \mathcal{D}_1(P, L))$.

Proposition 3.2.1. *[KS06] Let $(-\Delta_1, \mathcal{D}_1(A, B))$ be a self-adjoint realisation of the one-particle Laplacian on a compact quantum graph. Then, its resolvent is a compact operator and hence the spectrum is purely discrete.*

Most importantly, on one-particle quantum graphs, one can calculate the (positive) eigenvalues directly as roots of the so-called *secular function*. This property is crucial, for example, for the derivation of the trace formula on graphs [KS97b, BE09]. Following the presentation in [KS06, BE09], we define the *scattering matrix* of the graph by

$$S(k) = -(A + ikB)^{-1}(A - ikB) \tag{3.2.1}$$

or, in terms of the maps P and L,

$$S(k) = -P - Q(L + ik)^{-1}(L - ik)Q, \tag{3.2.2}$$

see [BE09]. Note that the scattering matrix (3.2.1) is unitary for all $k \in \mathbb{R}\backslash\{0\}$

[KS06]. Furthermore, we define

$$T(\mathbf{l};k) = \begin{pmatrix} 0 & t(\mathbf{l};k) \\ t(\mathbf{l};k) & 0 \end{pmatrix} \qquad \text{with} \qquad t(\mathbf{l};k) = \begin{pmatrix} e^{ikl_1} & & \\ & \ddots & \\ & & e^{ikl_E} \end{pmatrix}, \tag{3.2.3}$$

where $k \in \mathbb{C}$ and set

$$U(k) = S(k)T(\mathbf{l};k). \tag{3.2.4}$$

Note that $U(k)$ is, for $k \in \mathbb{R}\backslash\{0\}$, a unitary matrix [BE09]. The secular function $F(k)$ is then defined by

$$F(k) = \det\left(\mathbb{1} - U(k)\right) \tag{3.2.5}$$

and we have the following statement.

Theorem 3.2.2. *[KS06] The number $k^2 > 0$ is an eigenvalue of $-\Delta_1$ iff k is a zero of (3.2.5), i.e. $F(k) = 0$. Moreover, the spectral multiplicity of the Laplace eigenvalue $k^2 > 0$ coincides with the multiplicity of the eigenvalue one of $U(k)$.*

Introducing the counting function

$$N(K) = \#\{n \in \mathbb{N} \mid k_n^2 \leq K^2\}, \tag{3.2.6}$$

where the eigenvalues are counted with their multiplicities, one has the following result.

Lemma 3.2.3. *[BE09] Let $(-\Delta_1, \mathcal{D}_1(P,L))$ be a self-adjoint realisation of the one-particle Laplacian on a compact quantum graph. Then, the corresponding counting function $N(K)$ fulfils the asymptotic law*

$$N(K) \sim \frac{\mathcal{L}}{\pi}K, \quad K \to \infty, \tag{3.2.7}$$

where $\mathcal{L} = \sum_{e=1}^{E} l_e$ is the length of the graph.

Proof. Without loss of generality, we restrict ourselves to an interval of length l. As a first step, we consider the Dirichlet-Laplacian, i.e. we choose $P_D = \mathbb{1}$ and

$L_D = 0$. In this case, the eigenvalues are $\left\{\frac{n^2\pi^2}{l^2}\right\}_{n\in\mathbb{N}}$ and therefore

$$\begin{aligned} N_D(K) = \#\left\{n \in \mathbb{N} \mid n \leq \frac{Kl}{\pi}\right\} &= \left\lfloor \frac{Kl}{\pi} \right\rfloor \\ &= \frac{Kl}{\pi} - \mu(K), \end{aligned} \tag{3.2.8}$$

with $|\mu(K)| \leq 1$. From this, we readily see that the asymptotic law (3.2.7) is indeed fulfilled. As a next step, we consider the Robin-Laplacian, i.e. we choose $P_R = 0$ and $L_R = \lambda \mathbb{1}$ with $\lambda = \|L\|_{op}$. As shown in [BE09], its positive eigenvalues (which have multiplicity one) are the squares of the (positive) solutions $k_n > 0$ of

$$\left(\frac{\lambda - ik_n}{\lambda + ik_n}\right)^2 e^{2ik_n l} = 1. \tag{3.2.9}$$

Now, solving (3.2.9) yields the condition

$$\tan(k_n l) = \frac{2\lambda k_n}{\lambda^2 - k_n^2} \tag{3.2.10}$$

from which we can infer that large eigenvalues k_n^2 differ only little from corresponding Dirichlet eigenvalues. More precisely, for all $k_n \geq K_0$ with $K_0 \in \mathbb{R}^+$ large enough, we can write

$$k_n = \frac{\pi n}{l} + \epsilon_n, \tag{3.2.11}$$

with $|\epsilon_n| \to 0$ for $n \to \infty$. In particular, we can assume that $|\epsilon_n| < \epsilon$ with $\epsilon > 0$ some small number. Now, defining

$$N(K_0, K) = \#\left\{n \in \mathbb{N} \,|K_0^2 \leq\ k_n^2 \leq K^2\right\}, \tag{3.2.12}$$

we obtain

$$N_D(K_0, K - \epsilon) \leq N_R(K_0, K) \leq N_D(K_0, K + \epsilon), \tag{3.2.13}$$

and hence $N_R(K)$ shows the asymptotic law (3.2.7). Finally, using the Dirichlet-Neumann bracketing for quadratic forms as described in [RS78], it was shown in [BE09] that

$$N_D(K) \leq N(K) \leq N_R(K), \tag{3.2.14}$$

and hence the asymptotic law (3.2.7) holds for all self-adjoint realisations of the

one-particle Laplacian. □

3.3 Fundamentals of chaos

In this section, we want give a brief introduction to fundamental concepts in classical chaos as well as quantum chaos [Ber89, KS97a]. We will also discuss the connection of quantum graphs with quantum chaos as introduced in [KS97b].
In classical mechanics, the phase space P of N particles moving in d dimensions is given by $P = \mathbb{R}^{dN} \times \mathbb{R}^{dN}$, with $\mathbf{q} \in \mathbb{R}^{dN}$ denoting the positions and $\mathbf{p} \in \mathbb{R}^{dN}$ the momenta of the particles. On the phase space, a sufficiently smooth *Hamiltonian* function $H : P \to \mathbb{R}$ is defined that governs the motion of the particles through the equations of motion, i.e.

$$\dot{\mathbf{q}} = \frac{\partial H(\mathbf{q}, \mathbf{p})}{\partial \mathbf{p}} , \qquad \dot{\mathbf{p}} = -\frac{\partial H(\mathbf{q}, \mathbf{p})}{\partial \mathbf{q}} . \tag{3.3.1}$$

Through these equations, the Hamiltonian function induces a flow $\Phi_t : P \to P$ on the phase space that describes the trajectories of the particles.

Definition 3.3.1. Let $H \in C^2(P)$ be a Hamiltonian function generating the flow Φ_t through the equations of motion (3.3.1). We then call (P, H, Φ_t) a *Hamiltonian system*.

In Hamiltonian systems, the total energy E is conserved under the flow Φ_t, i.e. the trajectory of the particles is restricted to a subset of P, called the *energy shell*, consisting of all points $(\mathbf{q}, \mathbf{p}) \in P$ for which

$$H(\mathbf{q}, \mathbf{p}) = E . \tag{3.3.2}$$

Chaotic motion of a system then manifests itself in the nature of the flow Φ_t that describes the trajectories of the particles. In general, one would like to distinguish between two different aspects of chaotic motion, i.e. hyperbolicity and ergodicity. Whereas hyperbolicity refers to the local instability of the trajectories as expressed in terms of Lyapunov exponents [BP00], ergodicity refers to a more global aspect of chaotic motion. Loosely speaking, a system exhibits ergodic motion if the trajectory $\mathbf{r}(t) = (\mathbf{q}(t), \mathbf{p}(t))$ covers the whole energy shell densely in the course of time. To introduce the notion of ergodicity in general, let (X, Σ, μ) be a probability

space where X is some set with σ-algebra Σ and probability measure μ [Kle08].

Definition 3.3.2. [Kle08] Let $\{\Phi_t\}_{t\in\mathbb{R}}$ be a one-parameter group of measure-preserving transformations, i.e.

$$\Phi_0 = \mathbb{1} \quad \text{and} \quad \Phi_{t_1} \circ \Phi_{t_2} = \Phi_{t_1+t_2} \tag{3.3.3}$$

as well as

$$\mu(\Phi_t(A)) = \mu(A), \quad \forall t \in \mathbb{R}, \forall A \in \Sigma. \tag{3.3.4}$$

Then (X, Σ, μ, Φ_t) is called a μ-invariant dynamical system.

Definition 3.3.3. [Kle08] Let (X, Σ, μ, Φ_t) be a μ-invariant dynamical system and consider the set of Φ_t-invariant sets, i.e.

$$I = \{A \in \Sigma \mid \forall t : \Phi_t(A) = A\}. \tag{3.3.5}$$

Then, the flow Φ_t is called ergodic if

$$\mu(A) \in \{0, 1\}, \quad \forall A \in I. \tag{3.3.6}$$

Note that ergodic systems are important in the context of statistical mechanics. Indeed, the famous *Ergodic hypothesis* as introduced by Boltzmann states that, for thermodynamical systems, the time-average of an observable should equal the ensemble (phase-space) average [GBG04, Far64]. For ergodic systems, this is in fact the case as expressed in the following theorem of Birkhoff.

Theorem 3.3.4. *[KS97a] Let (X, Σ, μ, Φ_t) be a μ-invariant dynamical system with an ergodic flow Φ_t. Then, for any function $f \in L^1(X, \Sigma, \mu)$, the limits*

$$\bar{f}^{\pm}(x) = \lim_{t\to\infty} \frac{1}{t} \int_0^t f(\Phi_{\pm s}(x)) \, \mathrm{d}s \tag{3.3.7}$$

exist for almost every $x \in X$. Also, one has

$$\bar{f}^{+}(x) = \bar{f}^{-}(x) := \bar{f}(x) \tag{3.3.8}$$

and

$$\bar{f}(x) = \int f(z) \, \mathrm{d}\mu(z). \tag{3.3.9}$$

Besides the notion of ergodicity, there exists another type of dynamics which is associated to chaotic motion. Indeed, systems with *mixing* dynamics exhibit a higher degree of chaos.

Definition 3.3.5. [Kle08] A μ-invariant dynamical system (X, Σ, μ, Φ_t) is called mixing if

$$\lim_{|t|\to\infty} \mu(\Phi_t(A) \cap B) = \mu(A)\mu(B), \quad \forall A, B \in \Sigma. \tag{3.3.10}$$

Lemma 3.3.6. *[Kle08] Mixing systems are ergodic.*

Having introduced concepts of chaotic motion in classical mechanics, one would like to establish similar concepts in the quantum mechanical description of a system. However, there are fundamental conceptual problems. For example, since the notion of a trajectory loses its meaning, the definition of chaos as a local instability of trajectories (hyperbolicity) seems not possible. Also, since there is no notion of phase space in quantum mechanics, our definition of ergodicity cannot be carried over directly to the quantum describtion. However, based on the correspondence principle, one should nevertheless be able to identify signatures of chaos in quantum mechanics [Haa91]. Indeed, to find and understand such signatures is the main object of quantum chaos [Ber89, Gut90, Haa91].
The quantum mechanical description of a system relies heavily on the eigenstates and the eigenspectrum of the corresponding Hamiltonian. It is therefore convenient, while searching for signatures of chaos, to study those quantities more closely. To this end, let $\Omega \subset \mathbb{R}^2$ be an open bounded convex subset (billiard) such that the unit normal vector has Lipschitz regularity [GL93] and consider, as a Hamiltonian, the two-dimensional Laplacian with Dirichlet boundary conditions. Interestingly enough, given the classical dynamics is ergodic, one can show that the quantum motion follows closely the classical one in the sense that the eigenfunctions become, in the high-energy limit, smeared evenly over the complete billiard.

Theorem 3.3.7. *[GL93] Let $\Omega \subset \mathbb{R}^2$ be a billiard of area $|\Omega|$ as introduced above with an ergodic billiard flow and let $\{\varphi_n\}_{n\in\mathbb{N}_0}$ be the eigenfunctions of the Dirichlet Laplacian with eigenvalues $\{\lambda_n\}_{n\in\mathbb{N}_0}$. Then, there exists a subsequence $\{n_k\}_{n_k\in\mathbb{N}} \subset \{n\}_{n\in\mathbb{N}}$ of asymptotic density one such that*

$$\lim_{n_k\to\infty} \int_{B\subset\Omega} |\varphi_{n_k}(x)|^2 \, \mathrm{d}x = \frac{|B|}{|\Omega|} \tag{3.3.11}$$

holds for all (Lebegue measurable) subsets $B \subset \Omega$ with area $|B|$.

Remark 3.3.8. Since Theorem 3.3.7 accounts for almost all eigenfunctions only, there may be eigenfunctions that are localised. This phenomenon is generally known as *scarring* [Hel84].

As already mentioned in the introduction, signatures of chaos can also be found in spectral correlations. Indeed, it was observed that the eigenvalues of a system whose classical counterpart belongs to an important class of non-ergodic systems, so called integrable systems, are distributed very differently than those of a system whose classical analogue is chaotic [Haa91]. Note that an N-particle system moving in d dimensions is called integrable if there exist Nd constants of motion which are in involution [Arn78]. Most importantly, for integrable systems, one can introduce action-angle variables (I_n, φ_n), $n = 1, ..., Nd$, such that the Hamiltonian function depends on the actions $\mathbf{I} = (I_1, ..., I_{Nd})^T$ only, i.e. $H = H(\mathbf{I})$. This then allows for a straightforward quantisation which is the reason why integrable system were of primary interest in the early days of quantum mechanics [Gut90]. More precisely, the quantisation rules are given by

$$I_l = \frac{1}{2\pi} \oint_{\Gamma_l} \mathbf{p} \cdot \mathrm{d}\mathbf{q} = \left(n_l + \frac{\mu_l}{4} \right) \hbar, \quad l = 1, ..., Nd, \tag{3.3.12}$$

where $n_l = 0, 1, 2, ...$ are natural quantum numbers and $\mu_l \in \mathbb{N}_0$ are the Maslov indices, i.e. integers characterised by the topology of the classical dynamics [Gut90, MF81]. Furthermore, $\Gamma_1, ..., \Gamma_{Nd}$ are topologically independent paths on the phase space which, as expressed in the famous theorem of Liouville-Arnold, foliates into invariant tori [Arn78, Kna12].

Remark 3.3.9. A simple system for which the quantisation rule (3.3.12) applies is the harmonic oscillator in one dimension. Indeed, already for this rather simple example, it is necessary to include the Maslov indices $\mu = 2$ in order to arrive at the correct energy eigenvalues.

Now, consider the nearest-neighbour level spacings distribution

$$P(s) = \lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N} \delta \left(s - (E_{n+1} - E_n) \right), \tag{3.3.13}$$

where the eigenvalues $\{E_n\}_{n\in\mathbb{N}_0}$ are rescaled such that the mean level density is one. Then, for an integrable system and according to the Berry-Tabor conjecture [BT77], it is expected that $P(s)$ follows Poisson statistics, i.e.

$$P(s) = e^{-s}. \tag{3.3.14}$$

This means that the eigenvalues of an integrable system tend to cluster since small spacings $s > 0$ are preferred. For a generic chaotic system, the situation is completely different. Following the conjecture of Bohigas-Gianonni-Schmit [BGS84], the level spacings distribution $P(s)$ is expected to be the same as for an ensemble of random matrices which is associated with the system according to its symmetries [Dys62, Stö99, Haa91]:

1. The Gaussian Unitary Ensemble (GUE) is associated with a system without time-reversal symmetry.

2. The Gaussian Orthogonal Ensemble (GOE) is associated with a system with time-reversal symmetry and $T^2 = 1$.

3. The Gaussian Symplectic Ensemble (GSE) is associated with a system with time-reversal symmetry and $T^2 = -1$.

Note that T denotes the (anti-unitary) time-reversal operator [Haa91]. In contrast to (3.3.14), the nearest-neighbour level spacings distribution of a system associated to one of the ensembles above is such that

$$P(s) \sim s^\beta, \quad s \to 0, \tag{3.3.15}$$

with $\beta = 1, 2, 4$ [Haa91]. Hence, in contrast to integrable systems, larger spacings $s > 0$ are preferred, i.e. one observes level-repulsion.
As illustrated above, the first quantisation rules (3.3.12) allowed to determine the eigenspectrum of an integrable systems based on classical properties only. For a chaotic system, however, these rules cannot be applied and no direct link to classical mechanics seems possible. Interestingly enough, using a semiclassical approximation, Gutzwiller was able to relate the eigenspectrum of a classically chaotic system to periodic orbits in phase space (here we shall assume that the periodic orbits are isolated and unstable) [Gut71, Gut90]. More precisely, writing

the spectral density of a system with eigenvalues $\{E_n\}_{n\in\mathbb{N}_0}$ as

$$\begin{aligned} d(E) &= \sum_n \delta(E - E_n), \\ &\underset{\hbar\to 0}{\sim} \bar{d}(E) + d_{osc}(E), \end{aligned} \tag{3.3.16}$$

where $\bar{d}(E)$ represents the smoothed density of states [Rob91], Gutzwiller established the relation

$$d_{osc}(E) = \frac{1}{\pi\hbar} \sum_{po} T_{ppo} A_{po} \cos\left(\frac{S_{po}}{\hbar} - \mu_{po}\frac{\pi}{2}\right). \tag{3.3.17}$$

Here the sum is taken over all periodic orbits (po) with energy E. Furthermore, T_{ppo} is the time period of the corresponding primitive periodic orbit, i.e. the time to travel around the orbit once. Note that a primitive periodic orbit is an orbit which is not a repetition of shorter periodic orbits. Also, A_{po} is an amplitude associated with each orbit (depending on its Lyapunov exponents) and μ_{po} is the Maslov index [Rob91]. The relation (3.3.17) is known as the *trace formula* and it played a vital role in understanding the connection between the quantum and the classical regime. For example, in [BT76], the quantisation rules (3.3.12) could be rediscovered from a similar trace formula valid for integrable systems. However, it must be kept in mind that the trace formula (3.3.17) is only a formal expression. Since the number of periodic orbits grows in general faster than the corresponding amplitudes A_{po} decay, the sum (3.3.17) may not converge [BK90, ASS88]. Another problem is, of course, the identification of all possible periodic orbits. However, evaluating the trace formula for only a finite number of periodic orbits can already yield valuable results [SA88, CC95].

To conclude this section, we want to comment on the connection between quantum graphs and quantum chaos as described in [KS97b]. For this, assume that we have a compact graph $\Gamma = \Gamma(\mathcal{V}, \mathcal{E})$ with rationally independent edge lengths. On the one-particle Hilbert space $L^2(\Gamma)$, we consider the Hamiltonian

$$\hat{H}_A = \left(-i\frac{\mathrm{d}}{\mathrm{d}x} - A\right)^2, \tag{3.3.18}$$

where $A \in \mathbb{R}$ introduces a breaking of time-reversal symmetry whenever $A \neq 0$. In order to have a self-adjoint operator, one demands Neumann boundary conditions

at the vertices of the graph, i.e. for each vertex one requires

$$\sum_{j=1}^{v} \left(-iA + \frac{\mathrm{d}}{\mathrm{d}x} \right) \Psi_j(x) \Big|_{x=0} = 0. \tag{3.3.19}$$

Here v is the number of edges connected to the vertex v and $\{\Psi_j\}_{j\in\mathbb{N}}$ are the corresponding incoming components of the wave function $\Psi \in L^2(\Gamma)$. Now, calculating a large number of eigenvalues numerically, it was shown in [KS97b] that the nearest-neighbour distribution (3.3.13) agrees very well with predictions of random matrix theory. Furthermore, graphs with broken time-reversal symmetry are associated with the GUE-ensemble whereas graphs without broken time-reversal symmetry follow GOE-predictions. Hence, based on the conjecture of Bohigas-Gianonni-Schmit as introduced above, quantum graphs can be considered as models of chaotic systems. Note that the origin of chaotic behaviour on a graph can also be understood from a classical point of view. Along any edge of the graph, the motion of the particle is simple. However, whenever the particle arrives at a vertex, it will be transmitted or reflected with some probability. Given the $2E \times 2E$ matrix $U_A(k)$, which is a generalisaton of (3.2.4) incorporating the magnetic potential A, the probability $T_{ee'}$ for the particle being transmitted from the (directed) edge e to the (directed) edge e' is given by

$$T_{ee'} = \left| (U_A)_{ee'}(k) \right|^2. \tag{3.3.20}$$

Here directed edges are obtained by associating to each edge $e \in \mathcal{E}$ two directed edges, one for each direction of travelling along the edge [KS97b, GS06, BE09]. Denoting the probability to occupy edge e at the (discrete) time t as $\rho_e(t)$, the classical evolution is described by the *master equation*

$$\rho_e(t+1) = \sum_{e'} T_{ee'} \rho_{e'}(t). \tag{3.3.21}$$

Note that the largest eigenvalue of the matrix T is one with eigenvector that corresponds to uniform distibution while all other eigenvalues have modulus less than one [KS97b]. Therefore the system will reach a state of uniform distribution exponentially fast [KS97b] which is an attribute of classically mixing systems (see Definition 3.3.5). Hence, on a classical level, the chaotic motion on graphs

originates in the probabilistic scattering at the vertices of the graph.

4. SINGULAR INTERACTIONS IN TWO-PARTICLE SYSTEMS ON COMPACT QUANTUM GRAPHS

In this chapter, we will consider two-particle systems on general quantum graphs in which the particles are interacting via singular interactions localised at the vertices. So far, most of the research conducted on quantum graphs focussed on one-particle systems [GS06]. However, Harmer investigated two-particle systems on star graphs with δ-like interactions [Har07, Har08] and Harrison *et al* studied the particle exchange symmetry in many-particle versions of finite-dimensional quantum graph models [HKR11]. Indeed, one of the first papers dealing with interacting two-particle systems on graphs was published by Melnikov and Pavlov [MP95]. They investigated two-particle scattering on a tree-like graph with two-particle interactions localised at the only vertex of the graph and their goal was to give a simple model for the effective electron-electron interaction in a solid. Since their model is related to our models of interacting particles, we will briefly illustrate the main steps in its construction. The graph considered by Melnikov and Pavlov consists of three edges of infinite length, connected in one vertex. Accordingly, the one-particle Hilbert space is given by

$$L^2(\Gamma) = \bigoplus_{j=1}^{3} L_j^2(\mathbb{R}^+), \tag{4.0.1}$$

and the two-particle Hilbert space is

$$L^2(\Gamma_2) = \bigoplus_{i,j=1}^{3} L_{ij}^2(\mathbb{R}_2^+), \tag{4.0.2}$$

where $\mathbb{R}_2^+ = \mathbb{R}^+ \times \mathbb{R}^+$. Hence, each two-particle wave function $\Psi \in L^2(\Gamma_2)$ consists of nine components $(\Psi)_{ij} = \psi_{ij}$. The Hamiltonian of the system is the two-particle

Laplacian $-\Delta_2$, acting on each function $\Psi \in H^2(\mathbb{R}_2^+)$ via

$$(-\Delta_2\Psi)_{ij} = -\frac{\partial^2\psi_{ij}}{\partial x_i^2} - \frac{\partial^2\psi_{ij}}{\partial x_j^2} \ . \tag{4.0.3}$$

As a first step, one constructs a self-adjoint realisation of the two-particle Laplacian $-\Delta_2$ corresponding to a system of non-interacting particles. For this, consider the one-particle boundary conditions

$$\psi_j(0) = -\frac{1}{3h}\sum_{i=1}^{3}\frac{\mathrm{d}\psi_i}{\mathrm{d}x_i}\bigg|_{x_i=0}, \quad j=1,2,3, \tag{4.0.4}$$

where $\Psi \in H^2(\Gamma)$ is a one-particle wave function and $h > 0$ is a parameter of the model. Denoting the set of all functions $\Psi \in H^2(\Gamma)$ that fulfil the boundary conditions (4.0.4) as Q_1, it follows that the operator $-\Delta_1$ with domain

$$\mathcal{D}(-\Delta_1) = \{\Psi |\ \Psi \in Q_1\} \tag{4.0.5}$$

is self-adjoint. Based on (4.0.5) one can now construct a self-adjoint realisation of the two-particle Laplacian such that the two-particle eigenfunctions are products of the one-particle eigenfunctions $\{u_n\}_{n\in\mathbb{N}_0}$, i.e.

$$\psi_{nm} = u_n \otimes u_m \ . \tag{4.0.6}$$

This self-adjoint realisation shall be denoted by $(-\Delta_2, \mathcal{D}_0(-\Delta_2))$. Note that, in such a system, the two particles are not interacting with each other. Now, in order to implement two-particle interactions which are only present whenever both particles are situated at the vertex, one remarks that any wave function $\Psi \in \mathcal{D}_0(-\Delta_2)$ which is zero at the vertex, should also be in the domain of the operator incorporating singular interactions. Hence, the idea is to consider the symmetric operator $-\Delta_2$ with domain

$$\tilde{\mathcal{D}}(-\Delta_2) = \mathcal{D}_0(-\Delta_2) \cap \{\Psi \in H^1(\Gamma_2) |\ \psi_{ij}(0,0) = 0\}. \tag{4.0.7}$$

Since this operator has finite deficiency indices [MP95], all self-adjoint realisation can be obtained using the von-Neumann scheme [Wei80]. Indeed, in the model of Melnikov and Pavlov, all self-adjoint realisation can be characterised by a real

parameter $\eta \in \mathbb{R}$ and, most importantly, those realisations correspond to a two-particle system with interactions localised at the vertex. Furthermore, it can be shown that each value of η represents a different asymptotic behaviour of functions $\Psi \in H^2(\Gamma_2)$ far away from the vertex which then allows to investigate the effect of the interaction on the scattering properties of the system [MP95].

As becomes clear from the model described above, singular interactions (on graphs) are physically important for modelling short-range particle-particle interactions. However, another motivation for the introduction of singular interactions on general quantum graphs, as mentioned already in the introduction, is to provide a useful model in order to understand the manifestation of chaos in a system of interacting particles, i.e. *many-particle quantum chaos*. An overview over this rapidly growing area of research can be found in [GKK$^+$11]. Interestingly enough, there are several new features appearing in many-particle quantum chaos that are absent or less emphasized in the one-particle case. One such difference is related to random matrix theory (RMT). Originally, random matrices were introduced by Wigner in the context of nuclear physics [Wig50, Wig67]. A nucleus is a many-particle system that is held together by strong interactions between the nucleons. However, the first models of the nucleus neglected the effect of many-particle interactions and it was soon discovered that, besides the success of those initial models, they were not sufficient to explain all the resonances observed in neutron scattering from certain nuclei [Meh91]. For this reason, it became necessary to include effects of many-particle interactions and since the actual structure of a nucleus is too difficult to approach directly, random matrices were soon recognised as a useful tool to circumvent some of the problems. However, often when applying RMT to chaotic (complex) systems, the Gaussian Ensembles as characterised by Dyson [Dys62] are considered [BGS84, Haa91]. But, as it turned out, the standard Gaussian ensembles are not fully appropriate to describe a system of interacting particles since they do not distinguish between two-particle and m-particle interactions [GKK$^+$11]. For this reason, one may use other ensembles such as the *embedded ensembles* EGOE(m) when interacting many-particle systems are considered [MF75, BW03, GKK$^+$11]. As an important consequence, it is not clear to what extent the Bohigas-Gianonni-Schmit conjecture covers chaotic many-particle systems.

The following chapter is organised as follows: In the first part, we will consider a

system of two (distinguishable) particles moving on the simplest compact graph, i.e. the interval of length l. Subsequently, we generalise the results to a system of two (distinguishable) particles moving on an arbitrary compact graph. We then implement exchange symmetry in order to describe either fermions or bosons on a graph and discuss spectral properties. Note that the presentation follows closely our paper [BK13b].

4.1 Two distinguishable particles on an interval

In this section, we will introduce the basic methods by considering the most simple compact graph, i.e. the interval of length l. For such a system, the configuration space of two particles is given by

$$D = (0, l) \times (0, l). \tag{4.1.1}$$

Accordingly, the two-particle Hilbert space is defined by

$$\mathcal{H}_2 = L^2(0, l) \otimes L^2(0, l) = L^2(D). \tag{4.1.2}$$

Remark 4.1.1. We will denote the two-particle Hilbert space also by $L^2(\Gamma_2)$.

On this Hilbert space, we consider the two-particle Laplacian $-\Delta_2$ acting on $\psi \in H^2(D)$ via

$$-\Delta_2\psi = -\frac{\partial^2\psi}{\partial x^2} - \frac{\partial^2\psi}{\partial y^2} \ . \tag{4.1.3}$$

Defining $-\Delta_2$ on the domain $\mathcal{D}(-\Delta_2) = C_0^\infty(D)$, we readily establish the following statement.

Proposition 4.1.2. *The operator $(-\Delta_2, C_0^\infty(D))$ is densely defined and symmetric.*

However, it is *not* self-adjoint and it will be the goal of this section to characterise self-adjoint extensions of $(-\Delta_2, C_0^\infty(D))$ that incorporate singular two-particle interactions. Note that the domain of its adjoint $-\Delta_2^*$ is given by

$$\mathcal{D}(-\Delta_2^*) = \{\psi \in L^2(D);\ \exists\chi \in L^2(D) \text{ s.t. } \langle\psi, -\Delta_2\varphi\rangle = \langle\chi, \varphi\rangle\ \forall\varphi \in C_0^\infty(D)\} \ . \tag{4.1.4}$$

As explained in Chapter 3, self-adjoint extensions of $(-\Delta_2, C_0^\infty(D))$ can be obtained by restricting the domain of its adjoint such that the resulting operator and *its* adjoint have the same domain. In the one-particle case, this was achieved by characterising all maximal symmetric extensions of $(-\Delta_1, C_0^\infty(\Gamma))$ [KS99]. As a result, the domains of all self-adjoint extensions are subsets of $H^2(\Gamma)$. However, it is not straightforward to generalise this approach to the two-particle case since we are now dealing with a partial differential operator rather than an ordinary differential operator. From (4.1.4) we can readily see that $H^2(D) \subset \mathcal{D}(-\Delta_2^*)$ but $\mathcal{D}(-\Delta_2^*) \neq H^2(D)$. It is therefore not clear if a self-adjoint realisation of $(-\Delta_2, C_0^\infty(D))$ has a domain that is a subset of $H^2(D)$. This difficulty, i.e. the problem of regularity as introduced in Chapter 2, is well-known in the theory of partial differential equations [GT83, Dob05]. Also, since the deficiency indices of $(-\Delta_2, C_0^\infty(D))$ are infinite, in contrast to $(-\Delta_1, C_0^\infty(\Gamma))$ where they are finite, it is not guaranteed that all maximal symmetric extension are self-adjoint [RS79].

Proposition 4.1.3. *The operator $(-\Delta_2, C_0^\infty(D))$ has infinite deficiency indices.*

Proof. We prove the proposition for n_-. Consider the set

$$\mathcal{D} = \left\{\psi \in L^2(D) |\ \psi(x,y) = e^{i(k_x x + k_y y)} \ \text{ s.t. } \ k_x^2 + k_y^2 = -i\right\}. \tag{4.1.5}$$

Since $\mathcal{D} \subset \mathcal{D}(-\Delta_2^*)$ and every $\psi \in \mathcal{D}$ fulfils the equation

$$(-\Delta_2^* + i)\psi = 0, \tag{4.1.6}$$

we have the inclusion $\mathcal{D} \subset \ker(-\Delta_2^* + i)$. Defining, for each $n \in \mathbb{N}$,

$$\kappa_n^2 = -i - \left(\frac{2\pi n}{l}\right)^2, \tag{4.1.7}$$

we see that the functions

$$\psi_n(x,y) = e^{i\left(\kappa_n x + \frac{2\pi n}{l} y\right)} \tag{4.1.8}$$

are such that $\langle \psi_n, \psi_m \rangle_{L^2(D)} = 0$ for $m \neq n$. Hence, we have an orthogonal set $\{\psi_n\}$ that contains infinitely many functions. From this, it follows that the Hilbert space dimension of $\ker(-\Delta_2^* + i)$ cannot be finite. □

In order to characterise self-adjoint extensions of $(-\Delta_2, C_0^\infty(D))$ that incorporate singular two-particle interactions, we will construct suitable quadratic forms. For this, let

$$\psi_{bv}(y) = \begin{pmatrix} \psi(0,y) \\ \psi(l,y) \\ \psi(y,0) \\ \psi(y,l) \end{pmatrix} \qquad \text{and} \qquad \psi'_{bv}(y) = \begin{pmatrix} \psi_x(0,y) \\ -\psi_x(l,y) \\ \psi_y(y,0) \\ -\psi_y(y,l) \end{pmatrix}, \tag{4.1.9}$$

be vectors containing the values of $\psi \in H^1(D)$ or, in addition if $\psi \in H^2(D)$, its (inner) normal derivative along the boundary ∂D. We then introduce two bounded and measurable maps $P, L : [0,l] \to \mathrm{M}(4,\mathbb{C})$ such that

1. $P(y)$ is an orthogonal projection,
2. $L(y)$ is self-adjoint endomorphism of $\ker P(y)$,

for a.e. $y \in [0,l]$. Moreover, we set $Q(y) = \mathbb{1}_4 - P(y)$.

Remark 4.1.4. For the maps P and L, measurable and bounded shall mean that each matrix element is a measurable and bounded function.

With the maps P and L, we associate two bounded and self-adjoint operators on $L^2(0,l) \otimes \mathbb{C}^4$, i.e.

$$\Pi : L^2(0,l) \otimes \mathbb{C}^4 \to L^2(0,l) \otimes \mathbb{C}^4, \chi(y) \mapsto P(y)\chi(y), \tag{4.1.10}$$

and

$$\Lambda : L^2(0,l) \otimes \mathbb{C}^4 \to L^2(0,l) \otimes \mathbb{C}^4, \chi(y) \mapsto L(y)\chi(y). \tag{4.1.11}$$

Now, introducing the domains

$$\begin{aligned} \mathcal{D}_2(P,L) = \{\psi \in H^2(D);\ & P(y)\psi_{bv}(y) = 0 \text{ and} \\ & Q(y)\psi'_{bv}(y) + L(y)Q(y)\psi_{bv}(y) = 0 \text{ for a.e. } y \in [0,l]\}, \end{aligned} \tag{4.1.12}$$

we can identify symmetric extensions of $(-\Delta_2, C_0^\infty(D))$.

Proposition 4.1.5. *The operator $(-\Delta_2, \mathcal{D}_2(P,L))$ is a densely defined and symmetric operator. Furthermore, it is an extension of the operator $(-\Delta_2, C_0^\infty(D))$.*

Proof. Since $C_0^\infty(D) \subset H^2(D)$, density follows directly. Now, let $\psi, \varphi \in \mathcal{D}_2(P, L)$ be two functions. We have

$$\begin{aligned}\langle \psi, -\Delta_2 \varphi \rangle_{L^2(D)} = \langle -\Delta_2 \psi, \varphi \rangle_{L^2(D)} \\ + \int_0^l \left(\overline{\psi}_x \varphi - \overline{\psi} \varphi_x\right)_{x=0}^{x=l} \, \mathrm{d}y + \int_0^l \left(\overline{\psi}_y \varphi - \overline{\psi} \varphi_y\right)_{y=0}^{y=l} \, \mathrm{d}x,\end{aligned} \tag{4.1.13}$$

and a change of variables yields

$$\begin{aligned}\langle \psi, -\Delta_2 \varphi \rangle_{L^2(D)} = \langle -\Delta_2 \psi, \varphi \rangle_{L^2(D)} \\ + \int_0^l \underbrace{\left(\overline{\psi}_x \varphi(x,y) - \overline{\psi} \varphi_x(x,y) + \overline{\psi}_y \varphi(y,x) - \overline{\psi} \varphi_y(y,x)\right)_{x=0}^{x=l}}_{=R(y)} \, \mathrm{d}y.\end{aligned} \tag{4.1.14}$$

Note that change of variables $(x, y) \to (y, x)$ in (4.1.14) is done after taking the derivatives. Now, for functions $\psi, \varphi \in \mathcal{D}_2(P, L)$, $R(y) = 0$ for a.e. $y \in [0, l]$. This follows from an analogy with one-particle quantum graphs. Indeed, given the one-particle wave functions $\Psi, \Phi \in L^2(\Gamma)$, the self-adjointness of $-\Delta_1$ on the domain $\mathcal{D}_1(P, L)$ (see (3.1.22)) implies

$$\sum_{e=1}^{E} \left(\overline{\psi}_e' \varphi_e - \overline{\psi}_e \varphi_e'\right)_{x=0}^{x=l_e} = 0, \tag{4.1.15}$$

see (3.1.1). Setting $E = 2$, $l_1 = l_2 = l$ and renaming the functions shows that $R(y) = 0$ for a.e. $y \in [0, l]$. □

As we will show later, for a certain class of maps P and L, the Laplacian $-\Delta_2$ will indeed be self-adjoint on the domain (4.1.12).

Remark 4.1.6. In the same way as for one-particle Laplacians (see Remark 3.1.9), an equivalent characterisation in terms of maps $A, B : [0, l] \to \mathrm{M}(4, \mathbb{C})$ is available. These maps are required to fulfil, for a.e. $y \in [0, l]$, that $\operatorname{rank}(A(y), B(y)) = 4$ and that $A(y)B(y)^*$ is self-adjoint. In that case, $P(y)$ is a projection onto $\ker B(y) \subseteq \mathbb{C}^4$ and the self-adjoint map is given by $L(y) = (B(y)|_{\operatorname{ran} B(y)^*})^{-1} A(y) Q(y)$ on $\mathbb{C}^4$. Furthermore, see Remark 3.1.9 for the construction of $(B(y)|_{\operatorname{ran} B(y)^*})^{-1}$.

We can now construct a suitable sesquilinear form as

$$\begin{aligned} Q^{(2)}_{P,L}[\psi,\phi] &= \langle \nabla\psi, \nabla\phi\rangle_{L^2(D)} - \langle \psi_{bv}, \Lambda\phi_{bv}\rangle_{L^2(0,l)\otimes\mathbb{C}^4} \\ &= \int_0^l \int_0^l \Big(\overline{\psi_x(x,y)}\, \phi_x(x,y) + \overline{\psi_y(x,y)}\, \phi_y(x,y) \Big)\, \mathrm{d}x\, \mathrm{d}y \\ &\quad - \int_0^l \langle \psi_{bv}(y), L(y)\phi_{bv}(y)\rangle_{\mathbb{C}^4}\, \mathrm{d}y \ . \end{aligned} \tag{4.1.16}$$

Note that we will refer to $Q^{(2)}_{P,L}[\psi,\psi] = Q^{(2)}_{P,L}[\psi]$ as the quadratic form.

Theorem 4.1.7. *Given maps $P, L : [0,l] \to \mathrm{M}(4,\mathbb{C})$ as above that are bounded and measurable. Then the quadratic form $Q^{(2)}_{P,L}[\cdot]$ with domain*

$$\mathcal{D}_{Q^{(2)}} = \{\psi \in H^1(D);\ P(y)\psi_{bv}(y) = 0 \text{ for a.e. } y \in [0,l]\} \tag{4.1.17}$$

is closed and semi-bounded.

Proof. As $L(y)$ is self-adjoint, the expression (4.1.16) obviously defines a symmetric quadratic form. We then observe that

$$\left| \int_0^l \langle \psi_{bv}(y), L(y)\psi_{bv}(y)\rangle_{\mathbb{C}^4}\, \mathrm{d}y \right| \leq L_{max}\, \|\psi_{bv}\|^2_{L^2(0,l)\otimes\mathbb{C}^4} \ , \tag{4.1.18}$$

where

$$L_{max} = \sup_{y\in[0,l]} \|L(y)\|_{op} \ . \tag{4.1.19}$$

Moreover, as a consequence of Lemma 8 in [Kuc04] (which is a variation of Theorem 2.2.13),

$$\|\psi_{bv}\|^2_{L^2(0,l)\otimes\mathbb{C}^4} \leq 4 \left(\frac{2}{\delta} \|\psi\|^2_{L^2(D)} + \delta \|\nabla\psi\|^2_{L^2(D)} \right) \tag{4.1.20}$$

holds for any $\delta \leq l$. Therefore,

$$Q^{(2)}_{P,L}[\psi] \geq \big(1 - 4\delta L_{max}\big) \|\nabla\psi\|^2_{L^2(D)} - \frac{8L_{max}}{\delta} \|\psi\|^2_{L^2(D)} \ . \tag{4.1.21}$$

Now choosing $\delta \leq \frac{1}{4L_{max}}$, there obviously exits $C > 0$ such that

$$Q^{(2)}_{P,L}[\psi] \geq -C\|\psi\|^2_{L^2(D)} \tag{4.1.22}$$

and hence the quadratic form is bounded from below. We denote the optimal such

constant by C_∞. Now, in order to show that the quadratic form (4.1.16) is closed, we observe that the (squared) form norm

$$\|\cdot\|^2_{Q^{(2)}_{P,L}} = Q^{(2)}_{P,L}[\cdot] + (C_\infty + 1)\,\|\cdot\|^2_{L^2(D)} \tag{4.1.23}$$

is equivalent to the Sobolev norm in $H^1(D)$. This follows from (4.1.20). Therefore, due to the completeness of $H^1(D)$, any Cauchy sequence $\{\psi_n\}_{n\in\mathbf{N}}$ in $\mathcal{D}_{Q^{(2)}} \subset H^1(D)$ with respect to the form-norm has a limit $\psi \in H^1(D)$. Then, taking the trace theorem 2.2.11 into account, we see that $\{\psi_{n,bv}\}$ converges to ψ_{bv} in $L^2(0,l)\otimes\mathbb{C}^4$. Finally, since the operator Π on $L^2(0,l)\otimes\mathbb{C}^4$ is bounded, one concludes that $P(\cdot)\psi_{n;bv} = 0$ converges to $P(\cdot)\psi_{bv}$ and hence $P(y)\psi_{bv}(y) = 0$ for a.e. $y \in [0,l]$. □

Due to the representation theorem of quadratic forms [Kat66], there is a unique self-adjoint operator $(H, \mathcal{D}(H))$ corresponding to each form characterised in Theorem 4.1.7. It will be the goal in the sequel to characterise the operator H and its domain $\mathcal{D}(H)$ in more detail. According to [Kat66], for each $\varphi \in \mathcal{D}(H)$ there exists a unique $\chi \in L^2(D)$ such that

$$Q^{(2)}_{P,L}[\varphi,\psi] = \langle\chi,\psi\rangle_{L^2(D)}, \quad \forall\psi \in \mathcal{D}_{Q^{(2)}}. \tag{4.1.24}$$

Hence, the action of the corresponding self-adjoint operator H is given by

$$H\varphi = \chi. \tag{4.1.25}$$

Now, based on results presented in [Sho77], we can give an abstract characterisation of the domain $\mathcal{D}(H)$. The first step is to split the quadratic form (4.1.16) into a volume part and a boundary part, i.e.

$$Q^{(2)}_{P,L}[\phi,\psi] = q_1[\phi,\psi] + q_2[\phi,\psi]\ , \tag{4.1.26}$$

where

$$q_1[\phi,\psi] = \langle\nabla\psi,\nabla\phi\rangle_{L^2(D)} \tag{4.1.27}$$

is the volume part and

$$q_2[\phi,\psi] = -\langle\psi_{bv},\Lambda\phi_{bv}\rangle_{L^2(0,l)\otimes\mathbb{C}^4} \tag{4.1.28}$$

the boundary part. We then introduce an abstract Green's operator ∂_n that can be regarded as a weak version of the standard normal derivative. To this end, we consider the trace map

$$\gamma : H^1(D) \to L^2(\partial D), \tag{4.1.29}$$

restricted to the Hilbert space $\mathcal{D}_{Q^{(2)}}$ (equipped with the form-norm), with kernel $\ker\gamma = \mathcal{D}_{Q^{(2)}} \cap H_0^1(D)$. Now, let

$$\mathcal{D}_0 = \{\psi \in \mathcal{D}_{Q^{(2)}};\ \Delta_2\psi \in L^2(D)\}\ , \tag{4.1.30}$$

then $\partial_n : \mathcal{D}_0 \to (\operatorname{ran}\gamma)'$, where $(\operatorname{ran}\gamma)'$ is the dual of $\operatorname{ran}\gamma$, is a linear map defined by the relation

$$q_1[\psi,\phi] - \langle -\Delta_2\psi, \phi\rangle_{L^2(D)} = \partial_n\psi[\gamma\phi], \quad \phi \in \mathcal{D}_{Q^{(2)}}\ . \tag{4.1.31}$$

Remark 4.1.8. For $\psi \in H^2(D)$ and $\phi \in \mathcal{D}_{Q^{(2)}}$ we have

$$\partial_n\psi[\gamma\phi] = \int_{\partial D} \frac{\partial\bar{\psi}}{\partial n}\,\phi\ \mathrm{d}\sigma, \tag{4.1.32}$$

involving the outer normal derivative of $\bar{\psi}$.

Applying Theorem 3.A from [Sho77] then yields

Proposition 4.1.9. *Let H be the unique self-adjoint, semi-bounded operator corresponding to the quadratic form $Q^{(2)}_{P,L}$. Then its domain is given by*

$$\mathcal{D}(H) = \{\psi \in \mathcal{D}_0;\ \partial_n\psi[\gamma\phi] + q_2[\psi,\phi] = 0,\ \forall\phi \in \mathcal{D}_{Q^{(2)}}\}\ . \tag{4.1.33}$$

Since, due to the presence of the abstract Green's operator, the characterisation of the domain $\mathcal{D}(H)$ in Proposition 4.1.9 is not very explicit, we aim at singling out cases where the domain can be characterised in more detail. Since the abstract Green's operator is given by (4.1.32), whenever we consider functions in $H^2(D)$, it would be interesting to know if the domain $\mathcal{D}(H)$ is a subset of $H^2(D)$. As mentioned beforehand, this is related to the issue of (elliptic) regularity as introduced in Chapter 2. We therefore define the following notion.

Definition 4.1.10. The quadratic form $Q^{(2)}_{P,L}$ is called *regular*, iff its associated self-adjoint operator H has a domain $\mathcal{D}(H) \subset H^2(D)$.

As a first step towards a more explicit characterisation of the domain $\mathcal{D}(H)$, we need to ensure that the kernel of the operator Π is under sufficient control. This is necessary since we require a pointwise characterisation as given in (4.1.12) rather than an integral characterisation as in Proposition 4.1.9.

Lemma 4.1.11. *Let $P : (0,l) \to \mathrm{M}(4,\mathbb{C})$ be such that its matrix entries are in $C^1(0,l)$, then $\mathrm{ran}(\gamma|_{\mathcal{D}_{Q^{(2)}}})$ is dense in $\ker\Pi$ with respect to the norm on $L^2(0,l)\otimes\mathbb{C}^4$.*

Proof. As $C_0^\infty(0,l)\otimes\mathbb{C}^4 \subset L^2(0,l)\otimes\mathbb{C}^4$ is dense, whenever $\chi \in \ker\Pi \subset L^2(0,l)\otimes\mathbb{C}^4$ there exists a sequence $\{\chi_n\} \subset C_0^\infty(0,l)\otimes\mathbb{C}^4$ that converges to χ. Moreover, any $\chi_n \in C_0^\infty(0,l)\otimes\mathbb{C}^4$ can be extended to some $\psi_n \in H^1(D)$, such that $\chi_n = \psi_{n,bv}$.

Using the orthogonal complement $\Pi^\perp$ to the projection Π we note that, by the assumption in the lemma, $\Pi^\perp\chi_n \in C_0^1(0,l)\otimes\mathbb{C}^4$. Again, $\Pi^\perp\chi_n$ can be extended to a function $\phi_n \in H^1(D)$, such that $\Pi^\perp\chi_n = \phi_{n,bv}$. By construction, $P(y)\phi_{n,bv}(y) = 0$ so that indeed $\phi_n \in \mathcal{D}_{Q^{(2)}}$. Therefore, identifying $\phi_{n,bv}$ with $\gamma\phi_n$ we conclude that $\Pi^\perp\chi_n \in \mathrm{ran}(\gamma|_{\mathcal{D}_{Q^{(2)}}})$.

Moreover, as Π is assumed to be bounded in operator norm there exits $K > 0$ such that

$$\|\Pi^\perp\chi_n - \chi\|_{L^2(0,l)\otimes\mathbb{C}^4} = \|\Pi^\perp\big(\chi_n - \chi\big)\|_{L^2(0,l)\otimes\mathbb{C}^4} \leq K\,\|\chi_n - \chi\|_{L^2(0,l)\otimes\mathbb{C}^4} \to 0\ , \tag{4.1.34}$$

as $n \to \infty$. Thus, $\mathrm{ran}(\gamma|_{\mathcal{D}_{Q^{(2)}}})$ is dense in $\ker\Pi$. □

We are now in position to state one of the main theorems of this section. As it turns out, for regular quadratic forms in the sense of Definition 4.1.10, the operator H is indeed the two-particle Laplacian $-\Delta_2$ with domain (4.1.12).

Theorem 4.1.12. *Suppose that the matrix entries of $P : (0,l) \to \mathrm{M}(4,\mathbb{C})$ are in $C^1(0,l)$ and that the quadratic form $Q^{(2)}_{P,L}$ is regular. Then the unique self-adjoint, semi-bounded operator H that is associated with this form is the two-particle Laplacian $-\Delta_2$ with domain $\mathcal{D}_2(P,L)$.*

Proof. Since, in the regular case, any $\psi \in \mathcal{D}(H)$ is in $H^2(D)$, the Green's operator ∂_n is the standard normal derivative (see Remark 4.1.8). This would allow us to state the 'boundary condition' contained in (4.1.33) immediately in an explicit way. However, following the one-particle approach developed in [Kuc04], we shall

now proceed in a more direct way. For this, we choose ψ in (4.1.24) to be smooth and compactly supported in D, vanishing in neighbourhoods of ∂D such that $\psi_{bv}(y) = 0$ for all $y \in [0, l]$. Thus

$$\langle \chi, \psi \rangle_{L^2(D)} = \int_0^l \int_0^l \big(\bar{\phi}_x(x,y)\, \psi_x(x,y) \; + \bar{\phi}_y(x,y)\, \psi_y(x,y) \big) \, \mathrm{d}x \, \mathrm{d}y \; . \tag{4.1.35}$$

An integration by parts then yields

$$\langle \chi, \psi \rangle_{L^2(D)} = \int_0^l \int_0^l \big(-\bar{\phi}_{xx}(x,y) - \bar{\phi}_{yy}(x,y) \big) \psi(x,y) \, \mathrm{d}x \, \mathrm{d}y \; , \tag{4.1.36}$$

so that $\chi = H\phi = -\Delta_2 \phi$. Hence the operator H acts as a two-particle Laplacian and every $\phi \in \mathcal{D}(H)$ must be in $\mathcal{D}(-\Delta^*_{2,0})$. Now, we choose $\psi \in \mathcal{D}_{Q^{(2)}}$ that is non-zero in a neighbourhood of ∂D. Then, in addition to the right-hand side of (4.1.36), an integration by parts yields the term

$$- \int_0^l \langle \phi'_{bv}(y) + L(y)\phi_{bv}(y), \psi_{bv}(y) \rangle_{\mathbb{C}^4} \, \mathrm{d}y = - \langle \phi'_{bv} + L\phi_{bv}, \psi_{bv} \rangle_{L^2(0,l)\otimes\mathbb{C}^4} \; , \tag{4.1.37}$$

which must vanish. Since $L(\cdot)$ is self-adjoint, one can rewrite this term as

$$\int_{\partial D} \frac{\partial \bar{\phi}}{\partial n} \, \psi \, \mathrm{d}\sigma + q_2[\phi, \psi] \; . \tag{4.1.38}$$

Hence its vanishing is precisely a more explicit version of the boundary condition in (4.1.33).

Furthermore, the condition $P(y)\psi_{bv}(y) = 0$, fulfilled by $\psi \in \mathcal{D}_{Q^{(2)}}$ for a.e. $y \in [0, l]$, implies that ψ_{bv} is in the kernel of the orthogonal projection Π on $L^2(0, l) \otimes \mathbb{C}^4$. Hence, the vanishing of (4.1.37) for all $\psi \in \mathcal{D}_{Q^{(2)}}$, together with the fact that by Lemma 4.1.11 $\mathrm{ran}(\gamma|_{\mathcal{D}_{Q^{(2)}}}) \subset \ker \Pi$ is dense, implies that $\phi'_{bv} + L(\cdot)\phi_{bv}$ is in the kernel of $\Pi^\perp$, or

$$Q(y)\phi'_{bv}(y) + Q(y)L(y)\phi_{bv}(y) = 0 \; . \tag{4.1.39}$$

Furthermore, as $L(y)$ is an endomorphism of $\mathrm{ran}\, Q(y) \subseteq \mathbb{C}^4$, a comparison with (4.1.12) shows that $\mathcal{D}(H) = \mathcal{D}_2(P, L)$. □

Remark 4.1.13. Note that, in the following we will, also in the case of a non-regular quadratic form $Q^{(2)}_{P,L}[\cdot]$, denote the domain of the corresponding operator as $\mathcal{D}_2(P, L)$.

We now want to discuss to what extent the representation of a quadratic form $Q^{(2)}_{P,L}[\cdot]$ by the maps P and L is unique. Since the domain of each quadratic form is a subset of $H^1(D)$, the traces of all functions $\varphi \in \mathcal{D}_{Q^{(2)}}$ exhibit some regularity along the boundary ∂D. Indeed, as proved in [Din96], the trace map $\gamma : H^1(D) \to L^2(\partial D)$ can be extended to

$$\gamma : H^1(D) \to H^{\frac{1}{2}}(\partial D), \tag{4.1.40}$$

where $H^{\frac{1}{2}}(\partial D)$ is the space of all functions $\varphi \in L^2(\partial D)$ such that

$$\|\varphi\|^2_{H^{\frac{1}{2}}(\partial D)} = \int_{\partial D} |\varphi(x)|^2 \, \mathrm{d}\sigma_x + \int_{\partial D \times \partial D} \frac{|\varphi(x) - \varphi(y)|^2}{|x-y|^2} \, \mathrm{d}\sigma_x \mathrm{d}\sigma_y < +\infty \ , \tag{4.1.41}$$

where $\mathrm{d}\sigma_{x/y}$ refers to the line segment of the boundary (see Definition 2.2.9). Accordingly, in order to establish uniqueness for a quadratic form $Q^{(2)}_{P,L}[\cdot]$, we have to require P to be smooth enough.

Proposition 4.1.14. *Suppose that the matrix entries of $P : (0,l) \to \mathrm{M}(4,\mathbb{C})$ are in $C^1(0,l)$. Then the parametrisation of the quadratic form $Q^{(2)}_{P,L}$ in terms of P and L according to* (4.1.16) *and* (4.1.17) *is unique with this property.*

Proof. The characterisation (4.1.17) of a domain $\mathcal{D}_{Q^{(2)}}$ involves only P. Suppose that a given domain can be characterised by two different maps $P_j : (0,l) \to \mathrm{M}(4,\mathbb{C})$, $j = 1,2$, both of which with matrix entries in $C^1(0,l)$. The associated projection operators Π_j on $L^2(0,l) \otimes \mathbb{C}^4$ are, therefore, different implying $\ker \Pi_1 \neq \ker \Pi_2$. We can hence assume that there exists $\chi \in \ker \Pi_1$ such that $\chi \notin \ker \Pi_2$. Now, following Lemma 4.1.11 there exists a sequence $\{\phi_n\}$ in $\mathcal{D}_{Q^{(2)}}$ such that $\phi_{n,bv}$ converges to χ. Moreover, following our assumption $\phi_n \in \mathcal{D}_{Q^{(2)}}$ means that $\phi_{n,bv} \in \ker \Pi_1 \cap \ker \Pi_2$. However, $\chi \notin \ker \Pi_2$ contradicts the fact that the $\phi_{n,bv} \in \ker \Pi_2$ converge to χ.
Now assume that a domain $\mathcal{D}_{Q^{(2)}}$ (with a unique C^1-map P) is given, but the form (4.1.16) can be characterised by two different maps $L_j : (0,l) \to \mathrm{M}(4,\mathbb{C})$, $j = 1,2$, yielding two different (bounded and self-adjoint) operators Λ_j on $L^2(0,l) \otimes \mathbb{C}^4$. Hence

$$\langle \phi_{bv}, \big(\Lambda_1 - \Lambda_2\big)\phi_{bv} \rangle_{L^2(0,l)\otimes\mathbb{C}^4} = 0 \ , \quad \text{for all } \phi \in \mathcal{D}_{Q^{(2)}} \ . \tag{4.1.42}$$

Again following Lemma 4.1.11, and using that, by definition, $L_j(y)$ vanishes on

$\big(\ker P(y)\big)^{\perp}$, this implies $\Lambda_1 = \Lambda_2$. □

Remark 4.1.15. In the regular case, when the associated operators are two-particle Laplacians with domains $\mathcal{D}_2(P, L)$, the same uniqueness results holds for the operators as the association between closed, semi-bounded quadratic forms and semi-bounded, self-adjoint operators is one-to-one [Kat66].

In the following, we will characterise some examples of regular forms (see Definition 4.1.10). Since the proof of the main theorem will be quite technical, it will be deferred to part B of the appendix. In a first step, we mention a few standard cases for which regularity is well established [Kon70, Neč67, Dau88, Gri11, Mgh92, BK06]:

1. A Dirichlet-Laplacian, in which case $P(y) = \mathbb{1}_4$ for all $y \in [0, l]$.
2. A Neumann-Laplacian, where $P(y) = 0 = L(y)$ for all $y \in [0, l]$.
3. A mixed Dirichlet-Neumann Laplacian, where $P(y)$ is independent of y and diagonal such the diagonal entries are either zero or one. Moreover, $L(y) = 0$ for all $y \in [0, l]$. In such a case, Dirichlet boundary conditions are imposed on the parts of the boundary that, via (4.1.9), correspond to a one on the diagonal of P, and Neumann boundary conditions on the remaining parts.
4. A Laplacian with standard Robin boundary condition follows when $P(y) = 0$ for all $y \in [0, l]$ and $L = \alpha\mathbb{1}_4$, where $\alpha < 0$. In that case the boundary conditions in (4.1.12) reduce to $\psi'_{bv}(y) + \alpha\psi_{bv}(y) = 0$.

As we will see later, these self-adjoint realisations correspond to systems of two non-interacting particles. Now, in order to establish regularity in a further class of examples, we require the map P to have the block-structure

$$P(y) = \begin{pmatrix} \tilde{P}(y) & 0 \\ 0 & \tilde{P}(y) \end{pmatrix} . \tag{4.1.43}$$

Note that this block structure will later be considered to implement exchange symmetry, i.e. to describe a system of two bosons or two fermions respectively. In general, we can assume that

$$\tilde{P}(y) = \begin{pmatrix} \beta(y) & \bar{\gamma}(y) \\ \gamma(y) & 1 - \beta(y) \end{pmatrix} , \tag{4.1.44}$$

where $0 \leq \beta(y) \leq 1$ and $|\gamma(y)|^2 = \beta(y) - \beta^2(y)$, i.e., when $\gamma(y) = 0$, $\beta(y)$ must be either one or zero. Hence, demanding that $\gamma(y) \to 0$ as $y \to 0$ and as $y \to l$, $\tilde{P}(y)$ approaches one of the two cases

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} , \quad \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} . \tag{4.1.45}$$

We will actually assume that on intervals $[0, \epsilon_1]$ and $[l - \epsilon_2, l]$, where $\epsilon_{1/2} > 0$ are some small constants, $\tilde{P}(y)$ assumes one of the forms (4.1.45). Note that the proof of the following theorem is given in part B of the appendix.

Theorem 4.1.16. *Let L be Lipschitz continuous on $[0, l]$ and let P be of the block-diagonal form (4.1.43). Assume that the matrix entries of $\tilde{P}$ are in $C^3(0, l)$. Moreover, when $y \in [0, \varepsilon_1] \cup [l - \varepsilon_2, l]$ with some $\varepsilon_1, \epsilon_2 > 0$, suppose that $L(y) = 0$ and that $\tilde{P}(y)$ is diagonal with diagonal entries that are either zero or one. Then the quadratic form $Q^{(2)}_{P,L}$ is regular.*

Finally, we want to distinguish between self-adjoint realisations $(-\Delta_2, \mathcal{D}_2(P, L))$ that correspond to a system of two non-interacting particles and such realisations that correspond to a system with genuine two-particle interactions. To illustrate this point in more detail, assume we have a one-particle realisation $(-\Delta_1, \mathcal{D}_1(P, L))$ with corresponding eigenfunctions $\{\varphi_n\}_{n \in \mathbb{N}_0}$. We then construct the two-particle states

$$\varphi_{mn} = \varphi_n \otimes \varphi_m \tag{4.1.46}$$

and define

$$\mathcal{D}_2(-\Delta_1) = \left\{ \Psi \in \mathcal{H}_2 \mid \Psi = \sum_{mn}^{\text{finite}} a_{mn}\, \varphi_{mn},\ a_{nm} \in \mathbb{C} \right\} . \tag{4.1.47}$$

Lemma 4.1.17. *The operator $(-\Delta_2, \mathcal{D}_2(-\Delta_1))$ is essentially self-adjoint.*

Proof. By definition $\mathcal{D}_2(-\Delta_1)$ is a dense subset of $\mathcal{H}_2$. Also, we can readily verify symmetry and semi-boundedness following from the semi-boundedness of $(-\Delta_1, \mathcal{D}_1(P, L))$. Now, since each element $\Psi \in \mathcal{D}_2(-\Delta_1)$ is an analytic vector, i.e. $-\Delta_2^n \Psi \in \mathcal{H}_2$ for all $n \in \mathbb{N}$, and

$$\sum_{n=1}^{\infty} \frac{\| - \Delta_N^n \Psi \|_{\mathcal{H}_2}}{n!} < \infty , \tag{4.1.48}$$

Nelson's analytic vector theorem (see Theorem 2.1.15) applies and the lemma follows. □

Definition 4.1.18. Let $Q^{(2)}_{P,L}$ be a quadratic form with corresponding self-adjoint operator $(-\Delta_2, \mathcal{D}_2(P,L))$. We say that $(-\Delta_2, \mathcal{D}_2(P,L))$ represents no interactions, i.e. corresponds to a system of non-interacting particles, iff

$$(-\Delta_2, \mathcal{D}_2(P,L)) = \overline{(-\Delta_2, \mathcal{D}_2(-\Delta_1))}, \tag{4.1.49}$$

where $\overline{(-\Delta_2, \mathcal{D}_2(-\Delta_1))}$ is the closure of a operator described in Lemma 4.1.17.

Now, let P_1 and L_1 be one-particle maps and define the two-particle maps

$$P(y) = \begin{pmatrix} P_1 & 0 \\ 0 & P_1 \end{pmatrix} \quad \text{and} \quad L(y) = \begin{pmatrix} L_1 & 0 \\ 0 & L_1 \end{pmatrix}, \tag{4.1.50}$$

for all $y \in [0,l]$.

Proposition 4.1.19. *Suppose that the matrix entries of $P : (0,l) \to \mathrm{M}(4,\mathbb{C})$ are in $C^1(0,l)$. Then, the two-particle Laplacian $-\Delta_2$ with domain $\mathcal{D}_2(P,L)$ represents no interactions iff P and L are block-diagonal as in* (4.1.50) *and are independent of y.*

Proof. Consider the operator $(-\Delta_2, \mathcal{D}_2(-\Delta_1))$ and the form $(Q^{(2)}_{P,L}, \mathcal{D}_{Q^{(2)}})$ with the maps (4.1.50). We see that $\mathcal{D}_2(-\Delta_1) \subset \mathcal{D}_{Q^{(2)}}$. On the domain $\mathcal{D}_2(-\Delta_1)$, we can then define a quadratic form by

$$Q_{-\Delta_2}[\varphi] = \langle \varphi, -\Delta_2 \varphi \rangle_{\mathcal{H}_2}, \quad \varphi \in \mathcal{D}_2(-\Delta_1). \tag{4.1.51}$$

This form is dense, symmetric and semi-bounded [BB93]. Since $\varphi \in \mathcal{D}_2(-\Delta_1) \subset H^2(D)$, we have

$$\langle \varphi, -\Delta_2 \varphi \rangle_{\mathcal{H}_2} = Q^{(2)}_{P,L}[\varphi], \quad \varphi \in \mathcal{D}_2(-\Delta_1). \tag{4.1.52}$$

Now, since the form norm $\|\cdot\|_{Q^{(2)}_{P,L}}$ is equivalent to the H^1-norm, $(Q^{(2)}_{P,L}, \mathcal{D}_{Q^{(2)}})$ forms a closed extension of $(Q^{(2)}_{P,L}, \mathcal{D}_2(-\Delta_1))$. Therefore, the self-adjoint operator $(-\Delta_2, \mathcal{D}_2(P,L))$ corresponding to $(Q^{(2)}_{P,L}, \mathcal{D}_{Q^{(2)}})$ forms a closed extension of $(-\Delta_2, \mathcal{D}_2(-\Delta_1))$ [BB93]. Hence, by Lemma 4.1.17, $(-\Delta_2, \mathcal{D}_2(P,L))$ represents

no interactions. Finally, taking Proposition 4.1.14 into account completes the proof. □

Based on Proposition 4.1.19, the cases of regular forms as mentioned beforehand clearly represent systems of non-interacting particles.

4.1.1 Two particles on a general compact metric graph

In this section, we shall generalise the results obtained in the previous section to general compact metric graphs. The methods are the same as in the last section and only a change of notation will be necessary. The two-particle Hilbert space $\mathcal{H}_2$ on a general graph is given by

$$\mathcal{H}_2 = L^2(\Gamma) \otimes L^2(\Gamma) = \bigoplus_{e_1 e_2} L^2(D_{e_1 e_2}) \ . \tag{4.1.53}$$

Hence, each two-particle state $\Psi \in \mathcal{H}_2$ consists of E^2 components $(\Psi)_{e_1 e_2} = \psi_{e_1 e_2}$ such that $\psi_{e_1 e_2} \in L^2(D_{e_1 e_2})$ with $D_{e_1 e_2} = (0, l_{e_1}) \times (0, l_{e_2})$.

Remark 4.1.20. We will denote the two-particle Hilbert space also by $L^2(\Gamma_2)$. Note that we will use an analogous notation also for other function spaces.

The Sobolev spaces on a general compact graph are defined by

$$H^m(\Gamma_2) = \bigoplus_{e_1 e_2} H^m(D_{e_1 e_2}), \quad m \in \mathbb{N}. \tag{4.1.54}$$

Note that each state $\Psi \in L^2(\Gamma_2)$ can be viewed as a function on the disjoint union

$$D_\Gamma = \dot{\bigcup_{e_1 e_2}} D_{e_1 e_2}, \tag{4.1.55}$$

whose boundary is given by

$$\partial D_\Gamma = \dot{\bigcup_{e_1 e_2}} \partial D_{e_1 e_2}. \tag{4.1.56}$$

Accordingly, the trace map $\gamma : H^1(\Gamma_2) \mapsto L^2(\partial D_\Gamma)$ as introduced in Chapter 2 associates boundary values with each state $\Psi \in H^1(\Gamma_2)$. As in the last section, the Hamiltonian of a two-particle system is given by the two-particle Laplacian $-\Delta_2$.

On functions $\Psi \in C_0^\infty(\Gamma_2)$, it acts via

$$(-\Delta_2\Psi)_{e_1e_2}(x_{e_1}, y_{e_2}) = -\frac{\partial^2\psi_{e_1e_2}(x_{e_1}, y_{e_2})}{\partial x_{e_1}^2} - \frac{\partial^2\psi_{e_1e_2}(x_{e_1}, y_{e_2})}{\partial y_{e_2}^2} \ . \tag{4.1.57}$$

As in Proposition 4.1.2, the operator $(-\Delta_2, C_0^\infty(\Gamma_2))$ is a densely defined and symmetric operator but it is *not* self-adjoint. To construct quadratic forms that yield self-adjoint realisations of $-\Delta_2$, we introduce two vectors of boundary values,

$$\Psi_{bv}(y) = \begin{pmatrix} \sqrt{l_{e_2}}\psi_{e_1e_2}(0, l_{e_2}y) \\ \sqrt{l_{e_2}}\psi_{e_1e_2}(l_{e_1}, l_{e_2}y) \\ \sqrt{l_{e_1}}\psi_{e_1e_2}(l_{e_1}y, 0) \\ \sqrt{l_{e_1}}\psi_{e_1e_2}(l_{e_1}y, l_{e_2}) \end{pmatrix} \qquad \text{and} \qquad \Psi'_{bv}(y) = \begin{pmatrix} \sqrt{l_{e_2}}\psi_{e_1e_2,x}(0, l_{e_2}y) \\ -\sqrt{l_{e_2}}\psi_{e_1e_2,x}(l_{e_1}, l_{e_2}y) \\ \sqrt{l_{e_1}}\psi_{e_1e_2,y}(l_{e_1}y, 0) \\ -\sqrt{l_{e_1}}\psi_{e_1e_2,y}(l_{e_1}y, l_{e_2}) \end{pmatrix} , \tag{4.1.58}$$

where $y \in [0,1]$. As a next step, we introduce measurable and bounded (see Remark 4.1.4) maps $P, L : [0,1] \to \mathrm{M}(4E^2, \mathbb{C})$ such that

1. $P(y)$ is an orthogonal projection,
2. $L(y)$ is a self-adjoint endomorphism on $\ker P(y)$,

for a.e. $y \in [0,1]$. In addition, we set $Q(y) = \mathbb{1}_{4E^2} - P(y)$. Moreover, with P and L, we associate two self-adjoint and bounded operators on the Hilbert space $L^2(0,1) \otimes \mathbb{C}^{4E^2}$ via

$$\Pi : L^2(0,1) \otimes \mathbb{C}^{4E^2} \to L^2(0,1) \otimes \mathbb{C}^{4E^2}, \chi(y) \mapsto P(y)\chi(y), \tag{4.1.59}$$

and

$$\Lambda : L^2(0,1) \otimes \mathbb{C}^{4E^2} \to L^2(0,1) \otimes \mathbb{C}^{4E^2}, \chi(y) \mapsto L(y)\chi(y). \tag{4.1.60}$$

Now we can define a quadratic form via

$$\begin{aligned} Q_{P,L}^{(2)}[\Psi] &= \langle \nabla\Psi, \nabla\Psi\rangle_{L^2(D_\Gamma)} - \langle \Psi_{bv}, \Lambda\Psi_{bv}\rangle_{L^2(0,1)\otimes\mathbb{C}^{4E^2}} \\ &= \sum_{e_1,e_2=1}^{E} \int_0^{l_{e_2}} \int_0^{l_{e_1}} \left(\left|\psi_{e_1e_2,x}(x,y)\right|^2 + \left|\psi_{e_1e_2,y}(x,y)\right|^2 \right) \mathrm{d}x\,\mathrm{d}y \\ &\qquad - \int_0^1 \langle \Psi_{bv}(y), L(y)\Psi_{bv}(y)\rangle_{\mathbb{C}^{4E^2}} \ \mathrm{d}y \ . \end{aligned} \tag{4.1.61}$$

We will later see that whenever the form $Q_{P,L}^{(2)}[\cdot]$ is regular (see Definition 4.1.10),

the corresponding operator is the two-particle Laplacian $-\Delta_2$ with domain

$$\begin{aligned}\mathcal{D}_2(P,L) = \{\Psi \in H^2(\Gamma_2);\ P(y)\Psi_{bv}(y) = 0 \text{ and} \\ Q(y)\Psi'_{bv}(y) + L(y)Q(y)\Psi_{bv}(y) = 0 \text{ for a.e. } y \in [0,1]\}.\end{aligned} \tag{4.1.62}$$

This hence establishes a close connection with the one-particle quadratic form (3.1.11).

Theorem 4.1.21. *Let $P, L : [0,1] \to \mathrm{M}(4E^2, \mathbb{C})$ be maps as introduced above that are bounded and measurable. Then, the quadratic form* (4.1.61) *with domain*

$$\mathcal{D}_{Q^{(2)}} = \{\Psi \in H^1(\Gamma_2);\ P(y)\Psi_{bv}(y) = 0 \text{ for a.e. } y \in [0,1]\} \tag{4.1.63}$$

is closed and semi-bounded.

The proof follows the same lines as the proof of Theorem 4.1.7. In order to characterise the self-adjoint operator $(H, \mathcal{D}(H))$ corresponding to the quadratic form $Q^{(2)}_{P,L}[\cdot]$, we first use the method developed in [Sho77] and introduced in the last section. It employs an abstract Green's operator ∂_n that associates to each function $\Psi \in \mathcal{D}_{Q^{(2)}}$ a functional $\partial_n\Psi[\cdot]$, acting on traces $\gamma\Phi \in L^2(\partial D_\Gamma)$ of functions $\Phi \in \mathcal{D}_{Q^{(2)}}$. More explicitly, one has

$$\partial_n\Psi[\gamma\Phi] = q_1[\Psi,\Phi] - \langle -\Delta_2\Psi, \Phi\rangle_{L^2(\Gamma_2)}, \quad \Phi \in \mathcal{D}_{Q^{(2)}}\ , \tag{4.1.64}$$

where $q_1[\Psi,\Phi] = \langle \nabla\Psi, \nabla\Phi\rangle_{L^2(\Gamma_2)}$. Note that, for functions $\Psi \in H^2(D_\Gamma)$, one has

$$\partial_n\Psi(\gamma\Phi) = \sum_{e_1e_2} \int_{\partial D_{e_1e_2}} \frac{\partial\bar{\psi}_{e_1e_2}}{\partial n}\, \phi_{e_1e_2}\ \mathrm{d}\sigma, \tag{4.1.65}$$

where the standard outer normal derivative of $\bar{\psi}_{e_1e_2}$ is involved. Setting

$$q_2[\Psi,\Phi] = -\int_0^1 \langle \Psi_{bv}(y), L(y)\Psi_{bv}(y)\rangle_{\mathbb{C}^{4E^2}}\ \mathrm{d}y\ , \tag{4.1.66}$$

we have the following statement.

Proposition 4.1.22. *Let H be the unique self-adjoint, semi-bounded operator corresponding to the quadratic form $Q^{(2)}_{P,L}$. Then its domain is given by*

$$\mathcal{D}(H) = \{\Psi \in \mathcal{D}_0;\ \partial_n\Psi[\gamma\Phi] + q_2[\Psi,\Phi] = 0,\ \forall\Phi \in \mathcal{D}_{Q^{(2)}}\}\ , \tag{4.1.67}$$

with $\mathcal{D}_0$ *defined as in* (4.1.30).

In order to arrive at a more explicit characterisation of the operator $(H, \mathcal{D}(H))$, we would like to establish regularity for some quadratic forms $Q^{(2)}_{P,L}[\cdot]$ (see Definition 4.1.10). Since we are also interested in a pointwise characterisation of the boundary conditions specifying the domain $\mathcal{D}(H)$ as given in (4.1.62), we have to ensure that the traces $\gamma\Phi$ of all functions $\Phi \in \mathcal{D}_{Q^{(2)}}$ form a dense subset of $L^2(\partial D_\Gamma)$.

Lemma 4.1.23. *Let* $P : (0,1) \to \mathrm{M}(4E^2, \mathbb{C})$ *be such that its matrix entries are in* $C^1(0,1)$*, then* $\mathrm{ran}(\gamma|_{\mathcal{D}_{Q^{(2)}}})$ *is dense in* $\ker \Pi$ *with respect to the norm on* $L^2(0,1) \otimes \mathbb{C}^{4E^2}$.

Whenever the form $Q^{(2)}_{P,L}[\cdot]$ is regular, we can establish the main result of this section.

Theorem 4.1.24. *Suppose that the matrix entries of* $P : (0,1) \to \mathrm{M}(4E^2, \mathbb{C})$ *are in* $C^1(0,1)$ *and that the quadratic form* $Q^{(2)}_{P,L}$ *is regular. Then the unique self-adjoint, semi-bounded operator* H *that is associated with this form is the two-particle Laplacian* $-\Delta_2$ *with domain* $\mathcal{D}_2(P, L)$.

Proof. The proof is in close analogy to the proof of Theorem 4.1.21, and leads to an obvious generalisation of (4.1.36). Performing the integration by part with some $\Psi \in \mathcal{D}_{Q^{(2)}}$ that does not vanish in a neighbourhood of ∂D_Γ one obtains the additional term

$$-\int_0^1 \langle \Phi'_{bv}(y) + L(y)\Phi_{bv}(y), \Psi_{bv}(y)\rangle_{\mathbb{C}^{4E^2}} \,\mathrm{d}y = -\langle \Phi'_{bv} + L\Phi_{bv}, \Psi_{bv}\rangle_{L^2(0,1)\otimes\mathbb{C}^{4E^2}} \,. \tag{4.1.68}$$

This is the explicit expression for $\partial_n\Psi[\gamma\Phi] + q_2[\Psi, \Phi]$ and is required to vanish. Again, the fact that $\mathrm{ran}(\gamma|_{\mathcal{D}_{Q^{(2)}}})$ is dense in $\ker\Pi$ implies the condition

$$Q(y)\Psi'_{bv}(y) + L(y)Q(y)\Psi_{bv}(y) = 0 \text{ for a.e. } y \in [0,1] \tag{4.1.69}$$

in (4.1.62). □

As in Proposition 4.1.14, given that the map P is of class C^1, we can establish uniqueness of the quadratic form and it associated operator H.

Proposition 4.1.25. *Suppose that the matrix entries of* $P : (0,1) \to \mathrm{M}(4E^2, \mathbb{C})$ *are in* $C^1(0,1)$*. Then the parametrisation of the quadratic form* $Q^{(2)}_{P,L}$ *in terms of* P *and* L *according to* (4.1.61) *and* (4.1.63) *is unique with this property.*

As a final result in this section, we want to construct a class of regular quadratic forms. The proof follows the same lines as the proof of Theorem 4.1.16 given in part B of the appendix. To this end, we assume that $P(y)$ is of form

$$P(y) = \begin{pmatrix} \tilde{P}(y) & 0 \\ 0 & \tilde{P}(y) \end{pmatrix} , \tag{4.1.70}$$

where $\tilde{P}(y)$ are blocks of dimension $2E^2$ acting on the upper or lower components of (4.1.58), respectively.

Theorem 4.1.26. *Let L be Lipschitz continuous on $[0,1]$ and let P be of the block-diagonal form (4.1.43). Assume that the matrix entries of $\tilde{P}$ are in $C^3(0,1)$. Moreover, when $y \in [0,\varepsilon_1] \cup [l-\varepsilon_2, l]$ with some $\varepsilon_1, \varepsilon_2 > 0$, suppose that $L(y) = 0$ and that $\tilde{P}(y)$ is diagonal with diagonal entries that are either zero or one. Then the quadratic form $Q^{(2)}_{P,L}$ is regular.*

4.2 Two identical particles on a graph

In this section, we will implement exchange symmetry in order to describe a pair of identical particles on a graph, i.e. fermions or bosons. The corresponding Hilbert spaces are denoted by $\mathcal{H}_{2,B}$ and $\mathcal{H}_{2,F}$, respectively. They are obtained by applying the projections

$$(\Pi_{B,F}\Psi)_{e_1e_2}(x_{e_1}, y_{e_2}) = \frac{1}{2}(\psi_{e_1e_2}(x_{e_1}, y_{e_2}) \pm \psi_{e_2e_1}(y_{e_2}, x_{e_1})), \tag{4.2.1}$$

to the full Hilbert space $\mathcal{H}_2$ where a minus sign is used in the fermionic case and a plus sign in the bosonic case.

Remark 4.2.1. We also write $L^2_B(\Gamma_2)$ for the bosonic two-particle Hilbert space and $L^2_F(\Gamma_2)$ for the fermionic two-particle Hilbert space. Again, we use an analogous notation for other function spaces.

Note that (4.2.1) implies the relation

$$\psi_{e_1e_2,x}(x_{e_1}, y_{e_2}) = \pm\psi_{e_2e_1,y}(y_{e_2}, x_{e_1}) \tag{4.2.2}$$

for functions $\Psi \in H^1_{B/F}(\Gamma_2)$. Here, the symmetric or antisymmetric Sobolev spaces

of order $m \in \mathbb{N}$ are defined by

$$H^m_{B/F}(\Gamma_2) = H^m(\Gamma_2) \cap L^2_{B/F}(\Gamma_2). \tag{4.2.3}$$

Due to exchange symmetry, the upper and lower components of (4.1.58) are no longer independent. We therefore assume that the maps P and L are of block structure

$$M(y) = \begin{pmatrix} \tilde{M}(y) & 0 \\ 0 & \tilde{M}(y) \end{pmatrix} , \tag{4.2.4}$$

where $M \in \{P, L\}$. Note that exchange symmetry would allow for more general forms of $M(y)$, i.e.

$$M(y) = \begin{pmatrix} \tilde{M}(y) & \tilde{N}(y) \\ \tilde{N}(y) & \tilde{M}(y) \end{pmatrix} . \tag{4.2.5}$$

However, for convenience, we will always restrict us to the case (4.2.4) in the following. We also introduce the restricted vector of boundary values

$$\tilde{\Psi}_{bv}(y) = \begin{pmatrix} \sqrt{l_{e_2}}\psi_{e_1e_2}(0, l_{e_2}y) \\ \sqrt{l_{e_2}}\psi_{e_1e_2}(l_{e_1}, l_{e_2}y) \end{pmatrix} \tag{4.2.6}$$

for functions $\Psi \in H^1_{B/F}(\Gamma_2)$ and, in addition,

$$\tilde{\Psi}'_{bv}(y) = \begin{pmatrix} \sqrt{l_{e_2}}\psi_{e_1e_2,x}(0, l_{e_2}y) \\ -\sqrt{l_{e_2}}\psi_{e_1e_2,x}(l_{e_1}, l_{e_2}y) \end{pmatrix} \tag{4.2.7}$$

for functions $\Psi \in H^2_{B/F}(\Gamma_2)$. Based on this notation, the quadratic form we want to introduce is

$$\begin{aligned} Q^{(2),B/F}_{P,L}[\Psi] = 2 \sum_{e_1,e_2=1}^{E} \int_0^{l_{e_2}} \int_0^{l_{e_1}} \left|\psi_{e_1e_2,x}(x,y)\right|^2 \,\mathrm{d}x\,\mathrm{d}y \\ - 2\int_0^1 \langle \tilde{\Psi}_{bv}(y), \tilde{L}(y)\tilde{\Psi}_{bv}(y)\rangle_{\mathbb{C}^{2E^2}} \,\mathrm{d}y \ , \end{aligned} \tag{4.2.8}$$

with domain

$$\mathcal{D}_{Q^{(2),B/F}} = \{\Psi \in H^1_{B/F}(\Gamma_2);\ \tilde{P}(y)\tilde{\Psi}_{bv}(y) = 0 \text{ for a.e. } y \in [0,1]\} \ . \tag{4.2.9}$$

Using the same steps as in the previous sections, we readily obtain the following

result.

Theorem 4.2.2. *The quadratic form $Q_{P,L}^{(2),B/F}[\cdot]$ with domain $\mathcal{D}_{Q^{(2),B/F}}$ is closed and semi-bounded.*

Furthermore, taking Definition 4.1.10 into account, we have:

Theorem 4.2.3. *Suppose that the matrix entries of $\tilde{P} : (0,1) \to \mathrm{M}(2E^2, \mathbb{C})$ are in $C^1(0,1)$ and that the quadratic form $Q_{P,L}^{(2),B/F}$ is regular. Then the unique self-adjoint, semi-bounded operator $H_{B/F}$ that is associated with this form is the bosonic or fermionic two-particle Laplacian $-\Delta_{2,B/F}$ with domain*

$$\begin{aligned}\mathcal{D}_{2,B/F}(P,L) = \{\Psi \in H^2_{B/F}(\Gamma_2);\ \tilde{P}(y)\tilde{\Psi}_{bv}(y) = 0 \text{ and} \\ \tilde{Q}(y)\tilde{\Psi}'_{bv}(y) + \tilde{L}(y)\tilde{Q}(y)\tilde{\Psi}_{bv}(y) = 0 \text{ for a.e. } y \in [0,1]\}\ .\end{aligned} \tag{4.2.10}$$

Remark 4.2.4. Examples of regular quadratic forms follow immediately from Theorem 4.1.26. Also, in the following, we will denote the self-adjoint operator corresponding to the form $Q_{P,L}^{(2),B/F}$ as $(-\Delta_{2,B/F}, \mathcal{D}_{2,B/F}(P,L))$, irrespective of regularity.

In order to identify self-adjoint realisations that correspond to a system with genuine two-particle interactions (see Definition 4.1.18 and Proposition 4.1.19), we decompose the space of boundary values V as

$$V = \bigoplus_{e_2=1}^{E} V_{e_2}\ , \tag{4.2.11}$$

where V_{e_2} is the subspace of boundary values in (4.1.58) corresponding to fixed e_2. Furthermore, each block V_{e_2} is ordered as the vectors of bounday values (3.1.4) in the one-particle case. Based on this, we have the following statement.

Proposition 4.2.5. *Suppose that the matrix entries of $\tilde{P} : (0,1) \to \mathrm{M}(2E^2, \mathbb{C})$ are in $C^1(0,1)$. Then, the two-particle Laplacian $-\Delta_{2,B/F}$ with domain $\mathcal{D}_{2,B/F}(P,L)$ represents no interactions iff $\tilde{P}$ and $\tilde{L}$ are block-diagonal with respect to the decomposition* (4.2.11) *with blocks that are identical and represent corresponding one-particle maps.*

Remark 4.2.6. Proposition 4.2.5 can readily be generalised to a system of distinguishable particles on general compact graphs as described in the last section.

4.2.1 Local two-particle interactions

So far, the maps P and L were allowed to be arbitrary matrices. Only to establish regular quadratic forms, we require P and L to exhibit the block structure (4.1.70). However, whenever P and L are arbitrary, it can be seen from (4.2.10) that so called *non-local* couplings are introduced. For example, the boundary values of the two components $\psi_{e_1e_2}$ and $\psi_{\tilde{e}_1\tilde{e}_2}$ could be coupled, *independent* of the connectivity of the graph, i.e. it could be that edges e_1 and e_2 do not have a common vertex with edges $\tilde{e}_1$ and $\tilde{e}_2$. For a one-particle system, locality means that the one-particle maps $P \in \mathbb{C}^{2E\times 2E}$ and $L \in \mathbb{C}^{2E\times 2E}$ are block diagonal with respect to the decomposition

$$V = \bigoplus_{v\in\mathcal{V}} V_v \ , \tag{4.2.12}$$

where the subspace V_v only contains components of the wave function $\Psi \in L^2(\Gamma)$ that start or end in the vertex v [BE09]. In the two-particle case, locality can be introduced as follows: In a first step, we carry over the notion of locality from the one-particle case in order to respect the connectivity of the graph. To this end, we decompose the components in (4.2.6) and (4.2.7) as

$$V = \bigoplus_{v\in\mathcal{V}} V_v \ , \tag{4.2.13}$$

where the subspace V_v contains all components $\psi_{e_1e_2}$ such that the first variable is related to the vertex v. Thus all components in V_v are such that the particle described by the first coordinate is located at vertex v. However, the second particle could still be on any other edge which is not necessarily connected to v. A weak version of two-particle locality would then require that

$$V_v = \bigoplus V_{weak}(v), \tag{4.2.14}$$

where $V_{weak}(v)$ only contains components $\psi_{e_1e_2}$ and $\psi_{e_1'e_2'}$ such that the first particle sits at vertex v and e_2 and e_2' are connected. Since the weak notion of locality does not take into account that both particles may be 'far' from each other, a stronger notion of locality might be applied. To arrive at this stronger notion of locality,

we demand that the subspace $V_{weak}(v)$ is further decomposed as

$$V_{weak}(v) = V_{strong}(v) \oplus \tilde{V}_{weak}(v). \tag{4.2.15}$$

Here the subspace $V_{strong}(v)$ only contains components $\psi_{e_1e_2}$ and $\psi_{e_1'e_2'}$ such that the first coordinate forms the common vertex v and the second coordinate lives on an edge connected to v. All other components of $V_{weak}(v)$ that do not allow for a stronger notion of locality are contained in $\tilde{V}_{weak}(v)$.

4.2.2 An Example

In this section, we want to illustrate the nature of the singular interactions introduced above. For this, we choose a simple graph consisting of two edges of infinite length joined at one common vertex. Strictly speaking, since this is not a compact graph, our results do not cover this example. However, since we are only interested in local properties of the interactions, it is enough to consider a graph of this form. Furthermore, instead of using maps P and L to characterise the boundary conditions, we use maps A and B as explained in Remark 4.1.6.
Since the graph has two edges, the (bosonic or fermionic) wave-function $\Psi = (\psi_{e_1e_2}) \in (L^2(\mathbb{R}^2_+) \otimes \mathbb{C}^4)_{B/F}$ has four components and the boundary values of Ψ are encoded in vectors

$$\tilde{\Psi}_{bv}(y) = \begin{pmatrix} \psi_{11}(0,y) \\ \psi_{21}(0,y) \\ \psi_{12}(0,y) \\ \psi_{22}(0,y) \end{pmatrix} \quad \text{and} \quad \tilde{\Psi}'_{bv}(y) = \begin{pmatrix} \psi_{11,x}(0,y) \\ \psi_{21,x}(0,y) \\ \psi_{12,x}(0,y) \\ \psi_{22,x}(0,y) \end{pmatrix} . \tag{4.2.16}$$

Note that only the values of the wave function at 0 have to be included since the edges are of infinite length. We furthermore choose the maps $A, B : [0,\infty) \to \mathrm{M}(4,\mathbb{C})$ as

$$A(y) = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & v(0,y) & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & v(0,-y) \end{pmatrix} \quad \text{and} \quad B(y) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 \end{pmatrix} , \tag{4.2.17}$$

where $v \in C_0^\infty(\mathbb{R}^2)$ with $v(x,y) = v(y,x)$. The boundary conditions, in terms of maps A and B, then read

$$A(y)\tilde{\Psi}_{bv}(y) + B(y)\tilde{\Psi}'_{bv}(y) = 0. \tag{4.2.18}$$

Note that this implies the continuity relations

$$\begin{aligned} \psi_{11}(0,y) &= \psi_{21}(0,y), \\ \psi_{12}(0,y) &= \psi_{22}(0,y). \end{aligned} \tag{4.2.19}$$

Furthermore, writing out (4.2.18), we get

$$\begin{aligned} -\psi_{11,x}(0,y) - \psi_{21,x}(0,y) &= -v(0,y)\psi_{21}(0,y), \\ -\psi_{12,x}(0,y) - \psi_{22,x}(0,y) &= -v(0,-y)\psi_{22}(0,y). \end{aligned} \tag{4.2.20}$$

We now rearrange the four components defined on $\mathbb{R}^2_+$, such that we end up with one function defined on $\mathbb{R}^2$, i.e.

$$\begin{aligned} \psi(x,y) &= \psi_{11}(x,y), \\ \psi(-x,-y) &= \psi_{22}(x,y), \\ \psi(x,-y) &= \psi_{12}(x,y), \\ \psi(-x,y) &= \psi_{21}(x,y). \end{aligned} \tag{4.2.21}$$

Using those relations, we can see that the boundary conditions fulfilled by ψ equal those induced by the formal Hamiltonian

$$\hat{H} = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + v(x,y)[\delta(x) + \delta(y)] \ . \tag{4.2.22}$$

As can be seen from (4.2.22), the delta-functions lead to a strong localisation in the sense that the interaction is present only whenever at least one of the particles hits the vertex. Furthermore, it is worth mentioning the close connection of (4.2.22) with the model presented in [MP95]. If we choose the function $v(x,y)$ with a support close to the origin, the particles only interact whenever they are both close to the vertex. In this sense, the interactions are similar to those introduced in [MP95] where the particles interact whenever *both* particles are situated at the vertex.

4.3 Spectral properties

In this section, we shall discuss spectral properties of the self-adjoint operators $(-\Delta_2, \mathcal{D}_2(P,L))$ corresponding to quadratic forms $Q^{(2)}_{P,L}[\cdot]$ as described in Theorems 4.1.21 and 4.2.2. Note that we do *not*, as mentioned in Remark 4.1.13, require the forms to be regular. First of all, one would like to know whether the spectrum of an operator $(-\Delta_2, \mathcal{D}_2(P,L))$ is purely discrete. Since we are concerned with compact quantum graphs, one would indeed expect the spectrum to be purely discrete. However, since the boundary conditions as expressed in (4.1.62) are non-trivial, one would like to prove this. Furthermore, it would be interesting to know if the corresponding eigenvalue count exhibits standard Weyl asymptotics [Wey11, AE09]. To introduce the standard Weyl law, let $\Omega \subset \mathbb{R}^2$ be a bounded convex domain with boundary $\partial\Omega$. On this domain, consider the *Helmholtz* equation

$$(-\Delta_2 + \lambda)\varphi(x) = 0, \quad \lambda \in \mathbb{R}, \tag{4.3.1}$$

with Dirichlet boundary conditions, i.e. $\varphi(x) = 0$ for $x \in \partial\Omega$. It is well known that equation (4.3.1) allows for a non-trivial solution only for a discrete set $\{\lambda_n\}_{n\in\mathbb{N}_0}$, with corresponding solutions $\{\varphi_n\}_{n\in\mathbb{N}_0}$. Defining the counting function

$$N(\lambda) = \#\{\lambda_n \leq \lambda\}, \tag{4.3.2}$$

where the eigenvalues are counted with their corresponding multiplicities, one has the following statement.

Theorem 4.3.1. *[RS78] Given that $\{\lambda_n\}_{n\in\mathbb{N}_0}$ is the set of values for which there exists a solution of the boundary-value problem* (4.3.1)*. Then the counting function $N(\lambda)$ allows for the expansion*

$$N(\lambda) = \frac{|\Omega|}{4\pi}\,\lambda + o(\lambda), \tag{4.3.3}$$

where $|\Omega|$ is the area of the domain $\Omega \in \mathbb{R}^2$ and $o(\cdot)$ is the Landau symbol.

In a first step, assume that the two-particle Laplacian $(-\Delta_2, \mathcal{D}_2(P,L))$ describes a system of non-interacting particles as characterised in Propositions 4.1.19 and 4.2.5 (see also Remark 4.2.6). For such self-adjoint realisations, the two-

particle spectrum is discrete with eigenvalues

$$\lambda_{nm} = k_n^2 + k_m^2, \quad n, m \in \mathbb{N}_0, \tag{4.3.4}$$

where $\{k_n^2\}_{n\in\mathbb{N}_0}$ are the corresponding one-particle eigenvalues.

Lemma 4.3.2. *Let $(-\Delta_2, \mathcal{D}_2(P, L))$ be a self-adjoint realisation describing a system of non-interacting particles. Then the eigenvalues $\{\lambda_{nm} : (n, m) \in \mathbb{N}_0^2\}$ of $-\Delta_2$ are distributed according to the Weyl law,*

$$N_2(\lambda) = \{(n, m) \in \mathbb{N}_0^2;\ \lambda_{nm} \leq \lambda\} \sim \frac{\mathcal{L}^2}{4\pi}\lambda\ , \qquad \lambda \to \infty\ , \tag{4.3.5}$$

where $\mathcal{L} = l_1 + \cdots + l_E$ is the sum of the edge lengths of the graph. It is understood that $N_2(\lambda)$ counts eigenvalues with their respective multiplicities.

Proof. As established in Lemma 3.2.3, the eigenvalue count for the one-particle Laplacian $-\Delta_1$ with eigenvalues $\{k_n^2\}_{n\in\mathbb{N}_0}$ follows the asymptotics

$$N_1(k) = \{n \in \mathbb{N}_0;\ k_n^2 \leq k^2\} \sim \frac{\mathcal{L}}{\pi}k\ , \qquad k \to \infty\ . \tag{4.3.6}$$

Via a Tauberian theorem [Kar31], this asymptotic law is equivalent to

$$\sum_n \mathrm{e}^{-k_n^2 t} \sim \frac{\mathcal{L}}{\sqrt{4\pi t}}\ , \qquad t \to 0+\ . \tag{4.3.7}$$

Squaring both sides of (4.3.7) and using the equivalence between eigenvalue asymptotics and heat-trace asymptotics in the opposite direction immediately yields (4.3.5). □

Using a bracketing argument for quadratic forms [RS78, Dob05], we can now generalise this lemma to arbitrary self-adjoint realisations.

Theorem 4.3.3. *A self-adjoint realisation of the two-particle Laplacian $-\Delta_2$ with domain $\mathcal{D}_2(P, L)$ has compact resolvent and, therefore, possesses a purely discrete spectrum. Moreover, the eigenvalue asymptotics follow the Weyl law* (4.3.5).

Proof. The proof is based on a comparison with two operators (quadratic forms). Both comparison operators describe a system of non-interacting particles and hence are covered by Lemma 4.3.2. The first operator $(-\Delta_2, \mathcal{D}_2(P_D, L_D))$ is the

Dirichlet-Laplacian, characterised by the projector $P_D = \mathbb{1}_{4E^2}$ as well as $L_D = 0$. The second operator $(-\Delta_2, \mathcal{D}_2(P_R, L_R))$ is the Robin-Laplacian and is characterised by the projector $P_R = 0$ and $L_R = \|\Lambda\|_{op}\mathbb{1}_{4E^2}$, where $\|\Lambda\|_{op}$ is the operator norm of Λ (4.1.60) (see also [BE09]). For every operator $(-\Delta_2, \mathcal{D}_2(P, L))$, the associated quadratic form satisfies the inclusion

$$\mathcal{D}_{Q^{(2)}_{P_D,L_D}} \subseteq \mathcal{D}_{Q^{(2)}_{P,L}} \subseteq \mathcal{D}_{Q^{(2)}_{P_R,L_R}} \ . \tag{4.3.8}$$

This means, in the sense of [RS78], that

$$(-\Delta_2, \mathcal{D}_2(P_D, L_D)) \geq (-\Delta_2, \mathcal{D}_2(P, L)) \geq (-\Delta_2, \mathcal{D}_2(P_R, L_R)) \ . \tag{4.3.9}$$

Now, for every self-adjoint, semi-bounded operator H on a Hilbert space $\mathcal{H}$, one can define

$$\mu_n(H) = \sup_{\varphi_1,\dots,\varphi_{n-1}\in\mathcal{H}} \inf_{\substack{\psi\in[\varphi_1,\dots,\varphi_{n-1}]^\perp \\ \psi\in Q_H, \|\psi\|=1}} \langle\psi, H\psi\rangle_{\mathcal{H}} \ , \tag{4.3.10}$$

see Theorem 2.1.27. Then (4.3.9) implies that

$$\mu_n(-\Delta_2)_D \geq \mu_n(-\Delta_2) \geq \mu_n(-\Delta_2)_R \ . \tag{4.3.11}$$

Using that the Dirichlet- as well as the Robin-Laplacian have compact resolvent, one concludes (with Theorem XIII.64 in [RS78]) that $\mu_n(-\Delta_2)_{R,D} \to \infty$ as $n \to \infty$; hence the same is true for $\mu_n(-\Delta_2)$. By the same theorem, this implies that $(-\Delta_2, \mathcal{D}_2(P, L))$ has compact resolvent. Furthermore, (4.3.9) implies for the eigenvalue counting functions that

$$N_2^D(\lambda) \leq N_2(\lambda) \leq N_2^R(\lambda) \ . \tag{4.3.12}$$

As both N_2^D and N_2^R count eigenvalues of a two-particle Laplacian that correspond to non-interacting systems, they both satisfy the Weyl asymptotics (4.3.5). Hence the same asymptotics holds for N_2. □

Finally, we want to consider symmetric or antisymmetric realisations of the two-particle Laplacian, i.e. $(-\Delta_2, \mathcal{D}_{2,B/F}(P, L))$. For self-adjoint realisations that correspond to non-interacting systems, the (anti-)symmetric eigenfunctions are

given by

$$\psi_n \otimes \psi_m \pm \psi_m \otimes \psi_n, \tag{4.3.13}$$

and hence the two eigenvalues λ_{nm} and λ_{mn} are identified. Accordingly, the corresponding eigenvalue counting function $N_{2,B/F}$ fulfils

$$N_{2,B/F}(\lambda) \sim \frac{\mathcal{L}^2}{8\pi}\lambda\ , \qquad \lambda \to \infty\ , \tag{4.3.14}$$

where the factor of one half comes from the identification of λ_{nm} and λ_{mn}. Using the same arguments as in the proof of Theorem 4.3.3, we can now prove the same asymptotic for any realisation $(-\Delta_2, \mathcal{D}_{2,B/F}(P,L))$.

Theorem 4.3.4. *A self-adjoint, bosonic or fermionic realisation of the two-particle Laplacian $-\Delta_2$ on a domain $\mathcal{D}_{2,B/F}(P,L)$ has compact resolvent and, therefore, possesses a purely discrete spectrum. Moreover, the eigenvalue asymptotics follow the Weyl law* (4.3.14).

5. CONTACT INTERACTIONS ON COMPACT QUANTUM GRAPHS

In this chapter, we will introduce contact interactions between the particles. In contrast to the singular interactions localised at the vertices of the graph, contact interactions are also present along the edges, i.e. whenever two particles are at the same position.

Contact interactions play an important role in various areas of physics. For example, the Gross-Pitaevskii equation that describes the spatial extension of a Bose-Einstein condensate [LSSY05, Ued10] is derived from the Schrödinger equation by considering point-like contact interactions. Indeed, the interaction potential between two particles with positions $\vec{r}_1 \in \mathbb{R}^3$ and $\vec{r}_2 \in \mathbb{R}^3$ is modelled as

$$V(\vec{r}_1, \vec{r}_2) = \frac{4\pi\hbar^2 a}{m}\, \delta(\vec{r}_1 - \vec{r}_2), \tag{5.0.1}$$

where a is the scattering length and m is the mass of the particles. Another important model, that incorporates point-like contact interactions and plays a prominent role in the description of one-dimensional Bose-Einstein condensation [CCG$^+$11], is the Lieb-Liniger model [LL63]. For a system of two particles, the Hamiltonian in the Lieb-Liniger model is given by

$$\hat{H} = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \alpha\delta(x - y), \tag{5.0.2}$$

where $\alpha \in \mathbb{R}$ is the interaction strength and $x, y \in \mathbb{R}$ are the positions of the particles. Note that the limit $\alpha \to \infty$ corresponds to (repulsive) *hard-core* interactions, effectively leading to Dirichlet boundary conditions for the wave function at $x = y$. Also, note that the Hamiltonian (5.0.2) is only a formal expression since the delta-distribution $\delta(x - y)$ is not properly defined as an operator on $L^2(\mathbb{R}^2)$. However, there are various possibilities to circumvent this difficulty. For example, Lieb and Liniger [LL63] considered the Hamiltonian (5.0.2) for N bosons on

an interval with periodic boundary conditions and, using a Bethe ansatz, they constructed the eigenfunctions explicitly. On a graph, however, the boundary conditions are not always periodic in the vertices and it is therefore not possible to use the same approach. Indeed, we will use that the delta-function in (5.0.2) can effectively be expressed in terms of boundary conditions. As a first step, note that the interaction term in (5.0.2) is only important whenever the particles are at the same position, i.e. whenever $x = y$. This in turn means that (5.0.2) acts as the standard Laplacian on functions that vanish along the diagonal. Accordingly, the idea is to divide the configuration space $\mathbb{R}^2$ into two subdomains

$$\begin{aligned} \mathbb{R}^2_+ &= \{(x,y) \in \mathbb{R}^2 |\ x > y\}, \\ \mathbb{R}^2_- &= \{(x,y) \in \mathbb{R}^2 |\ x < y\}, \end{aligned} \tag{5.0.3}$$

and to characterise self-adjoint realisations of the Laplacian based on this dissected configuration space. Formally, the action of the operator (5.0.2) is given by

$$\langle \varphi, \hat{H}\varphi \rangle_{L^2(\mathbb{R}^2)} = \langle \varphi, -\Delta_2 \varphi \rangle_{L^2(\mathbb{R}^2)} + \alpha \int_{\mathbb{R}} |\varphi(x,x)|^2 \, \mathrm{d}x \tag{5.0.4}$$

which implies that the quadratic form corresponding to the formal Hamiltonian (5.0.2) is constructed from the form of the free Laplacian by adding the term proportional to α, i.e.

$$Q_\delta[\varphi] = \int_{\mathbb{R}^2} |\nabla \varphi|^2 \, \mathrm{d}x\mathrm{d}y + \alpha \int_{\mathbb{R}} |\varphi(x,x)|^2 \, \mathrm{d}x. \tag{5.0.5}$$

To see how the δ-interaction in (5.0.2) affects the continuity properties of functions and their derivatives, we define the form (5.0.5) on the domain

$$\mathcal{D}_{Q_\delta} = \left\{ \varphi \in H^1(\mathbb{R}^2) |\ \varphi_\pm \in H^2(\mathbb{R}^2_\pm) \right\}. \tag{5.0.6}$$

Here $\varphi_\pm$ denote the restrictions of φ to $\mathbb{R}^2_\pm$. Note that, by construction, functions $\varphi \in \mathcal{D}_{Q_\delta}$ are continuous along the diagonal, i.e. $\varphi_+(x,x) = \varphi_-(x,x)$. Furthermore,

integrating by parts gives

$$\begin{aligned} Q_\delta[\varphi] = \langle \varphi, -\Delta_2 \varphi \rangle_{L^2(\mathbb{R}^2)} + \alpha \int_{\mathbb{R}} |\varphi_+(x,x)|^2 \mathrm{d}x \\ + \sqrt{2} \int_{\mathbb{R}} \bar{\varphi}_+ \left(\frac{\partial \varphi_+}{\partial \vec{n}} + \frac{\partial \varphi_-}{\partial \vec{n}} \right) \mathrm{d}x, \end{aligned} \tag{5.0.7}$$

where the plus sign in the outer (unit) normal derivatives refers to $\mathbb{R}^2_+$ and the minus sign refers to $\mathbb{R}^2_-$. Finally, since the form (5.0.7) shall correspond to a self-adjoint realisation of the Laplacian $-\Delta_2$, the last two terms on the right of (5.0.7) must vanish, implying the boundary conditions

$$\left(\frac{\partial \varphi_+}{\partial \vec{n}} + \frac{\partial \varphi_-}{\partial \vec{n}} \right) + \frac{\alpha}{\sqrt{2}} \varphi_+ = 0 \tag{5.0.8}$$

along the diagonal. Hence, a two particle delta-interaction as in (5.0.2) induces a jump in the normal derivatives along the diagonal of $\mathbb{R}^2$. This is similar to the case of the one-dimensional delta-interaction which also induces a jump in the derivatives (see (3.1.10)). Note that contact interactions of the form (5.0.8) for identical particles were also discussed in [LM77].

Note that contact interactions on a graph are also important in the context of many-particle quantum chaos. As established in [KS97b] and outlined in Chapter 3, chaos on a one-particle graph originates in the scattering of the particle in the vertices. However, in a one-particle system, the motion along the edges is simple. To investigate properties of many-particle effects, we have so far introduced singular two-particle interactions localised at the vertices of the graph. But since at least one of the particles had to be at the vertex, the motion along the edges remained unaffected given that both particles were situated in the interior of an edge. Contact interactions, on the other hand, lead to a non-trivial motion along the edges since scattering takes place whenever two particles hit each other. For this reason, they lead to another possibility for investigating properties of many-particle chaos. In that context, it is worth mentioning interesting numerical results concerning the quantum chaotic behaviour of two-particle systems with short-range interactions [VSCdL01, XSdS$^+$04]. In [VSCdL01], the authors considered

two particles on an interval with Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2\gamma m}\frac{\partial^2}{\partial y^2} + \alpha\delta(x-y), \tag{5.0.9}$$

where $\alpha \in \mathbb{R}$ is the interaction strength and γ the mass ratio. Furthermore, the boundary conditions where chosen to be either Dirichlet or periodic. The authors then numerically calculated the eigenvalues and plotted the nearest-neighbour level spacings distribution $P(s)$ (see (3.3.13)), finally comparing it to either Poisson statistics or random matrix predictions. The results were as follows:

1. In the case of Dirichlet boundary conditions, the system is non-chaotic for $\gamma = 1$ and chaotic for $\gamma \neq 1$ and α large enough.

2. In the case of periodic boundary conditions, the system is non-chaotic for all values γ.

We hence see that the choice of boundary conditions, as well as the mass ratio, play an important role in the development of quantum chaos. Note that similar results were obtained in [XSdS$^+$04]. In that paper, the authors considered two particles in a circular domain interacting via Yukawa short-range potentials and subject to a constant magnetic field. Numerically evaluating the eigenvalues of the interacting system, and plotting the nearest-neighbour level spacing distribution $P(s)$, the results were as follows:

1. For a mass ratio $\gamma = 1$, the system is non-chaotic and the level-spacing distribution follows Poisson statistics.

2. For a mass ratio of $\gamma = 15$, the system is chaotic and the level-spacing distribution follows GOE predictions.

3. For increasing values of γ, the degree of chaos measured in terms of a suitable function, increases as well. However, the curve showing the increase of chaos is oscillating yielding a more integrable behaviour at certain values of γ.

In this thesis, we will only consider particles of equal mass. However, since the lengths of the edges can be chosen arbitrarily, one can nevertheless introduce a similar breaking of symmetry. To see this, assume that one particle is located on edge e_1 with length l_1 and the second particle is located on edge e_2 with length

$l_2 = \gamma l_1$, where $\gamma \in \mathbb{R}$ is a scaling parameter. The corresponding components of $-\Delta_2$ then read

$$\begin{aligned}(-\Delta_2)_{e_1e_2} &= -\frac{\partial^2}{\partial x_{e_1}^2} - \frac{\partial^2}{\partial x_{e_2}^2} \\ &= -\frac{1}{l_{e_1}^2}\frac{\partial^2}{\partial y_{e_1}^2} - \frac{1}{\gamma^2 l_{e_1}^2}\frac{\partial^2}{\partial y_{e_2}^2},\end{aligned} \tag{5.0.10}$$

where $y_{e_1}, y_{e_2} \in (0,1)$ are rescaled coordinates. A comparison with (5.0.9) hence shows that the metric of the graph can cause a breaking of symmetry similar to a mass ratio unequal to one.

This chapter is organised as follows: In the first part, we will introduce contact interactions on general quantum graphs, also discussing regularity results and spectral properties of the self-adjoint operators. In the second part, we then introduce exchange symmetry in order to describe contact interactions in a system of two bosons. In the third part, we extend the results to a system of N bosons, finally obtaining a generalisation of the Lieb-Liniger model to general quantum graphs. Note that the presentation in this chapter follows closely our paper [BK13c].

5.1 Contact interactions in a system of two distinguishable particles

We want to implement interactions that are present whenever two particles on a graph are located on the same edge and at the same position. Given the two-particle configuration space

$$D_\Gamma = \dot{\bigcup_{e_1e_2}} D_{e_1e_2}, \tag{5.1.1}$$

these interactions have to be implemented on the squares $\{D_{ee}\}_{e\in\mathcal{E}}$. As explained above, this will be achieved by a dissection of each D_{ee} while imposing suitable matching conditions for functions and their (normal) derivatives along the diagonal. To this end, we introduce the *dissected* configuration space

$$D_\Gamma^* = \left(\dot{\bigcup_{e_1\neq e_2}} D_{e_1e_2}\right) \dot{\bigcup_e} \left(D_{ee}^+ \dot{\cup} D_{ee}^-\right), \tag{5.1.2}$$

where $D_{ee}^{+} = \{(x,y) \in D_{ee};\ x > y\}$ and $D_{ee}^{-} = \{(x,y) \in D_{ee};\ x < y\}$. Functions on D_{Γ}^{*} are denoted as $\Psi = (\psi_{e_1e_2})$. Note that components defined on $D_{e_1e_2}$, with $e_1 \neq e_2$, are given by $\psi_{e_1e_2}$, whereas components on D_{ee} are given by $\psi_{ee} = (\psi_{ee}^{+}, \psi_{ee}^{-})$ with $\psi_{ee}^{\pm}$ defined on $D_{ee}^{\pm}$. Accordingly, the (dissected) two-particle Hilbert space $\mathcal{H}_2^*$ is given by

$$L^2(\Gamma_2^*) = \left(\bigoplus_{e_1 \neq e_2} L^2(D_{e_1e_2}) \right) \bigoplus_{e} \left(L^2(D_{ee}^{+}) \oplus L^2(D_{ee}^{-}) \right). \tag{5.1.3}$$

Introducing Sobolev spaces in the same fashion, boundary values of functions $\Psi \in H^1(\Gamma_2^*)$ will be characterised by vectors

$$\Psi_{bv}(y) = \big(\psi_{e_1e_2,bv}(y)\big) \qquad \text{and} \qquad \Psi'_{bv}(y) = \big(\psi'_{e_1e_2,bv}(y)\big). \tag{5.1.4}$$

For $e_1 \neq e_2$, no contact interactions are present and we set

$$\psi_{e_1e_2,bv}(y) = \begin{pmatrix} \sqrt{l_{e_2}}\psi_{e_1e_2}(0, l_{e_2}y) \\ \sqrt{l_{e_2}}\psi_{e_1e_2}(l_{e_1}, l_{e_2}y) \\ \sqrt{l_{e_1}}\psi_{e_1e_2}(l_{e_1}y, 0) \\ \sqrt{l_{e_1}}\psi_{e_1e_2}(l_{e_1}y, l_{e_2}) \end{pmatrix}, \tag{5.1.5}$$

as well as

$$\psi'_{e_1e_2,bv}(y) = \begin{pmatrix} \sqrt{l_{e_2}}\psi_{e_1e_2,x}(0, l_{e_2}y) \\ -\sqrt{l_{e_2}}\psi_{e_1e_2,x}(l_{e_1}, l_{e_2}y) \\ \sqrt{l_{e_1}}\psi_{e_1e_2,y}(l_{e_1}y, 0) \\ -\sqrt{l_{e_1}}\psi_{e_1e_2,y}(l_{e_1}y, l_{e_2}) \end{pmatrix}. \tag{5.1.6}$$

On the other hand, for $e_1 = e_2$, boundary values along the diagonal have to be added. Noting that the inward normal derivatives on the diagonal are

$$\psi_{ee,n}^{\pm} = \frac{\pm 1}{\sqrt{2}} \big(\psi_{ee,x}^{\pm} - \psi_{ee,y}^{\pm}\big), \tag{5.1.7}$$

we set

$$\psi_{ee,bv}(y) = \begin{pmatrix} \sqrt{l_e}\psi^-_{ee}(0, l_e y) \\ \sqrt{l_e}\psi^+_{ee}(l_e, l_e y) \\ \sqrt{l_e}\psi^+_{ee}(l_e y, 0) \\ \sqrt{l_e}\psi^-_{ee}(l_e y, l_e) \\ \sqrt{l_e}\psi^+_{ee}(l_e y, l_e y) \\ \sqrt{l_e}\psi^-_{ee}(l_e y, l_e y) \end{pmatrix} \quad \text{and} \quad \psi'_{ee,bv}(y) = \begin{pmatrix} \sqrt{l_e}\psi^-_{ee,x}(0, l_e y) \\ -\sqrt{l_e}\psi^+_{ee,x}(l_e, l_e y) \\ \sqrt{l_e}\psi^+_{ee,y}(l_e y, 0) \\ -\sqrt{l_e}\psi^-_{ee,y}(l_e y, l_e) \\ \sqrt{2l_e}\psi^+_{ee,n}(l_e y, l_e y) \\ \sqrt{2l_e}\psi^-_{ee,n}(l_e y, l_e y) \end{pmatrix}, \tag{5.1.8}$$

for $y \in [0, 1]$. Altogether, the vectors (5.1.4) of boundary values have $n(E) = 4E^2 + 2E$ components.

In the following, we will always assume a certain ordering of boundary values that allows us to distinguish clearly between contact interactions and interactions related to vertices. In detail, we assume the structure

$$\mathbb{C}^{n(E)} = V_{contact} \oplus V_{vertex}, \tag{5.1.9}$$

with $\dim V_{contact} = 2E$ and $\dim V_{vertex} = 4E^2$. Here V_{vertex} consists of all components of (5.1.5) and (5.1.6) as well as the upper four components of (5.1.8). As can be seen from their arguments, they are related to the vertices of the graph. On the other hand, $V_{contact}$ consists of the lower two components of (5.1.8), hence representing the contact interaction part. As a next step, we introduce two bounded and measurable maps $P, L : [0, 1] \to \mathrm{M}(n(E), \mathbb{C})$ that are required to fulfil

1. $P(y)$ is an orthogonal projection,
2. $L(y)$ is a self-adjoint endomorphism on $\ker P(y)$,

for a.e. $y \in [0, 1]$. Moreover, we set $Q(y) = \mathbb{1}_{n(E)} - P(y)$. On $L^2(0, 1) \otimes \mathbb{C}^{n(E)}$, we associate two bounded and self-adjoint operators with P and L, i.e.

$$\Pi : L^2(0, 1) \otimes \mathbb{C}^{n(E)} \to L^2(0, 1) \otimes \mathbb{C}^{n(E)}, \chi(y) \mapsto P(y)\chi(y), \tag{5.1.10}$$

and

$$\Lambda : L^2(0, 1) \otimes \mathbb{C}^{n(E)} \to L^2(0, 1) \otimes \mathbb{C}^{n(E)}, \chi(y) \mapsto L(y)\chi(y). \tag{5.1.11}$$

In order to avoid a coupling of vertex interactions and contact interactions, we will throughout this chapter assume that the maps P and L are of the form

$$M = M_{contact} \oplus M_{vertex}, \tag{5.1.12}$$

with regard to the decomposition (5.1.9) and $M \in \{P, L\}$. Also, to avoid contact interactions across different edges, we assume that $M_{contact}$ is block-diagonal with respect to the decomposition

$$M_{contact} = \bigoplus_e M_{contact,e}, \tag{5.1.13}$$

where $M_{contact,e}$ contains the lower two components of (5.1.8) for the edge $e \in \mathcal{E}$. Our aim is now to characterise self-adjoint realisations of the two-particle Laplacian $-\Delta_2$ that represent two-particle contact interactions. They will be symmetric extensions of $(-\Delta_2, C_0^\infty(\Gamma_2^*))$ and, in analogy to the one-particle case (3.1.22), as well as the case of singular interactions covered in the last chapter (4.1.62), their domains should be given in the form

$$\begin{aligned}\mathcal{D}_2(P, L) = \{\Psi \in H^2(\Gamma_2^*);\ & P(y)\Psi_{bv}(y) = 0 \text{ and} \\ & Q(y)\Psi'_{bv}(y) + L(y)Q(y)\Psi_{bv}(y) = 0 \text{ for a.e. } y \in [0,1]\}.\end{aligned} \tag{5.1.14}$$

However, before we generate a quadratic form that will (under certain conditions) yield a self-adjoint realisation of $-\Delta_2$ with a domain (5.1.14), we single out two classes of particular importance.

Definition 5.1.1. Let $\alpha : [0,1] \to \mathbb{R}$ be Lipschitz continuous. A contact interaction is said to be of

(i) *δ-type with (variable) strength α*, if $\Psi \in H^2(\Gamma_2^*)$ is continuous across diagonals,

$$\psi^+_{ee}(l_e y, l_e y) = \psi^-_{ee}(l_e y, l_e y), \tag{5.1.15}$$

and satisfies jump conditions for the normal derivatives,

$$\psi^+_{ee,n}(l_e y, l_e y) + \psi^-_{ee,n}(l_e y, l_e y) = \frac{\alpha(y)}{\sqrt{2}}\ \psi^\pm_{ee}(l_e y, l_e y). \tag{5.1.16}$$

(ii) *hard-core type*, if it satisfies Dirichlet boundary conditions along diagonals.

To relate those classes of contact interactions to the formalism introduced before, we set

$$P_{contact,e}(y) = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \tag{5.1.17}$$

and

$$L_{contact,e}(y) = -\frac{1}{2}\,\alpha(y)\,\mathbb{1}_2, \tag{5.1.18}$$

to obtain δ-like contact interactions. On the other hand, to obtain hard-core interactions, we set $P_{contact,e}(y) = \mathbb{1}_2$ and $L_{contact,e}(y) = 0$. Now, in order to identify self-adjoint realisations of the two-particle Laplacian $-\Delta_2$, we will generate a suitable quadratic form.

Proposition 5.1.2. *Assume that the maps $P, L : [0,1] \to \mathrm{M}(n(E), \mathbb{C})$ are bounded and measurable. Then the quadratic form*

$$Q^{(2)}_{P,L}[\psi] = \langle \nabla\Psi, \nabla\Psi\rangle_{L^2(\Gamma_2^*)} - \int_0^1 \langle \Psi_{bv}(y), L(y)\Psi_{bv}(y)\rangle_{\mathbb{C}^{n(E)}}\ \mathrm{d}y\ , \tag{5.1.19}$$

with domain

$$\mathcal{D}_{Q^{(2)}} = \{\Psi \in H^1(\Gamma_2^*);\ P(y)\Psi_{bv}(y) = 0 \text{ for a.e. } y \in [0,1]\} \tag{5.1.20}$$

is closed and semi-bounded.

Proof. The proof follows the same lines as the proof of Theorem 4.1.7. Only the estimate

$$\left| \int_0^1 \langle \Psi_{bv}(y), L(y)\Psi_{bv}(y)\rangle_{\mathbb{C}^{n(E)}}\ \mathrm{d}y \right| \leq \|\Lambda\|_{op}\, \|\Psi_{bv}\|^2_{L^2(0,1)\otimes\mathbb{C}^{n(E)}} \tag{5.1.21}$$

needs some consideration. Since we work on the dissected Hilbert space (5.1.3), we have to be a somewhat more careful in order to establish an upper bound for the right-hand side. Indeed, we require the bound

$$\|\Psi_{bv}\|^2_{L^2(0,1)\otimes\mathbb{C}^{n(E)}} \leq K\,\left(\frac{2}{\delta}\,\|\Psi\|^2_{L^2(\Gamma_2^*)} + \delta\,\|\nabla\Psi\|^2_{L^2(\Gamma_2^*)}\right), \tag{5.1.22}$$

to hold for all $\delta \leq \delta_0$, where $K, \delta_0 > 0$. Note that the contribution from rectangles $D_{e_1e_2}$ with $e_1 \neq e_2$ is estimated as done in the proof of Theorem 4.1.7. Concerning the triangles $D^{\pm}_{ee}$, we note that their contribution cannot be estimated in the same

way. However, to estimate the non-diagonal boundary values one can always reflect functions $\psi_{ee}^{\pm}$ across the diagonal, define them on the square D_{ee} and then apply the bound as before for the rectangles. Also, to estimate the boundary values along the diagonal, one continues the function again by reflection onto a square such that the diagonal is the outer boundary of that square. The proof then continues as the proof of Theorem 4.1.7. Note that the estimate (5.1.22) can also be obtained by applying Theorem 2.2.13. □

According to the representation theorem of quadratic forms [Kat66], we conclude that each form $Q_{P,L}^{(2)}[\cdot]$ is associated with a unique self-adjoint operator on $L^2(\Gamma_2^*)$ which shall be denoted as $(H, \mathcal{D}(H))$. To actually identify this operator as well as its domain, we would like to know if $\mathcal{D}(H) \subset H^2(\Gamma_2^*)$.

Definition 5.1.3. Let $Q_{P,L}^{(2)}[\cdot]$ be a quadratic form covered by Proposition 5.1.2. If its associated self-adjoint operator has domain $\mathcal{D}(H) \subset H^2(\Gamma_2^*)$, we call the form *regular*.

As mentioned in previous sections, it is in general very difficult to show that a quadratic form is regular. Loosely speaking, in order to render a regular quadratic form, the boundary conditions in terms of the maps P and L must be chosen smooth enough. Furthermore, whenever a quadratic form is regular, we would like to show that the corresponding operator has a domain of the form (5.1.14).

Theorem 5.1.4. *Suppose that the map P is of class C^1 and that the quadratic form $Q_{P,L}^{(2)}$ with domain $\mathcal{D}_{Q^{(2)}}$ is regular. Then the unique, self-adjoint and semibounded operator that is associated with this form is the two-particle Laplacian $-\Delta_2$ with domain $\mathcal{D}_2(P, L)$.*

Proof. The proof follows the same lines as the proof of Theorem 4.1.24. It is based on the representation theorem for quadratic forms, which implies that for each $\Psi \in \mathcal{D}(H)$ there exists a unique $\chi \in L^2(\Gamma_2^*)$ such that

$$Q_{P,L}^{(2)}[\Psi, \Phi] = \langle \chi, \Phi \rangle \ , \quad \forall \Phi \in \mathcal{D}_{Q^{(2)}} \ . \tag{5.1.23}$$

When $\Phi \in C_0^\infty(\Gamma_2^*)$, an integration by parts shows that H acts as a two-particle Laplacian $-\Delta_2$. For an arbitrary function $\Psi \in \mathcal{D}_{Q^{(2)}}$, the integration by parts

yields an additional boundary term, i.e.

$$-\int_0^1 \langle \Psi'_{bv}(y) + L(y)\Psi_{bv}(y), \Phi_{bv}(y)\rangle_{\mathbb{C}^{n(E)}}\, \mathrm{d}y \ , \tag{5.1.24}$$

that is required to vanish. Following Lemma 4.1.23, which has an immediate generalisation to the present case, the set $\{\Psi_{bv};\ \Psi \in \mathcal{D}_{Q^{(2)}}\}$ is dense in $\ker\Pi \subset L^2(0,1)^{n(E)}$. Hence, $\Psi'_{bv} + \Lambda\Psi_{bv} \in \ker\Pi^\perp$, or

$$Q(y)\Psi'_{bv}(y) + Q(y)L(y)\Psi_{bv}(y) = 0 \ . \tag{5.1.25}$$

This condition finally implies that $\mathcal{D}(H) = \mathcal{D}_2(P,L)$. □

In the following theorem, we will establish regularity for δ- as well as hard-core interactions. The proof will use the same techniques as the proof given in part B of the appendix that corresponds to the Theorem 4.1.26 of the last chapter.

Theorem 5.1.5. *In addition to the assumption made for the maps P and L above, suppose that P_{vertex} has the block structure* (4.1.70) *and is of class C^3. In addition, L shall be Lipschitz continuous. Furthermore, for $y \in [0,\epsilon_1]\cup[1-\epsilon_2,1]$ with some $\epsilon_1,\epsilon_2 > 0$ assume that the restriction of P to V_{vertex} is diagonal with diagonal entries zero or one as well as $L_{vertex} = 0$, and, in the case of δ-type interactions, that $\alpha(y) = \alpha_0 > 0$. Then the quadratic form $Q^{(2)}_{P,L}$ is regular.*

Proof. First note that it is enough to show regularity near the corners of $D_{ee} = D^+_{ee}\cup D^-_{ee}$ adjacent to the diagonal. The regularity away from those corners of D_{ee}, as well as the regularity in the rectangles $D_{e_1e_2}$ with $e_1 \neq e_2$, is established with the methods employed in the proof of Theorem 4.1.26. Now, the assumptions made on P imply that functions in $\mathcal{D}_{Q^{(2)}}$ satisfy either Dirichlet- or Neumann boundary conditions near the corners of the squares D_{ee}. As a next step, consider

$$\begin{aligned}\psi_{ee,B}(x,y) :=& \frac{1}{2}\tau(r)\big[\psi_{ee}(x,y) + \psi_{ee}(y,x)\big],\\ \psi_{ee,F}(x,y) :=& \frac{1}{2}\tau(r)\big[\psi_{ee}(x,y) - \psi_{ee}(y,x)\big],\end{aligned} \tag{5.1.26}$$

where, using polar coordinates at the corner of consideration, $\tau \in C^\infty(0,1)$ is a (cut-off) test function with $0 \le \tau(r) \le 1$, $\tau(r) = 1$ for $r \le r_0$ and $\tau(r) = 0$ for r close to 1. The goal is then to show that both $\psi_{ee,B}$ and $\psi_{ee,F}$ are in $H^2(D^*_{ee})$.

This in turn implies that $\psi_{ee} \in H^2(D^*_{ee})$. For this, we recall the conditions (5.1.16) which imply that, on the diagonal,

$$\partial_n \psi^{\pm}_{ee,B} - \frac{\alpha}{\sqrt{2}} \psi^{\pm}_{ee,B} = 0 \ , \tag{5.1.27}$$

i.e., $\psi^{\pm}_{ee,B}$ satisfies (variable) Robin boundary conditions on the diagonal. By construction, $\psi^{\pm}_{ee,F}$ vanishes on the diagonal so that near the corners of $D^{\pm}_{ee}$ adjacent to the diagonal, where α is supposed to be constant, $\psi^{\pm}_{ee,B/F}$ satisfies a combination of Dirichlet-, Neumann- or standard Robin-boundary conditions. In all such cases regularity is well known to hold [Neč67, Gri11, Dau88]. □

As a next step, we want to discuss spectral properties of the self-adjoint operators corresponding to quadratic forms as described in Proposition 5.1.2.

Remark 5.1.6. Let $Q^{(2)}_{P,L}[\cdot]$ be a quadratic form as described in Proposition 5.1.2. In the following we will, irrespective of regularity, denote the corresponding self-adjoint operator by $(-\Delta_2, \mathcal{D}_2(P, L))$.

First of all, we would like to know if the spectrum of each operator $(-\Delta_2, \mathcal{D}_2(P, L))$ is purely discrete. In addition, given the spectrum is purely discrete with eigenvalues $\{\lambda_n\}_{n\in\mathbb{N}_0}$, we would like to establish Weyl asymptotics for the corresponding eigenvalue counting function

$$N(\lambda) = \#\{n; \lambda_n \leq \lambda\}, \tag{5.1.28}$$

where the eigenvalues are counted according to their multiplicities.

Proposition 5.1.7. *Let $(-\Delta_2, \mathcal{D}_2(P, L))$ be a self-adjoint realisation of the two-particle Laplacian describing contact interactions. Then this operator has compact resolvent. In particular, its spectrum is purely discrete and only accumulates at infinity. Furthermore, the counting function* (5.1.28) *obeys the Weyl law*

$$N(\lambda) \sim \frac{\mathcal{L}^2}{4\pi} \lambda \ , \quad \lambda \to \infty \ , \tag{5.1.29}$$

where $\mathcal{L} = \sum_{e=1}^{E} l_e$ is the total length of the graph.

Proof. We first note that the Hilbert space $H^1(\Gamma^*_2)$ is compactly embedded in $L^2(\Gamma^*_2)$ [Dob05]. Accordingly, since the form norm $||\cdot||_{Q^{(2)}}$ is equivalent to the

$H^1(\Gamma_2^*)$ norm, it follows that the Hilbert space $(\mathcal{D}_{Q^{(2)}}, ||\cdot||_{Q^{(2)}})$ is also compactly embedded in $L^2(\Gamma_2^*)$. Hence the operator associated with the quadratic form has compact resolvent [Dob05].
The Weyl law then follows from a standard bracketing argument [RS78] based on a comparison with two suitable operators (quadratic forms) (see also [BE09, BK13b]). The first operator, $(-\Delta_2, \mathcal{D}_2(P_D, L_D))$, is the Dirichlet-Laplacian and is characterised by the projection $P_D = \mathbb{1}_{n(E)}$ as well as $L_D = 0$. The second comparison operator, $(-\Delta_2, \mathcal{D}_2(P_R, L_R))$, is the Robin-Laplacian characterised by the projection $P_R = 0$ as well as

$$L_R = \mathrm{diag}(\underbrace{\sqrt{2}\lambda, \ldots, \sqrt{2}\lambda}_{2E-\text{times}}, \underbrace{\lambda, \ldots, \lambda}_{4E^2-\text{times}}) \ , \tag{5.1.30}$$

where $\lambda = ||\Lambda||_{\mathrm{op}}$. The associated quadratic forms therefore satisfy the following inclusions of their domains, i.e.

$$\mathcal{D}_2(P_D, L_D) \subseteq \mathcal{D}_2(P, L) \subseteq \mathcal{D}_2(P_R, L_R) \ . \tag{5.1.31}$$

Hence [RS78], it follows that the related eigenvalue-counting functions satisfy

$$N_D(\lambda) \leq N(\lambda) \leq N_R(\lambda) \ . \tag{5.1.32}$$

As both N_D and N_R satisfy the Weyl law (5.1.29), the same asymptotics holds for $N(\lambda)$. Note that the Weyl asymptotics for the Robin-Laplacian was established in [Zay98]. □

5.2 Contact interactions in a system of two bosons

In this section, we want to implement a particle exchange symmetry in order to investigate a system of two bosons interacting via contact interactions. For this, let Π_B be the projection operator acting via

$$(\Pi_B \Psi)_{e_1 e_2}(x_{e_1}, y_{e_2}) = \frac{1}{2}\big(\psi_{e_1 e_2}(x_{e_1}, y_{e_2}) + \psi_{e_2 e_1}(y_{e_2}, x_{e_1})\big), \tag{5.2.1}$$

on components $\psi_{e_1e_2}$ with $e_1 \neq e_2$ and

$$(\Pi_B\Psi)^{\pm}_{ee}(x_e, y_e) = \frac{1}{2}\big(\psi^{\pm}_{ee}(x_e, y_e) + \psi^{\mp}_{ee}(y_e, x_e)\big), \tag{5.2.2}$$

on components $\psi_{e_1e_2}$ with $e_1 = e_2$. Accordingly, the symmetric Hilbert space is given by

$$L^2_B(\Gamma^*_2) = \Pi_B L^2(\Gamma^*_2). \tag{5.2.3}$$

In the same fashion, we introduce the (symmetric) Sobolev spaces $H^m_B(\Gamma^*_2)$ of order $m \in \mathbb{N}$ by

$$H^m_B(\Gamma^*_2) = H^m(\Gamma^*_2) \cap L^2_B(\Gamma^*_2). \tag{5.2.4}$$

Note that all functions $\Psi \in H^1_B(D^*_\Gamma)$ fulfil

$$\psi_{e_1e_2,x}(x_{e_1}, y_{e_2}) = \psi_{e_2e_1,y}(y_{e_2}, x_{e_1}). \tag{5.2.5}$$

In order to introduce a suitable quadratic form, we first introduce vectors of boundary values. For components $\psi_{e_1e_2} = (\Psi)_{e_1e_2}$ with $e_1 \neq e_2$, we write

$$\psi_{e_1e_2,bv}(y) = \begin{pmatrix} \sqrt{l_{e_2}}\psi_{e_1e_2}(0, l_{e_2}y) \\ \sqrt{l_{e_2}}\psi_{e_1e_2}(l_{e_1}, l_{e_2}y) \end{pmatrix}, \tag{5.2.6}$$

and

$$\psi'_{e_1e_2,bv}(y) = \begin{pmatrix} \sqrt{l_{e_2}}\psi_{e_1e_2,x}(0, l_e y) \\ -\sqrt{l_{e_2}}\psi_{e_1e_2,x}(l_{e_1}, l_{e_2}y) \end{pmatrix}, \tag{5.2.7}$$

whereas for components ψ_{ee} we have

$$\psi_{ee,bv}(y) = \begin{pmatrix} \sqrt{l_e}\psi^-_{ee}(0, l_e y) \\ \sqrt{l_e}\psi^+_{ee}(l_e, l_e y) \\ \sqrt{l_e}\psi^+_{ee}(l_e y, l_e y) \end{pmatrix} \qquad \text{and} \qquad \psi'_{ee,bv}(y) = \begin{pmatrix} \sqrt{l_e}\psi^-_{ee,x}(0, l_e y) \\ -\sqrt{l_e}\psi^+_{ee,x}(l_e, l_e y) \\ \sqrt{2l_e}\psi^+_{ee,n}(l_e y, l_e y) \end{pmatrix}, \tag{5.2.8}$$

with $y \in [0, 1]$. The space of boundary values therefore has dimension $n_B(E) = 2E^2 + E$ and decomposes in analogy to (5.1.9).

As a next step, we introduce two bounded and measurable maps $P, L : [0, 1] \to M(n_B(E), \mathbb{C})$ such that:

1. $P(y)$ is an orthogonal projection,

2. $L(y)$ is a self-adjoint endomorphism on $\ker P(y)$,

for a.e. $y \in [0,1]$. Moreover, we set $Q(y) = \mathbb{1}_{n_B(E)} - P(y)$. Also, we assume that P, L have the block-structure (5.1.12) in order to avoid a coupling of vertex-interactions and contact interactions. In order to avoid a coupling between contact interactions along different edges, we also assume that the decomposition (5.1.13) holds. Now, since the restriction of P to each subspace $M_{contact,e}$ is one-dimensional, we have

$$P_{contact,e} \in \{0,1\}, \tag{5.2.9}$$

where 0 corresponds to δ-interactions and 1 to hard-core interactions since Dirichlet boundary conditions are induced. Furthermore, we associate two bounded and self-adjoint operators Π and Λ on the Hilbert space of boundary values with the maps P and L, i.e.

$$\Pi : L^2(0,1) \otimes \mathbb{C}^{n_B(E)} \to L^2(0,1) \otimes \mathbb{C}^{n_B(E)}, \chi(y) \mapsto P(y)\chi(y), \tag{5.2.10}$$

and

$$\Lambda : L^2(0,1) \otimes \mathbb{C}^{n_B(E)} \to L^2(0,1) \otimes \mathbb{C}^{n_B(E)}, \chi(y) \mapsto L(y)\chi(y). \tag{5.2.11}$$

Using all the notation introduced above, we can now define a suitable quadratic form for a system of two bosons on a graph.

Proposition 5.2.1. *The quadratic form*

$$Q^{(2),B}_{P,L}[\psi] = 2\langle \Psi_x, \Psi_x \rangle_{L^2_B(D^*_\Gamma)} - 2\int_0^1 \langle \Psi_{bv}(y), L(y)\Psi_{bv}(y) \rangle_{\mathbb{C}^{n_B(E)}} \, \mathrm{d}y \ , \tag{5.2.12}$$

with domain

$$\mathcal{D}_{Q^{(2),B}} = \left\{ \Psi \in H^1_B(\Gamma^*_2);\ P(y)\Psi_{bv}(y) = 0 \text{ for a.e. } y \in [0,1] \right\}. \tag{5.2.13}$$

is closed and semi-bounded.

The proof is equivalent to the proof of Proposition 5.1.2. Note that the factor of 2 appears due to the bosonic symmetry as can also be understood from the reduced dimension of the vectors containing the boundary values. Furthermore,

given the form $Q^{(2),B}_{P,L}[\cdot]$ is regular in the sense of Definition 5.1.3, we have the following statement.

Proposition 5.2.2. *Let $Q^{(2),B}_{P,L}[\cdot]$ be the quadratic form as described in Proposition 5.1.2. Assume that P is of class C^1 and that the quadratic form is regular in the sense of Definition 5.1.3. Then the operator associated to the form is the two-particle Laplacian $-\Delta_2$ with domain*

$$\begin{aligned}\mathcal{D}_{2,B}(P,L) = \{\Psi \in H^2_B(\Gamma_2^*);\ & P(y)\Psi_{bv}(y) = 0 \text{ and} \\ & Q(y)\Psi'_{bv}(y) + L(y)Q(y)\Psi_{bv}(y) = 0 \text{ for a.e. } y \in [0,1]\}.\end{aligned} \tag{5.2.14}$$

The proof follows the same steps as the proof of Proposition 5.1.4.

Remark 5.2.3. Note that the regular forms characterised in Theorem 5.1.5 carry over directly to the bosonic case.

Finally, regarding the spectrum we readily establish:

Corollary 5.2.4. *Assume that $(-\Delta_2, \mathcal{D}_{2,B}(P,L))$ is, irrespective of regularity, the self-adjoint operator corresponding to the form $Q^{(2),B}_{P,L}[\cdot]$ as described in Proposition 5.1.2. Then its spectrum is purely discrete, only accumulating at infinity. Furthermore, the counting function*

$$N_B(\lambda) = \#\{n; \lambda_n \leq \lambda\}, \tag{5.2.15}$$

where the eigenvalues are counted according to their multiplicities, fulfils the Weyl law

$$N_B(\lambda) \sim \frac{\mathcal{L}^2}{8\pi}\lambda, \quad \lambda \to \infty. \tag{5.2.16}$$

As we can see from (5.2.16), the bosonic symmetry leads to a factor of one half.

5.3 Contact interactions in a system of N bosons

The goal of this section is to generalise the methods of the previous section to a system of an arbitrary number of particles. This will finally allow us to extend the Lieb-Liniger model [LL63] to general compact quantum graphs. Note that we will, for the sake of readability, refer in some proofs to part A of the Appendix. There, singular interactions in systems of N non-distinguishable particles are introduced

in the same way as discussed in Chapter 4 for the case of two particles. Since we will establish quadratic forms for N bosons which incorporate contact as well as singular interactions, similar methods are used in the proofs which therefore allows us to refer to the Appendix.
For N bosons, the (formal) operator we want to consider is given by

$$\hat{H}_N = -\Delta_N + \sum_{i<j} \alpha(x_i)\,\delta(x_i - x_j)\ , \tag{5.3.1}$$

where $\alpha : \mathbb{R} \to \mathbb{R}$ is the (possibly coordinate dependent) interaction strength. Note that the original Lieb-Liniger model is only concerned with constant $\alpha \in \mathbb{R}$. On a graph, the action of the Hamiltonian corresponding to (5.3.1) is such that

$$\begin{aligned}\langle \Psi, \hat{H}_N \Psi\rangle_{\mathcal{H}_2} &= \langle \Psi, -\Delta_N \Psi\rangle_{\mathcal{H}_2} \\ &+ \frac{N(N-1)}{2} \sum_{e_2 \dots e_N} \int_0^{l_{e_2}} \dots \int_0^{l_{e_N}} \alpha(x^2_{e_2}) |\psi_{e_2 e_2 \dots e_N}(x^2_{e_2}, x^2_{e_2}, \dots, x^N_{e_N})|^2 \, \mathrm{d}x^2_{e_2} \dots \mathrm{d}x^N_{e_N}\ .\end{aligned} \tag{5.3.2}$$

We see that the interaction part in (5.3.1) is realised by an integration along hypersurfaces characterised by the fact that two particles are at the same position, i.e. $x^1_e = x^2_e$ for some $e \in \mathcal{E}$. Note that, due to bosonic symmetry, it is enough to consider only the corresponding hypersurface for the first two coordinates. Now, in order to construct a quadratic form that will, due to the graph structure, also contain possible interactions in the vertices, we have to construct a dissected Hilbert space similar to (5.1.3). The configuration space for N distinguishable particles is given by

$$D^N_\Gamma = \dot{\bigcup_{e_1 e_2 \dots e_N}} D_{e_1 e_2 \dots e_N}, \tag{5.3.3}$$

with $D_{e_1 e_2 \dots e_N} = (0, l_{e_1}) \times \dots \times (0, l_{e_N})$. With each domain $D_{e_1 e_2 \dots e_N}$, we associate the vector $(n_1, \dots, n_E)^T \in \mathbb{N}^E$ that lists the numbers of particles situated on each edge $e \in \mathcal{E}$. Furthermore, the map

$$\sigma_e : (1, \dots, n_e) \mapsto \left(x^{\sigma_e(1)}_e, \dots, x^{\sigma_e(n_e)}_e\right) \tag{5.3.4}$$

associates to each particle on edge $e \in \mathcal{E}$ its coordinate label. We then single out a polyhedral subdomain of $D_{e_1e_2...e_N}$, called the *fundamental* domain, by requiring

$$x_e^{\sigma_e(1)} < \cdots < x_e^{\sigma_e(n_e)} \ , \quad \forall e \in \{1, \ldots, E\}. \tag{5.3.5}$$

Note that there are $n_1!...n_E!$ equivalent domains which are obtained from (5.3.5) by a permutation of the particle labels. Accordingly, each domain $D_{e_1e_2...e_N}$ can be written as the (dissected) union

$$D^*_{e_1...e_N} = \dot{\bigcup_{\eta}} D^{\eta}_{e_1...e_N}, \tag{5.3.6}$$

where $\eta \in \{1, ..., (n_1!...n_E!)\}$ and $D^{\eta}_{e_1...e_N}$ are the domains obtained via (5.3.5). Now, based on the dissected domains (5.3.6), the N-particle Hilbert space is given by

$$L^2(\Gamma^*_N) = \bigoplus_{e_1e_2...e_N} L^2(D^*_{e_1e_2...e_N}). \tag{5.3.7}$$

In the same way, the Sobolev space of order $m \in \mathbb{N}$ is defined by

$$H^m(\Gamma^*_N) = \bigoplus_{e_1e_2...e_N} H^m(D^*_{e_1e_2...e_N}). \tag{5.3.8}$$

According to (5.3.7), each component $(\Psi)_{e_1...e_N} = \psi_{e_1...e_N}$ consists of $n_1!...n_E!$ subcomponents. However, to keep the notation simple, we shall only write $\psi_{e_1...e_N}$ without explicitly writing out all subcomponents.

Since we want to describe a system of N bosons, we shall now introduce exchange symmetry. For this, let Π_B be the projection operator acting on a state $\Psi \in L^2(\Gamma^*_N)$ via

$$(\Pi_B\Psi)_{e_1...e_N} = \frac{1}{N!} \sum_{\pi \in S_N} \psi_{\pi(e_1)...\pi(e_N)}(x^{\pi(1)}_{\pi(e_1)}, ..., x^{\pi(N)}_{\pi(e_N)}), \tag{5.3.9}$$

and write

$$L^2_B(\Gamma^*_N) = \Pi_B L^2(\Gamma^*_N). \tag{5.3.10}$$

As in the previous sections, we now introduce vectors containing boundary values of any state $\Psi \in H^1(\Gamma^*_N)$ or $\Psi \in H^2(\Gamma^*_N)$ respectively. Note that these boundary values consist of two different parts: boundary values along the surfaces of $D_{e_1...e_N}$ corresponding to interactions in the vertices and boundary values along the hy-

persurfaces characterised by $x_e^1 = x_e^2$ corresponding to contact interactions. The boundary values associated with interactions in the vertices are then given by

$$\Psi_{bv,vert}(\boldsymbol{y}) = \begin{pmatrix} \sqrt{l_{e_2} \dots l_{e_N}} \psi_{e_1 \dots e_N}(0, l_{e_2} y_1, \dots, l_{e_N} y_{N-1}) \\ \sqrt{l_{e_2} \dots l_{e_N}} \psi_{e_1 \dots e_N}(l_{e_1}, l_{e_2} y_1, \dots, l_{e_N} y_{N-1}) \end{pmatrix}, \tag{5.3.11}$$

and

$$\Psi'_{bv,vert}(\boldsymbol{y}) = \begin{pmatrix} \sqrt{l_{e_2} \dots l_{e_N}} \psi_{e_1 \dots e_N, x^1_{e_1}}(0, l_{e_2} y_1, \dots, l_{e_N} y_{N-1}) \\ -\sqrt{l_{e_2} \dots l_{e_N}} \psi_{e_1 \dots e_N, x^1_{e_1}}(l_{e_1}, l_{e_2} y_1, \dots, l_{e_N} y_{N-1}) \end{pmatrix}. \tag{5.3.12}$$

Note that, due to bosonic symmetry, it is enough to consider boundary values for $x^1_{e_1} = 0$ and $x^1_{e_1} = l_{e_1}$ only.
As a next step, we introduce bounded and measurable maps $P_{vert}, L_{vert} : [0,1]^{N-1} \to \mathrm{M}(2E^N, \mathbb{C})$ that act on these vertex related boundary values. They are required to fulfil

1. $P_{vert}(\boldsymbol{y})$ is an orthogonal projection,

2. $L_{vert}(\boldsymbol{y})$ is a self-adjoint endomorphism on $\ker P_{vert}(\boldsymbol{y})$,

for a.e. $\boldsymbol{y} \in [0,1]^{N-1}$. Moreover, we set $Q_{vert}(\boldsymbol{y}) = \mathbb{1}_{2E^N} - P_{vert}(\boldsymbol{y})$. Now, in accordance with (5.3.2), we can introduce a suitable quadratic form incorporating δ-like contact interactions as well as singular interactions in the vertices of the graph. Setting $\boldsymbol{y_1} = (l_{e_2} y_1, l_{e_3} y_2, \dots, l_{e_N} y_{N-1})$, we have the following statement.

Theorem 5.3.1. *Let the maps $P_{vert}, L_{vert} : [0,1]^{N-1} \to \mathrm{M}(2E^N, \mathbb{C})$ as well as the function $\alpha : [0,1] \to \mathbb{C}$ be bounded and measurable. Then the quadratic form*

$$\begin{aligned} Q_B^{(N)}[\Psi] = N \sum_{e_1 \dots e_N} \int_0^{l_{e_1}} \dots \int_0^{l_{e_N}} |\psi_{e_1 \dots e_N, x^1_{e_1}}(x^1_{e_1}, \dots, x^N_{e_N})|^2 \, \mathrm{d}x^1_{e_1} \dots \mathrm{d}x^N_{e_N} \\ - N \int_{[0,1]^{N-1}} \langle \Psi_{bv,vert}, L_{vert}(\boldsymbol{y}) \Psi_{bv,vert} \rangle_{\mathbb{C}^{2E^N}} \mathrm{d}\boldsymbol{y} \\ + \frac{N(N-1)}{2} \sum_{e_2 \dots e_N} \int_{[0,1]^{N-1}} \alpha(y_1) \, |\sqrt{l_{e_2} \dots l_{e_N}} \psi_{e_2 e_2 \dots e_N}(l_{e_2} y_1, \boldsymbol{y_1})|^2 \, \mathrm{d}\boldsymbol{y}, \end{aligned} \tag{5.3.13}$$

defined on the domain

$$\mathcal{D}_{Q_B^{(N)}} = \left\{ \Psi \in H_B^1(\Gamma_N^*);\ P_{vert}(\boldsymbol{y})\Psi_{bv,vert}(\boldsymbol{y}) = 0 \text{ for a.e. } \boldsymbol{y} \in [0,1]^{N-1} \right\}, \quad (5.3.14)$$

is closed and semi-bounded.

Proof. Due to the bosonic symmetry, each function $\Psi \in H_B^1(\Gamma_N^*)$ can be considered as a function $\Psi \in H_B^1(\Gamma_N)$. Accordingly, the proof follows the same lines as the proof of Theorem A.0.16 and we therefore comment on the estimates regarding the contact interaction part of (5.3.13) only, i.e. we consider

$$A := \frac{N(N-1)}{2} \sum_{e_2 \dots e_N} \int_{[0,1]^{N-1}} \alpha(y_1)\ |\sqrt{l_{e_2} \dots l_{e_N}} \psi_{e_2 e_2 \dots e_N}(l_{e_2} y_1, \boldsymbol{y_1})|^2 \ \mathrm{d}\boldsymbol{y}. \quad (5.3.15)$$

For each component $\psi_{e_1 e_2 \dots e_N}(l_{e_2} y_1, \boldsymbol{y_1})$, we have

$$\begin{aligned} \|\sqrt{l_{e_2} \dots l_{e_N}} \psi_{e_2 e_2 \dots e_N}(l_{e_2} y_1, \boldsymbol{y_1})\|^2_{L^2(0,1)^{N-1}} \leq & \frac{2K}{\delta} \|\psi_{e_2 e_2 \dots e_N}\|^2_{L^2(D_{e_2 e_2 \dots e_N})} \\ & + K\delta \|\nabla \psi_{e_2 e_2 \dots e_N}\|^2_{L^2(D_{e_2 e_2 \dots e_N})}, \end{aligned} \quad (5.3.16)$$

for $K \in \mathbb{R}$ large enough and for all $\delta \leq \delta_0$ with $\delta_0 > 0$ some constant. Note that this estimate can be obtained by extending the component $\psi_{e_2 e_2 \dots e_N}(x^1_{e_2} > x^2_{e_2})$ in the first two coordinates onto a square, such that $\psi_{e_2 e_2 \dots e_N}(l_{e_2} y_1, \boldsymbol{y_1})$ are the boundary values on the outer surfaces of this square (see also the proof of Proposition 5.1.2). Subsequently, one can apply the standard estimate (A.0.11), finally arriving at (5.3.16). Combining everything, we have the desired estimate

$$|A| \leq c_1 \|\nabla \Psi\|^2_{L^2(D_N^*)} + c_2 \|\Psi\|^2_{L^2(D_N^*)} \quad (5.3.17)$$

with c_1 arbitrarily small. Note that (5.3.17) can also be obtained by applying Theorem 2.2.13. □

As a next step, we generate a quadratic form that incorporates hard-core interactions (see Definition 5.1.1).

Definition 5.3.2. Let $m \in \mathbb{N}$. The space $H^m_{0,B}(\Gamma_N^*)$ consists of all functions $\Psi \in H^m_B(\Gamma_N^*)$ that vanish along the hypersurfaces for which $x^i_e = x^j_e$ for some pair $i \neq j$ and $e \in \mathcal{E}$.

Theorem 5.3.3. *Let the maps $P_{vert}, L_{vert} : [0,1]^{N-1} \to \mathrm{M}(2E^N, \mathbb{C})$ be bounded and measurable. Then the quadratic form*

$$\begin{aligned} Q_B^{(N)}[\Psi] = N \sum_{e_1 \dots e_N} \int_0^{l_{e_1}} \dots \int_0^{l_{e_N}} |\psi_{e_1 \dots e_N, x^1_{e_1}}(x^1_{e_1}, \dots, x^N_{e_N})|^2 \, \mathrm{d}x^1_{e_1} \dots \mathrm{d}x^N_{e_N} \\ - N \int_{[0,1]^{N-1}} \langle \Psi_{bv,vert}, L_{vert}(\boldsymbol{y}) \Psi_{bv,vert} \rangle_{\mathbb{C}^{2E^N}} \, \mathrm{d}\boldsymbol{y}, \end{aligned} \tag{5.3.18}$$

defined on the domain

$$\mathcal{D}_{Q_B^{(N)}} = \left\{ \Psi \in H^1_{0,B}(\Gamma_N^*);\ P_{vert}(\boldsymbol{y}) \Psi_{bv,vert}(\boldsymbol{y}) = 0 \text{ for a.e. } \boldsymbol{y} \in [0,1]^{N-1} \right\}, \tag{5.3.19}$$

is closed and semi-bounded.

Proof. Note again that each function $\Psi \in H^1_{0,B}(\Gamma_N^*)$ can be considered as a function $\Psi \in H^1_{0,B}(\Gamma_N)$ (here $H^1_{0,B}(\Gamma_N)$ is defined analoguously to $H^1_{0,B}(\Gamma_N^*)$). Taking the completeness of $H^1_{0,B}(\Gamma_N)$ into account, the proof follows the same lines as the proof of Theorem A.0.16. □

For δ-interactions, given that the map P_{vertex} is of class C^1 and the form (5.3.13) is regular (see Definition 4.1.10), we can readily show that the corresponding operator is the N-particle Laplacian $-\Delta_N$ with domain

$$\begin{aligned} \mathcal{D}_N^{\alpha}(P, L) = \{ \Psi \in H^2_B(\Gamma_N^*);\ P(\boldsymbol{y}) \Psi_{bv}(\boldsymbol{y}) = 0 \text{ and} \\ Q(\boldsymbol{y}) \Psi'_{bv}(\boldsymbol{y}) + L(\boldsymbol{y}) Q(\boldsymbol{y}) \Psi_{bv}(\boldsymbol{y}) = 0 \text{ for a.e. } \boldsymbol{y} \in [0,1]^{N-1} \}, \end{aligned} \tag{5.3.20}$$

and $M = M_{contact} \oplus M_{vert}$ with $M \in \{P, L, Q\}$. For hard-core interactions, on the other hand, we have

$$\begin{aligned} \mathcal{D}_N^{\infty}(P, L) = \{ \Psi \in H^2_{0,B}(\Gamma_N^*);\ P_{vert}(\boldsymbol{y}) \Psi_{bv,vert}(\boldsymbol{y}) = 0 \text{ and} \\ Q_{vert}(\boldsymbol{y}) \Psi'_{bv,vert}(\boldsymbol{y}) + L_{vert}(\boldsymbol{y}) Q_{vert}(\boldsymbol{y}) \Psi_{bv,vert}(\boldsymbol{y}) = 0 \text{ for a.e. } \boldsymbol{y} \in [0,1]^{N-1} \}. \end{aligned} \tag{5.3.21}$$

Remark 5.3.4. Note that we will, irrespective of regularity, denote the operator corresponding to a form (5.3.13) or (5.3.18) by $(-\Delta_N, \mathcal{D}_N^{\alpha}(P, L))$. Furthermore, the notation $\alpha \equiv \infty$ shall refer to hard-core interactions.

Finally, regarding the spectrum of each operator $(-\Delta_N, \mathcal{D}_N^\alpha(P,L))$, we establish the following statement.

Proposition 5.3.5. *Assume that the map L_{vert} is negative definite and the function $\alpha : [0,1]^{N-1} \to \mathbb{C}$ strictly positive or $\alpha \equiv \infty$. Then the spectrum of the operator $(-\Delta_N, \mathcal{D}_N^\alpha(P,L))$ is purely discrete, only accumulating at infinity. Furthermore, the eigenvalue counting function*

$$N(\lambda) = \#\{n; \lambda_n \leq \lambda\}, \tag{5.3.22}$$

where the eigenvalues are counted according to their multiplicities, obeys the Weyl law

$$N(\lambda) \sim \frac{\mathcal{L}^N}{N!(4\pi)^{N/2}\Gamma(1+\frac{N}{2})}\,\lambda^{N/2}\ , \quad \lambda \to \infty\ . \tag{5.3.23}$$

Proof. The proof is based on the Dirichlet-Neumann bracketing of quadratic forms [RS78]. Since $\alpha : [0,1]^{N-1} \to \mathbb{C}$ is strictly positive (or $\alpha \equiv \infty$) and L_{vert} is negative definite, the two comparison operators are the Dirichlet-Laplacian ($P_{vert} = \mathbb{1}_{2E^N}$ and $L_{vert} = 0$) and the Neumann-Laplacian ($P_{vert} = 0$ and $L_{vert} = 0$). For both operators, the asymptotics (5.3.23) are well-known. The proposition then follows using the same arguments as, for example, in the proof of Proposition 5.1.7. □

6. BOSE-EINSTEIN CONDENSATION ON GENERAL COMPACT QUANTUM GRAPHS

In this chapter, we will discuss Bose-Einstein condensation (BEC) on general compact quantum graphs. We will identify many-particle systems that show condensation and other systems that do not. As a final result, we will prove that there is no condensation in a system of bosons interacting via repulsive hard-core interactions. Note that our results are summarised in [BK13a].

6.1 Basics of Bose-Einstein condensation

It was Einstein who predicted condensation in a free gas of bosons in three dimensions [Ein25]. He observed that for particle densities larger than some critical particle density, i.e. $\rho \geq \rho_{\text{crit}}$, the one-particle ground state becomes macroscopically occupied, i.e. the fraction of particles in the ground state is given by $\rho - \rho_{crit}$. As we will see later, the macroscopic occupation of a one-particle state is indeed the characteristic feature of Bose-Einstein condensation [PO56, Mic07].

Remark 6.1.1. Note that there is no Bose-Einstein condensation in a free Bose gas in one dimension at any finite temperature. Only at zero temperature, all particles occupy the one-particle ground state which implies condensation.

Bose-Einstein condensation is a phenomenon in statistical mechanics. In particular, it will be necessary to choose an appropriate ensemble in which BEC can be described. Mostly, we will work in the grand-canonical ensemble [Gal99]. A great advantage of this ensemble is that the particle number is not fixed. However, it requires the introduction of the Fock space $\mathcal{F}$ [Sch95, MR04]. Given the symmetric N-particle Hilbert space

$$\mathcal{H}_N^B = \Pi_B(\underbrace{\mathcal{H}_1 \otimes ... \otimes \mathcal{H}_1}_{N-\text{times}}), \tag{6.1.1}$$

where Π_B is the projection that projects onto the totally symmetric subspace, the (symmetric) Fock space is defined by

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{H}_N^B, \tag{6.1.2}$$

where $\mathcal{H}_0^B := \mathbb{C}$. In particular, Ψ with $(\Psi)_N = \Psi_N \in \mathcal{H}_N^B$ is an element of $\mathcal{F}$ if and only if

$$\sum_{N=0}^{\infty} \|\Psi_N\|^2_{\mathcal{H}_N^B} < \infty. \tag{6.1.3}$$

Furthermore, for two states $\Psi, \Phi \in \mathcal{F}$, the scalar product on $\mathcal{F}$ is defined by

$$\langle \Psi, \Phi \rangle_{\mathcal{F}} = \sum_{N=0}^{\infty} \langle \Psi_N, \Phi_N \rangle_{\mathcal{H}_N^B}. \tag{6.1.4}$$

Remark 6.1.2. The vector $\Omega = (1, 0, ...)$ is called the *vacuum*.

Since a state $\Psi \in \mathcal{F}$ does not correspond to a fixed particle number, it is necessary to introduce a particle number operator $\hat{N}$ whose expectation value is interpreted as the particle number in the state Ψ. More precisely, one defines

$$(\hat{N}\Psi)_N = N\Psi_N, \tag{6.1.5}$$

with domain

$$\mathcal{D}(\hat{N}) = \left\{ \Psi \in \mathcal{F} \,\middle|\, \sum_{N=0}^{\infty} N^2 \|\Psi_N\|^2_{\mathcal{H}_N^B} < \infty \right\}. \tag{6.1.6}$$

Accordingly, the particle number in a (normalised) state $\Psi \in \mathcal{F}$ is

$$\langle \hat{N} \rangle_{\Psi} = \sum_{N=0}^{\infty} N \|\Psi_N\|^2_{\mathcal{H}_N^B}. \tag{6.1.7}$$

In the framework of second quantisation [Sch95], it is customary to introduce creation and annihilation operators which then allow to express the Hamiltonian of the system in a clear way. For a one-particle state $\varphi \in \mathcal{H}_1$, the creation operator

$\hat{a}^\dagger_\varphi : \mathcal{F} \to \mathcal{F}$ is defined by

$$\begin{aligned}(\hat{a}^\dagger_\varphi \Psi)_N &= \sqrt{N}\ \Pi_B(\varphi \otimes \Psi_{N-1}), \quad \forall N \in \mathbb{N}, \\ (\hat{a}^\dagger_\varphi \Psi)_0 &= 0.\end{aligned} \tag{6.1.8}$$

Furthermore, the annihilation operator $\hat{a}_\varphi : \mathcal{F} \to \mathcal{F}$ of this state is defined by

$$(\hat{a}_\varphi \Psi)_N = \sqrt{N+1}\ \langle \varphi, \Psi_{N+1} \rangle_{\mathcal{H}_1}, \quad \forall N \in \mathbb{N}_0. \tag{6.1.9}$$

Here the scalar product $\langle \varphi, \Psi_{N+1} \rangle_{\mathcal{H}_1}$ is evaluated in the first coordinate of Ψ_{N+1}, i.e. whenever the one-particle Hilbert space $\mathcal{H}_1$ is a L^2-space one has

$$\langle \varphi, \Psi_{N+1} \rangle_{\mathcal{H}_1} = \int \overline{\varphi}(x) \Psi_{N+1}(x, x_1, ..., x_N)\ \mathrm{d}x. \tag{6.1.10}$$

Now, using creation and annihilation operators, it is straightforward to express the Hamiltonian of a system. In the grand-canonical ensemble, the Hamiltonian $\hat{H}_0 : \mathcal{D}(\hat{H}_0) \to \mathcal{F}$ of a gas of non-interacting bosons is given by

$$\hat{H}_0 = \sum_{n=0}^{\infty} \epsilon_n \hat{a}^\dagger_{\varphi_n} \hat{a}_{\varphi_n} - \mu \hat{N}. \tag{6.1.11}$$

Here $\{\hat{a}^\dagger_{\varphi_n}, \hat{a}_{\varphi_n}\}$ are the creation and annihilation operators of the one-particle eigenstates $\{\varphi_n\}_{n \in \mathbb{N}_0}$, $\{\epsilon_n\}_{n \in \mathbb{N}_0}$ are the corresponding eigenvalues and $\mu \in (-\infty, \epsilon_0)$ is the chemical potential [Sch06]. At inverse temperature $\beta = \frac{1}{T}$, the density matrix of the system at thermal equilibrium is given by

$$\hat{\rho}_\beta = \frac{e^{-\beta \hat{H}_0}}{\mathrm{Tr}\,(e^{-\beta \hat{H}_0})}\ . \tag{6.1.12}$$

Accordingly, the number of particles is

$$\begin{aligned}\langle \hat{N} \rangle_{\hat{\rho}_\beta} &= \mathrm{Tr}\,(\hat{N} \hat{\rho}_\beta) \\ &= \sum_{n=0}^{\infty} \frac{1}{e^{\beta(\epsilon_n - \mu)} - 1}\ .\end{aligned} \tag{6.1.13}$$

Note that the expected number of particles occupying the n-th one-particle eigen-

state is given by

$$\langle \hat{a}^\dagger_{\varphi_n} \hat{a}_{\varphi_n} \rangle_{\hat{\rho}_\beta} = \frac{1}{e^{\beta(\epsilon_n - \mu)} - 1} \ . \tag{6.1.14}$$

The statistical description of a system involves a thermodynamic limit [Gal99]. In the grand-canonical ensemble, the thermodynamic limit is obtained by taking the limit $V \to \infty$. Here V is the volume of the one-particle configuration space. Note that the particle number will also become infinite. However, the particle density ρ remains finite and can be chosen arbitrarily. In particular, for a given value of ρ, the chemical potential must be chosen such that

$$\rho = \lim_{V \to \infty} \frac{\langle \hat{N} \rangle_{\hat{\rho}_\beta}}{V} \ . \tag{6.1.15}$$

Remark 6.1.3. Note that, in some situations, the chemical potential may also depend on the volume [LW79, LSSY05]. This means that one has to define a sequence $\{\mu_V\}$ such that (6.1.15) is fulfilled.

We can now establish a definition of BEC that holds for non-interacting systems. For this, we will assume that the considered self-adjoint one-particle Hamiltonian $\hat{H}_1$ has compact resolvent, i.e. its spectrum is purely discrete.

Definition 6.1.4. Let $\hat{H}_1$ be a one-particle Hamiltonian with eigenstates $\{\varphi_n\}_{n \in \mathbb{N}_0}$ and eigenvalues $\{\epsilon_n\}_{n \in \mathbb{N}_0}$. Given that the ground state energy converges in the thermodynamic limit, i.e.

$$\lim_{V \to \infty} \epsilon_0 = \delta, \tag{6.1.16}$$

the corresponding Bose gas is said to display Bose-Einstein condensation (at inverse temperature β) iff there exists a finite set $A = \{n_1, ..., n_{|A|}\} \in \mathbb{N}_0^{|A|}$ such that the reduced particle density

$$\begin{aligned} \rho_{red}(\beta, \mu) &= \lim_{V \to \infty} \rho^V_{red}(\beta, \mu) \\ &= \lim_{V \to \infty} \frac{1}{V} \sum_{n \notin A} \frac{1}{e^{\beta(\epsilon_n - \mu)} - 1} \end{aligned} \tag{6.1.17}$$

is bounded from above, i.e. $\exists \lambda_\beta > 0$ such that

$$\rho_{red}(\beta, \mu) \leq \lambda_\beta, \quad \forall \mu \in (-\infty, \delta). \tag{6.1.18}$$

Remark 6.1.5. Note that Definition 6.1.4 implies that, in the case BEC is dis-

played, one or more states become macroscopically occupied as soon as the particle density ρ is larger than λ_β. In other words, the particles *condense* into these states.

We can now reformulate the classical result that establishes BEC in a Bose gas in three dimensions [Ein25, Sch06].

Theorem 6.1.6. *Consider the self-adjoint one-particle Hamiltonian $-\Delta_3$, i.e. the three-dimensional Laplacian, with domain*

$$\mathcal{D}(-\Delta_3) = \left\{\varphi \in H^2(\Lambda) |\ \varphi(x) = 0,\ x \in \partial\Lambda\right\}, \tag{6.1.19}$$

where $\Lambda = (0, L)^3$ and $L \in \mathbb{R}^+$. Then the system shows Bose-Einstein condensation.

Proof. We note that, due to the Dirichlet boundary conditions, the eigenvalues and eigenfunctions can be constructed explicitly [Sch06], i.e. the eigenvalues are $k^2_{n_x n_y n_z} = \frac{\pi^2}{L^2}(n_x^2 + n_y^2 + n_z^2)$ with $n_x, n_y, n_z = 1, 2, ...$ being natural numbers. The particle density is

$$\begin{aligned}\rho(\beta, \mu) &= \lim_{L\to\infty} \frac{1}{L^3} \sum_{n_x,n_y,n_z} \frac{1}{e^{\beta\left(\frac{\pi^2}{L^2}(n_x^2+n_y^2+n_z^2)-\mu\right)} - 1} \\ &= \sqrt{\frac{1}{\beta^3}} \frac{\Gamma(\frac{3}{2})}{4\pi^2} g_{\frac{3}{2}}(z),\end{aligned} \tag{6.1.20}$$

where Γ is the Gamma-function, $z = e^{\beta\mu}$ the fugacity and

$$g_{\frac{3}{2}}(z) = \frac{1}{\Gamma(\frac{3}{2})} \int_0^\infty \frac{x^{\frac{1}{2}}}{\frac{1}{z}e^x - 1}\, \mathrm{d}x. \tag{6.1.21}$$

It can be checked that $g_{\frac{3}{2}}(z)$ is, for $z \in [0, 1]$, bounded from above [Sch06]. This then implies that the particle density (6.1.20) is also bounded from above and hence the theorem follows. □

As a consequence of the proof of Theorem 6.1.6, the particle density in the ground state is given by

$$\rho_0(\beta) = (\rho - \rho_{crit})\, \Theta\left(\rho - \rho_{crit}\right), \tag{6.1.22}$$

where $\Theta : \mathbb{R} \to \mathbb{R}$ is the Heaviside function and

$$\rho_{crit} = \sqrt{\frac{1}{\beta^3}} \frac{\Gamma(\frac{3}{2})}{4\pi^2} g_{\frac{3}{2}}(1) \tag{6.1.23}$$

the critical density. Hence, for densities $\rho > \rho_{crit}$, the ground state is macroscopically occupied which implies Bose-Einstein condensation.
For a free Bose gas with one-particle configuration space $(0, L)$, the eigenvalues $\{k_n^2\}_{n\in\mathbb{N}_0}$ of the Laplacian can again be explicitly given when Dirichlet or Neumann boundary conditions are imposed. However, it is possible generalise the standard approach to establish the absence of BEC in one dimension (for finite temperatures) without explicit knowledge of the spectrum and the Hamiltonian. For this, let $\hat{H}_1$ be a self-adjoint one-particle Hamiltonian describing a system with one-particle configuration space $(0, L)$. Furthermore, its resolvent shall be compact and the eigenvalues shall be purely positive.

Lemma 6.1.7. *Let $\{k_n^2 > 0\}_{n\in\mathbb{N}_0}$ be the positive eigenvalues (counted with multiplicity) of a one-particle Hamiltonian $\hat{H}_1$ as described above. Assume that*

$$\begin{aligned} k_{n+1}(L) - k_n(L) &\leq \frac{c}{L}, \qquad \forall n \in \mathbb{N}_0, \\ k_0(L) &\leq \frac{c}{L}, \end{aligned} \tag{6.1.24}$$

where $c > 0$ is some constant. Then the system does not show Bose-Einstein condensation.

Proof. Let $A = \{n_1, ..., n_{|A|}\} \in \mathbb{N}_0^{|A|}$ be any finite set of indices. We have

$$\begin{aligned} \rho_{red}^L(\beta, \mu) &= \frac{1}{c} \sum_{n\notin A}^{\infty} \frac{1}{e^{\beta(k_n^2-\mu)} - 1} \cdot \frac{c}{L} \\ &\geq \frac{1}{c} \sum_{n\notin A}^{\infty} \frac{1}{e^{\beta(k_n^2-\mu)} - 1} \cdot (k_{n+1} - k_n) \\ &\xrightarrow{L\to\infty} \frac{1}{c} \int_0^{\infty} \frac{1}{e^{\beta(k^2-\mu)} - 1} \, \mathrm{d}k \end{aligned} \tag{6.1.25}$$

in the sense of Riemann integrals. The integral on the right-hand side can be

evaluated using generalised Bose-Einstein functions [Sch06] and one obtains

$$\rho_{red}(\beta,\mu) \geq \frac{\Gamma(\frac{1}{2})}{2c\sqrt{\beta}} \cdot g_{\frac{1}{2}}(z), \tag{6.1.26}$$

where $z = e^{\beta\mu}$ and

$$g_{\frac{1}{2}}(z) = \frac{1}{\Gamma(\frac{1}{2})} \int_0^\infty \frac{x^{-\frac{1}{2}}}{\frac{1}{z}e^x - 1}\, \mathrm{d}x. \tag{6.1.27}$$

It is well known that $g_{\frac{1}{2}}(z)$ is, for $z \in (0,1)$, not bounded from above [Sch06]. Due to (6.1.26), the same holds for $\rho_{red}(\beta,\mu)$ which then implies the absence of BEC. □

We have already mentioned that Definition 6.1.4 covers systems of non-interacting bosons only. This follows from the fact that equation (6.1.13) is valid only for non-interacting systems. From a physical point of view, the reason is that in a system of interacting bosons, the eigenstates of the full system are not (tensor) products of one-particle eigenstates. It is therefore not clear into what one-particle states the particles may condense. A general definition of Bose-Einstein condensation, which also covers systems of interacting particles, was finally given by Penrose and Onsager [PO56]. In particular, they identified a special set of one-particle states for which condensation is investigated. Note that the definition of Penrose and Onsager is formulated in the setting of the canonical ensemble. In this ensemble, one works on the (symmetric) N-particle Hilbert space $\mathcal{H}_N^B$ instead of working on the full Fock space. The thermodynamic limit is then obtained by letting $V \to \infty$ as well as $N \to \infty$ in such a way that the particle density remains fixed [Gal99]. In the following, let $\hat{H}_N$ be a self-adjoint operator on the symmetric N-particle Hilbert-space $\mathcal{H}_N^B$ whose resolvent shall be compact, i.e. its spectrum shall be purely discrete.

Definition 6.1.8. Let $\hat{H}_N$ be a self-adjoint operator on $\mathcal{H}_N^B$ as introduced above with eigenstates $\{|\Psi_n\rangle\}_{n\in\mathbb{N}_0}$ and eigenvalues $\{E_n\}_{n\in\mathbb{N}_0}$. The thermal density matrix of the system is then defined by

$$\hat{\rho}_N = \frac{1}{Z} \sum_{n=0}^{\infty} e^{-\beta E_n} \left|\Psi_n\right\rangle \left\langle\Psi_n\right|, \tag{6.1.28}$$

where $Z = \sum_{n=0}^{\infty} e^{-\beta E_n}$ is the partition function. Furthermore,

$$\hat{\rho}_1 = N \operatorname{Tr}_{2\ldots N} (\hat{\rho}_N) \tag{6.1.29}$$

is called the reduced one-particle density matrix.

Remark 6.1.9. In Definition 6.1.8, $\operatorname{Tr}_{2\ldots N}$ refers to taking the partial trace [Mic07]. Regarding (6.1.28) as an integral operator, the partial trace is obtained by integrating out all degrees of freedom except one.

Note that the one-particle density matrix (6.1.29) is a trace-class operator on the one-particle Hilbert space $\mathcal{H}_1$ [Mic07]. In the following, we will denote its eigenvectors by $\{\varphi_n\}_{n\in\mathbb{N}_0}$ and its eigenvalues by $\{\lambda_n\}_{n\in\mathbb{N}_0}$.

Definition 6.1.10 (**Penrose and Onsager**). Consider a system with thermal density matrix $\hat{\rho}_N$. Then the system is said to display Bose-Einstein condensation in the state φ_n and at inverse temperature β if there exist some positive constants c_1, c_2 such that the inequality

$$c_1 < \frac{\lambda_n(\beta)}{N} < c_2 \tag{6.1.30}$$

holds for all $N > N_0$ in the thermodynamic limit.

Remark 6.1.11. Note that $\frac{\lambda_n}{N}$ is the fraction of particles in the state φ_n. This means that the criterion of Penrose and Onsager defines BEC as the macroscopic occupation of an eigenstate of the reduced one-particle density matrix. For other possible definitions of Bose-Einstein condensation and further discussion see [Mic07].

Although the criterion of Penrose and Onsager can also be applied to interacting systems, it is in general difficult to establish BEC rigorously in the sense of Definition 6.1.10. This is due to the fact that the eigenstates of the full system are hard to construct. Therefore, another approach to BEC related to phase transitions is often pursued in literature [BP86, BdSP83]. To introduce the notion of a phase transition, let $\{g_n(\beta)\}_{n\in\mathbb{N}}$ be a sequence of functions such that $g_n(\beta) \in C^\infty(\mathbb{R}^+)$ for all $n \in \mathbb{N}$ and assume that the limiting function

$$g(\beta) = \lim_{n\to\infty} g_n(\beta) \tag{6.1.31}$$

exists for all $\beta \in (0, \infty)$. If $g(\beta)$ is differentiable almost everywhere, we say that $g(\beta)$ is a thermodynamical function. Furthermore, we say that a thermodynamical function $g(\beta)$ displays a phase transition at all values of $\beta \in (0, \infty)$ for which it is not differentiable. As standard in statistical mechanics [Sch06], suitable sequences of functions $g_N^V(\beta)$ are constructed from the partition function or the free energy density. In the canonical ensemble, the partition function is given by

$$Z_N^V(\beta) = \mathrm{Tr}(e^{-\beta \hat{H}_N}) = \sum_{n=0}^{\infty} e^{-\beta E_n}, \tag{6.1.32}$$

and the free energy density by

$$f_N^V(\beta) = -\frac{1}{\beta V} \ln Z_N^V(\beta). \tag{6.1.33}$$

Possible candidates for functions that exhibit a phase transition are the free energy density itself, the internal energy per particle

$$u_N^V(\beta) = -\frac{1}{N} \frac{\partial \ln Z_N^V(\beta)}{\partial \beta}, \tag{6.1.34}$$

or the specific heat per volume

$$c_N^V(\beta) = \frac{N}{V} \left(\frac{\partial u_N^V(\beta)}{\partial T} \right)_V. \tag{6.1.35}$$

Remark 6.1.12. It is important to note that discontinuities (and hence phase transitions) can only occur *after* taking the thermodynamic limit [YL52]. For example, the *sharp* onset of the occupation of the ground state in a three dimensional Bose gas above the critical density (6.1.22) is due to taking the thermodynamic limit [KvD96].

For the non-interacting Bose gas in three dimensions, it is well known that besides the macroscopic occupation of the one-particle ground state (6.1.22), there is also a phase transition occurring at a critical temperature [Sch06]. Also, in [IRH76], the authors established Bose-Einstein condensation as well as the presence of a phase transition in a one-dimensional system with an attractive impurity centre. In general, one might wonder if Bose-Einstein condensation in the sense of Definition 6.1.10 will always leads to a phase transition. This in turn would

mean that the absence of a phase transition implies the absence of Bose-Einstein condensation. Now, in order to give a formal argument for the presence of a phase transition if Bose-Einstein condensation is displayed above some critical inverse temperature β_{crit}, we consider a system of bosons with two-particle interactions. Let

$$\hat{V} : \mathcal{H}_2 \to \mathcal{H}_2 \tag{6.1.36}$$

be a (bounded) interaction operator. The Hamiltonian $\hat{H}_{\mathcal{F}} : \mathcal{D}(\hat{H}_{\mathcal{F}}) \to \mathcal{F}$ on the Fock space can then, in the standard formalism of second quantisation [MR04], be written as

$$\begin{aligned} \hat{H}_{\mathcal{F}} = &\sum_{mn} \langle \varphi_m, \hat{H}_1 \varphi_n \rangle_{\mathcal{H}_1} \ \hat{a}^\dagger_{\varphi_m} \hat{a}_{\varphi_n} \\ &+ \frac{1}{2} \sum_{klmn} \langle \varphi_k \otimes \varphi_l, \hat{V}(\varphi_m \otimes \varphi_n) \rangle_{\mathcal{H}_2} \ \hat{a}^\dagger_{\varphi_k} \hat{a}^\dagger_{\varphi_l} \hat{a}_{\varphi_m} \hat{a}_{\varphi_n}, \end{aligned} \tag{6.1.37}$$

where $\{\hat{a}_{\varphi_n}, \hat{a}^\dagger_{\varphi_n}\}$ are the annihilation and creation operators of the eigenstates of the reduced one-particle density matrix $\{\varphi_n\}_{n \in \mathbb{N}_0}$.

Remark 6.1.13. Note that we can also consider the operator (6.1.37) as a representation of the N-particle Hamiltonian on $\mathcal{H}^B_N$ by identifying each function $\varphi \in \mathcal{H}^B_N$ with $(0, ..., 0, \varphi, 0, ...) \in \mathcal{F}$.

Now, assume that we have condensation into the state φ_0 for inverse temperatures $\beta \geq \beta_{crit}$. Starting from (6.1.37), we calculate the internal energy

$$\begin{aligned} U^V_N(\beta) &= \langle \hat{H}_{\mathcal{F}} \rangle_{\hat{\rho}_\beta} \\ &= \langle \varphi_0, \hat{H}_1 \varphi_0 \rangle_{\mathcal{H}_1} \langle \hat{a}^\dagger_{\varphi_0} \hat{a}_{\varphi_0} \rangle_{\hat{\rho}_\beta} \\ &\quad + \langle \hat{H}_{\mathcal{F}} \rangle^{\text{rest}}_{\hat{\rho}_\beta}, \end{aligned} \tag{6.1.38}$$

where $\langle \hat{H}_{\mathcal{F}} \rangle^{\text{rest}}_{\hat{\rho}_\beta}$ contains all other terms. Hence, the specific heat per volume (6.1.35) is given by

$$\begin{aligned} c^V_N(\beta) = &\langle \varphi_0, \hat{H}_1 \varphi_0 \rangle_{\mathcal{H}_1} \frac{1}{V} \frac{\partial \langle \hat{a}^\dagger_{\varphi_0} \hat{a}_{\varphi_0} \rangle_{\hat{\rho}_\beta}}{\partial T} \\ &+ \frac{\partial \langle \varphi_0, \hat{H}_1 \varphi_0 \rangle_{\mathcal{H}_1}}{\partial T} \frac{\langle \hat{a}^\dagger_{\varphi_0} \hat{a}_{\varphi_0} \rangle_{\hat{\rho}_\beta}}{V} \\ &+ \frac{1}{V} \frac{\partial \langle \hat{H}_{\mathcal{F}} \rangle^{\text{rest}}_{\hat{\rho}_\beta}}{\partial T} \ . \end{aligned} \tag{6.1.39}$$

Now, according to (6.1.14), the average density of particles in the state φ_0 is

$$\rho^V_{\varphi_0}(\beta) = \frac{\langle \hat{a}^\dagger_{\varphi_0} \hat{a}_{\varphi_0} \rangle_{\hat{\rho}_\beta}}{V} \tag{6.1.40}$$

and, by assumption, φ_0 is macroscopically occupied for $\beta \geq \beta_{crit}$. As a consequence,

$$\lim_{\substack{N,V\to\infty \\ \frac{N}{V}=const.}} \frac{\partial}{\partial T} \frac{\langle \hat{a}^\dagger_{\varphi_0} \hat{a}_{\varphi_0} \rangle_{\hat{\rho}_\beta}}{V} \tag{6.1.41}$$

is expected to be discontinuous at $\beta = \beta_{crit}$ and hence there is a phase transition in the specific heat per volume. Note that, although this derivation is not rigorous, it nevertheless sheds some light on basic processes. For example, in [Kim07], it was shown that the specific heat is indeed discontinuous in the presence of weak interactions. Also, in the one-dimensional model considered in [IRH76], the system displays BEC as well as a discontinuity in the specific heat per volume. Hence, instead of establishing Bose-Einstein condensation rigorously in the sense of Definition 6.1.10, one can also look for possible phase transitions. An absence of phase transitions would then indicate an absence of BEC. However, it must be kept in mind that this approach is not completely equivalent to the approach based on the criterion of Penrose and Onsager and hence can only provide strong indications towards the existence or absence of BEC. One important difference between the two approaches lies in the fact that only the spectrum enters the partition function, whereas in the criterion of Penrose and Onsager, the wave functions play also an important role.

So far, we have introduced the general criterion for the occurrence of Bose-Einstein condensation and repeated the main argument that establishes BEC in a free gas of bosons in three dimensions (see Theorem 6.1.6). However, the concept of a free gas is somehow pathological. Firstly, in a real gas the particles are never free in the strict sense. Secondly, we have to require boundary conditions which effectively describe an interaction with external potentials (see Remark 3.1.5). Most importantly, however, it is not clear how robust Bose-Einstein condensation is with respect to any additional (two-particle) interactions [dS86, BdSP83] or a change of boundary conditions [FGKE00] (p.91-111). Therefore, it is of fundamental importance to understand the occurrence or absence of Bose-Einstein condensation in a

system of interacting particles. In that context, it is interesting to mention some results. For example, in [BP85], it is shown that condensation in a Bose gas in one dimension is destroyed as soon as the particles have some hard core, i.e. whenever they are modelled as hard balls with some diameter $a > 0$. Note that, in their one-dimensional model, the presence of condensation before the introduction of the hard cores is due to attractive interactions with external potentials. Furthermore, starting with the same one-dimensional model exhibiting condensation, it is shown in [dS86] that the condensation is destroyed through the implementation of arbitrarily small repulsive two-particle interactions. More precisely, the one-particle ground state remains no longer macroscopically occupied after repulsive two-particle interactions were switched on. Note that, in three dimensional models, the condensate may not be destroyed by implementing two-particle interactions given there was a gap in the one-particle spectrum [BdSP83, JLZ03]. Indeed, the presence of a gap leads to Bose-Einstein condensation also in a one-dimensional system. To illustrate this, let $\hat{H}_1$ be a self-adjoint one-particle Hamiltonian describing a system with one-particle configuration space $(0, L)$. We shall assume that $\hat{H}_1$ has compact resolvent and that the ground state eigenvalue $-k_0^2(L)$ with $k_0^2 > 0$ converges, in the limit $L \to \infty$, to $-\Theta$ where $\Theta > 0$ is some constant. Furthermore, the multiplicity of the ground state shall be one.

Proposition 6.1.14. *Let $\hat{H}_1$ be the one-particle Hamiltonian described above with spectrum*

$$\sigma(\hat{H}_1) = \{-k_0^2\} \cup \{k_n^2 > 0\}_{n\in\mathbb{N}}, \tag{6.1.42}$$

where the eigenvalues shall have multiplicity one and are such that

$$\frac{c_1}{L} \leq k_{n+1}(L) - k_n(L) \leq \frac{c_2}{L}, \qquad \forall n \in \mathbb{N}, \tag{6.1.43}$$

with $c_2 > c_1 > 0$ some constants. Then the system shows Bose-Einstein condensation.

Proof. For the particle density at finite volume $\rho_L(\beta,\mu)$, we have

$$\begin{aligned}\rho_L(\beta,\mu) &= \frac{1}{c}\sum_{n=1}^{\infty}\frac{1}{e^{\beta(k_n^2-\mu)}-1}\cdot\frac{c}{L} \\ &\quad + \frac{1}{L}\frac{1}{e^{\beta(-k_0^2-\mu)}-1} \\ &\leq \frac{1}{c}\sum_{n=1}^{\infty}\frac{1}{e^{\beta(k_n^2-\mu)}-1}\cdot(k_{n+1}-k_n) + \frac{1}{L}\frac{1}{e^{\beta(-k_0^2-\mu)}-1} \\ &\overset{L\to\infty}{\longrightarrow} \frac{1}{c}\int_0^{\infty}\frac{1}{e^{\beta(k^2-\mu)}-1}\,\mathrm{d}k\end{aligned} \tag{6.1.44}$$

in the sense of Riemann integrals. As in the proof of Lemma 6.1.7, the integral on the right-hand side is calculated to be a multiple of the Bose-Einstein function $g_{\frac{1}{2}}(z)$. However, due to the negative eigenvalue $-\Theta$, there is now a shift in the chemical potential, i.e. $\mu \in (-\infty,-\Theta)$. Hence, since $g_{\frac{1}{2}}(z)$ is monotonic, the right-hand side of (6.1.44) is bounded by some multiple of $g_{\frac{1}{2}}(e^{-\beta\Theta}) < \infty$. □

6.2 Bose-Einstein condensation in non-interacting many-particle systems

In this section, we will consider non-interacting many-particle systems on quantum graphs in the sense of Definition 4.1.18. Note, however, that the corresponding self-adjoint realisation of the one-particle Laplacian nevertheless induces interactions with external potentials as described in Remark 3.1.5.
In the sequel, we will work in the grand canonical ensemble and since the volume of a graph is given by

$$\mathcal{L} = \sum_{e=1}^{E} l_e, \tag{6.2.1}$$

we define the following.

Definition 6.2.1. Let $\Gamma = \Gamma(\mathcal{V},\mathcal{E})$ be a compact graph with edge lengths $\{l_e\}_{e\in\mathcal{E}}$. Introducing a scaling parameter $n \in \mathbb{N}$ and replacing l_e by nl_e for all $e \in \mathcal{E}$, the limit of infinite volume is obtained by the limit $n \to \infty$. This limit will also be denoted as $\lim_{\mathcal{L}\to\infty}$.

To construct a system of N non-interacting bosons in the sense of Definition 4.1.18, let $(-\Delta_1, \mathcal{D}_1(P,L))$ be a self-adjoint realisation of the one-particle

Laplacian with eigenfunctions $\{\varphi_n\}_{n\in\mathbb{N}_0}$ and eigenvalues $\{k_n^2\}_{n\in\mathbb{N}_0}$. Introducing the domain

$$\mathcal{D}_N(-\Delta_1) = \left\{ \Psi \in \mathcal{H}_N^B \middle| \Psi = \sum_{n_1\ldots n_N}^{\text{finite}} a_{n_1\ldots n_N} \cdot \Pi_B(\varphi_{n_1} \otimes \ldots \otimes \varphi_{n_N}),\ a_{n_1\ldots n_N} \in \mathbb{C} \right\}, \tag{6.2.2}$$

we readily establish the analogue of Lemma 4.1.17.

Lemma 6.2.2. *The operator $(-\Delta_N, \mathcal{D}_N(-\Delta_1))$ is semi-bounded and essentially self-adjoint.*

Remark 6.2.3. Note that the closure of $(-\Delta_N, \mathcal{D}_N(-\Delta_1))$ can be represented in the form $\mathcal{D}_B^N(P, L)$ with suitable N-particle maps P and L (see Remark A.0.20).

In the first theorem, we show that no Bose-Einstein condensation occurs for systems of non-interacting bosons where the interactions with external potentials in the vertices are fully repulsive, i.e. where the corresponding one-particle Laplacian $-\Delta_1$ is characterised by a negative definite map L.

Theorem 6.2.4. *Let $(-\Delta_N, \mathcal{D}_N(-\Delta_1))$ be such that the corresponding one-particle operator $(-\Delta_1, \mathcal{D}_1(P, L))$ has a negative definite map L. Then no Bose-Einstein condensation is displayed.*

Proof. Let $A = \{n_1, ..., n_{|A|}\} \in \mathbb{N}_0^{|A|}$ be any finite set of indices. Since the one-particle map L is assumed to be negative definite, a standard Dirichlet-Neumann bracketing argument [RS78] yields

$$N'_D(K) \leq N'(K) \leq N'_N(K), \tag{6.2.3}$$

where $N'(K) = \#\{n \notin A; k_n^2 \leq K^2\}$ is the reduced eigenvalue counting function for the one-particle Laplacian $(-\Delta_1, \mathcal{D}_1(P, L))$ and $K \in \mathbb{R}$ some bound. Also, $N'_D(K)$ denotes the reduced counting function for Dirichlet boundary conditions ($P_D = \mathbb{1}_{2E}$, $L_D = 0$) and $N'_N(K)$ the reduced counting function for Neumann boundary conditions ($P_N = 0, L_N = 0$). Setting $\epsilon_n = k_n^2$, we have the identity ($\mu < 0$)

$$\sum_{n\notin A} \frac{1}{e^{\beta(\epsilon_n - \mu)} - 1} = \int_{\frac{\mu}{2}}^{\infty} \frac{1}{e^{\beta(\epsilon-\mu)} - 1}\, \mathrm{d}N'(\epsilon), \tag{6.2.4}$$

where $N'(\epsilon) = \#\{n \notin A; \epsilon_n \leq \epsilon\}$. Note that we were free to choose the lower bound on the right-hand side of (6.2.4) to be $\frac{\mu}{2} < 0$ since $N'(\epsilon) = 0$ for $\epsilon < 0$.

Now, using an integration by parts, while taking into account that the boundary terms vanish due to the Weyl asymptotic for $N(K)$ (see Lemma 3.2.3) as well as $N(\frac{\mu}{2}) = 0$, we have

$$\rho_{red}(\beta, \mu) = \rho_{red}^{D/N}(\beta, \mu). \tag{6.2.5}$$

Finally, taking into account that the one-particle Laplacian with Dirichlet or Neumann boundary conditions is covered by an extension of Lemma 6.1.7 to general graphs, the theorem follows. □

As demonstrated in Proposition 6.1.14, a gap in the one-particle spectrum leads to Bose-Einstein condensation even in the one-dimensional Bose gas. However, in order to generate such a gap in the thermodynamic limit, it is necessary for $-\Delta_1$ to possess negative eigenvalues. Note that an upper bound for the number of negative eigenvalues $n_-(-\Delta_1)$ of the one-particle Laplacian was proved in [KS06].

Lemma 6.2.5. *[KS06] Let $(-\Delta_1, \mathcal{D}_1(A, B))$ be a self-adjoint realisation of the one-particle Laplacian. Then, the number of negative eigenvalues $n_-(-\Delta_1)$ is bounded from above, i.e.*

$$n_-(-\Delta_1) \leq n_+(AB^*), \tag{6.2.6}$$

where $n_+(AB^*)$ is the number of positive eigenvalues of $AB^* \in \mathbb{C}^{2E\times 2E}$.

The exact number of negative eigenvalues of a self-adjoint realisation $(-\Delta_1, \mathcal{D}_1(P, L))$ was later determined in [BL10] where the matrix

$$M_0(l_1, \ldots, l_E) = \begin{pmatrix} m_1(l_1) & & 0 \\ & \ddots & \\ 0 & & m_E(l_E) \end{pmatrix}, \tag{6.2.7}$$

with

$$m_e(l_e) = \frac{1}{l_e}\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{6.2.8}$$

was introduced. It was shown that

$$n_-(-\Delta_1) = n_+(L + QM_0Q), \tag{6.2.9}$$

where the right-hand side denotes the number of positive eigenvalues of the linear map $L + QM_0Q$ on $\ker P \subseteq \mathbb{C}^{2E}$.

On a graph, the eigenvalues may depend on the edge lengths and hence it is not clear that a gap present at finite volume will persist when taking the thermodynamic limit. However, in the following proposition we will indeed prove that a gap will remain present when taking the thermodynamic limit as soon as the one-particle map L has at least one positive eigenvalue.

Proposition 6.2.6. *Let $(-\Delta_1, \mathcal{D}_1(P,L))$ be a self-adjoint realisation of the one-particle Laplacian. Assume that L has at least one positive eigenvalue and denote the largest eigenvalue by $L_{\max}$. Then the ground state eigenvalue $k_0^2 < 0$ of the one-particle Laplacian converges to $-L_{\max}^2 < 0$ in the thermodynamic limit.*

Proof. As L is assumed to possess at least one positive eigenvalue, $n_+(L) \geq 1$, the relation (6.2.9) implies that the Laplacian has at least one negative eigenvalue if the edge lengths are chosen large enough. Hence, for any $\Phi \in \mathcal{D}_{Q_1}$,

$$-s^2 \leq k_0^2 \leq R[\Phi] \tag{6.2.10}$$

where $R[\Phi]$ is the Rayleigh-quotient

$$R[\Psi] = \frac{Q_1[\Psi]}{\|\Psi\|^2_{L^2(\Gamma)}} , \qquad \Psi \in \mathcal{D}_{Q_1}. \tag{6.2.11}$$

Here $-s^2$ is the lower bound for the spectrum of the one-particle Laplacian proved in [KS06], with s a solution of

$$s \tanh\left(\frac{s l_{\min}}{2}\right) = L_{\max} , \tag{6.2.12}$$

and $l_{\min}$ the shortest edge-length. In the thermodynamic limit, where $l_{\min} \to \infty$, the lower bound in (6.2.10) converges to $-L_{\max}^2$. To find an upper bound in (6.2.10), we need to determine the Rayleigh quotient of a suitable trial function. We assume that $P \neq \mathbb{1}_{2E}$ as this would correspond to Dirichlet boundary conditions in the vertices, where it is known that there are no negative eigenvalues. Hence, there exists a non-trivial vector

$$v = (c_1, \ldots, c_E, c_{E+1}, \ldots, c_{2E})^T \in \ker P . \tag{6.2.13}$$

Using the components of such a vector, we now define a trial function Φ with

components

$$\phi_e(x) = \begin{cases} c_e\big(1-\frac{x}{\lambda}\big)^\alpha & , \ x \le \lambda \\ 0 & , \ \lambda \le x \le l_e - \lambda \\ c_{e+E}\big(\frac{x}{\lambda}+1-\frac{l_e}{\lambda}\big)^\alpha & , \ x \ge l_e - \lambda \end{cases} , \qquad \alpha \ge 1 \ . \tag{6.2.14}$$

In the thermodynamic limit, given any value for λ, we can arrange that $l_e \ge 2\lambda$ for all $e = 1, \dots, E$. The boundary values of this function, therefore, are

$$\Phi_{bv} = (c_1, \dots, c_E, c_{E+1}, \dots, c_{2E})^T = v \in \ker P \ , \tag{6.2.15}$$

hence this function is in the domain $\mathcal{D}_{Q_1}$ of the quadratic form. We now intend to estimate the Rayleigh quotient of Φ, noting that we are free to choose $v \in \ker P$. The optimal choice for our purpose is to let $v = \Phi_{bv}$ be an eigenvector of L corresponding to its maximal eigenvalue $L_{\max} > 0$. Then,

$$\begin{aligned} Q_1[\Phi] &= \sum_{e=1}^{E} \int_0^{l_e} |\phi_e'(x)|^2 \, \mathrm{d}x - \langle \Phi_{bv}, L\Phi_{bv} \rangle_{\mathbb{C}^{2E}} \\ &= \frac{\alpha^2}{(2\alpha-1)\lambda} \sum_{e=1}^{E} \big(|c_e|^2 + |c_{e+E}|^2 \big) - L_{\max} \|\Phi_{bv}\|^2_{\mathbb{C}^{2E}} \\ &= \left(\frac{\alpha^2}{(2\alpha-1)\lambda} - L_{\max} \right) \|\Phi_{bv}\|^2_{\mathbb{C}^{2E}} \ . \end{aligned} \tag{6.2.16}$$

Moreover,

$$\|\Phi\|^2 = \sum_{e=1}^{E} \int_0^{l_e} |\phi_e(x)|^2 \, \mathrm{d}x = \frac{\lambda}{2\alpha+1} \sum_{e=1}^{E} \big(|c_e|^2 + |c_{e+E}|^2 \big) = \frac{\lambda}{2\alpha+1} \|\Phi_{bv}\|^2_{\mathbb{C}^{2E}} \ , \tag{6.2.17}$$

so that

$$R[\Phi] = \left(\frac{\alpha^2}{(2\alpha-1)\lambda} - L_{\max} \right) \frac{2\alpha+1}{\lambda} \ . \tag{6.2.18}$$

The right-hand side is negative when $\lambda > \frac{\alpha^2}{(2\alpha-1)L_{\max}}$ and has a minimum at $\lambda_{\min} = \frac{2\alpha^2}{(2\alpha-1)L_{\max}}$. With this optimal choice we find that

$$R[\Phi] = -\frac{4\alpha^2-1}{4\alpha^2} L_{\max}^2 \ . \tag{6.2.19}$$

As $\alpha \geq 1$ can be chosen arbitrarily large in the thermodynamic limit, the optimal upper bound in (6.2.10) approaches $-L^2_{\max}$. Hence, k_0^2 converges to $-L^2_{\max}$ in the thermodynamic limit. □

We are now in position to state the main result of this section which is a generalisation of Proposition 6.1.14. We will show that Bose-Einstein condensation is present for all non-interacting many-particle systems whose corresponding one-particle map L has at least one positive eigenvalue. Since we have shown, in Theorem 6.2.4, that no BEC occurs for systems with negative definite L, all possible (non-interacting) systems on quantum graphs are covered by our results.

Theorem 6.2.7. *Let $(-\Delta_N, \mathcal{D}_N(-\Delta_1))$ be such that the corresponding one-particle operator $(-\Delta_1, \mathcal{D}_1(P, L))$ has a map L with at least one positive eigenvalue. Then the system displays Bose-Einstein condensation.*

Proof. We first note that since L has at least one positive eigenvalue, the operator $(-\Delta_1, \mathcal{D}_1(P, L))$ has at least one negative eigenvalue. The particle number in the eigenstates with positive eigenvalues is then given by

$$N_+(\beta, \mu) = \sum_{k_n^2 \geq 0} \frac{1}{e^{\beta(k_n^2 - \mu)} - 1} \ . \tag{6.2.20}$$

In order to evaluate this expression, we use a preliminary version of the trace formula as established in [BE09], i.e.

$$\begin{aligned} \sum_{k_n^2 \geq 0}^{\infty} h(k_n) = \frac{\mathcal{L}}{2\pi} \int_{-\infty}^{\infty} h(k) \, \mathrm{d}k + \gamma h(0) - \frac{1}{4\pi} \int_{-\infty}^{\infty} h(k) \, s(k) \, \mathrm{d}k \\ + \sum_{l \neq 0} \frac{1}{4\pi i} \int_{-\infty}^{\infty} \mathrm{Tr}[\Lambda(k) U^l(k)] \, h(k) \, \mathrm{d}k \ . \end{aligned} \tag{6.2.21}$$

Here γ is a constant related to the multiplicity of the eigenvalue zero, Λ, U are matrix-valued functions involving the boundary conditions, and s is another function related to the boundary conditions. In this trace formula, h is a test function from a suitable test function space [BE09].
Now, choosing $h(k) = \frac{1}{e^{\beta(k^2-\mu)}-1}$, the left-hand side of (6.2.21) is $N_+(\beta, \mu)$. The right-hand side, on the other hand, provides four seperate contributions to $N_+(\beta, \mu)$ of which the second and the third term give no contributions to the particle density $\rho_+(\beta, \mu)$ in the thermodynamic limit. An estimate of the fourth term can be

found in the proof of Theorem 5.4 in [BE09],

$$\sum_{l\neq 0}\left|\int_{-\infty}^{\infty}\mathrm{Tr}[\Lambda(k)U^l(k)]\,h(k)\;\mathrm{d}k\right| = O\big(\mathrm{e}^{-\sigma l_{\min}}\big), \tag{6.2.22}$$

where $l_{\min}$ is the shortest edge-length and $\sigma > 0$ a constant. Therefore, in the thermodynamic limit, this term also gives no contribution to $\rho_+(\beta,\mu)$ and hence the only non-vanishing contribution comes from the first term (which also provides the Weyl term in the asymptotics of the eigenvalue count), i.e.

$$\rho_+(\beta,\mu) = \frac{1}{\pi}\int_0^{\infty}\frac{1}{\mathrm{e}^{\beta(k^2-\mu)}-1}\;\mathrm{d}k = \frac{1}{\sqrt{4\pi\beta}}\,g_{\frac{1}{2}}(\mathrm{e}^{\beta\mu})\;. \tag{6.2.23}$$

Since $\mu < k_0^2 \to -L_{max}^2$, where L_{max}^2 is the largest positive eigenvalue of the map L, $\rho_+(\beta,\mu)$ is bounded from above and since the number of eigenstates with negative eigenvalues is also bounded, the theorem follows. □

Finally, with the notation of the previous proof, we can derive an expression for the critical particle density above which the states of negative energy are populated. The total particle density is given by

$$\rho(\beta,\mu) = \rho_-(\beta,\mu) + \rho_+(\beta,\mu) \tag{6.2.24}$$

where $\rho_-(\beta,\mu)$ is the particle density in the states of negative energy. The critical density is the maximal density of particles that can be occupied in the excited states, i.e.

$$\rho_{crit} = \frac{1}{\sqrt{4\pi\beta}}\,g_{\frac{1}{2}}(e^{-\beta L_{\max}^2}). \tag{6.2.25}$$

Hence, whenever $\rho > \rho_{crit}$, the states of negative energy are macroscopically occupied, i.e. we have Bose-Einstein condensation.

6.3 Bose-Einstein condensation in interacting many-particle systems

In this section, we will investigate Bose-Einstein condensation in many-particle systems where the particles are interacting with each other, i.e. we will consider realisations $(-\Delta_N, \mathcal{D}_N^{\alpha}(P,L))$ as described in Chapter 5. Since, as mentioned in the

introduction of this chapter, it is in general very difficult to discuss Bose-Einstein condensation rigorously in the sense of Definition 6.1.10, we will approach the problem indirectly. In the first part, we investigate the effect of many-particle interactions on the ground-state energy density. In the second part, we generalise the Fermi-Bose mapping introduced by M. Girardeau [Gir60] to general quantum graphs and use the results to establish, in the third part, the absence of Bose-Einstein condensation (in the sense of phase transitions) for systems of particles interacting via repulsive hard-core interactions.

6.3.1 The ground state energy density

In this subsection, we will consider many-particle systems at zero temperature. Note that, regarding Bose-Einstein condensation, it is customary to consider first the simplified situation of zero temperature [LSSY05]. For example, the thermal density matrix (6.1.28) then takes on a simple form incorporating the many-particle ground state only. Also, from a physical point of view, the tendency of a Bose gas to form a condensate can be assumed to be higher at zero temperature than at finite temperatures. In this context, a very interesting model is the Bogoliubov model of the weakly imperfect gas [ZB01]. There, one starts with a free three-dimensional Bose gas at zero temperature showing complete condensation into the one-particle ground state. One then implements repulsive two-particle interactions and, while *assuming* that condensation persists, investigates the effects of the interactions on the condensate. As a result, repulsive interactions lower the fraction of particles forming the condensate and, at the same time, the ground state energy is increased. As a consequence, if many-particle interactions lead to a higher ground-state energy density compared to the free gas (in which case the ground state energy density usually is zero), one expects the degree of Bose-Einstein condensation to be lowered.
In this subsection, we will work in the canonical ensemble and we will consider two types of systems, i.e. systems of non-interacting bosons described by realisations $(-\Delta_N, \mathcal{D}_N(-\Delta_1))$ and systems of interacting bosons described by realisations $(-\Delta_N, \mathcal{D}_N^\alpha(P, L))$.

Definition 6.3.1. Let $\hat{H}_N$ be a (self-adjoint) N-particle Hamiltonian describing a system of N bosons on a compact quantum graph $\Gamma = \Gamma(\mathcal{V}, \mathcal{E})$ with edge lengths $\{l_e\}_{e\in\mathcal{E}}$. Furthermore, let $\langle \hat{O}_N \rangle_{\hat{\rho}_N}$ be the expectation value of an observable $\hat{O}_N$.

Introducing a scaling parameter $n \in \mathbb{N}$ and replacing l_e by nl_e for all $e \in \mathcal{E}$ and N by nN, the thermodynamic limit of $\langle \hat{O}_N \rangle_{\hat{\rho}_N}$ in the canonical ensemble is obtained as the limit $\lim_{n\to\infty} \langle \hat{O}_N \rangle_{\hat{\rho}_N}$.

Definition 6.3.2. Let $(-\Delta_N, \mathcal{D}_N^\alpha(P, L))$ or $(-\Delta_N, \mathcal{D}_N(-\Delta_1))$ be a realisation of the N-particle Laplacian as introduced above. The ground state energy density is then defined as

$$e_0^\infty(\rho) = \lim_{n\to\infty} \frac{E_0^N}{N}, \tag{6.3.1}$$

where E_0^N is the N-particle ground state energy.

We first consider realisations $(-\Delta_N, \mathcal{D}_N(-\Delta_1))$, i.e. systems of non-interacting bosons.

Lemma 6.3.3. *Let $(-\Delta_N, \mathcal{D}_N(-\Delta_1))$ be a realisation of the N-particle Laplacian describing a system of N non-interacting bosons. Then, given the corresponding one-particle map L is negative definite, we have*

$$e_0^\infty(\rho) = 0 \ . \tag{6.3.2}$$

Proof. Since we consider a system of non-interacting bosons, we have

$$E_0^N = k_0^2 + ... + k_0^2 = Nk_0^2 \tag{6.3.3}$$

where k_0^2 is the one-particle ground state eigenvalue (compare with (4.3.4)). We get

$$\begin{aligned} e_0^\infty(\rho) &= \lim_{n\to\infty} \frac{E_0^N}{N} \\ &= \lim_{\mathcal{L}\to\infty} k_0^2. \end{aligned} \tag{6.3.4}$$

Now, since L is negative definite, we can apply the min-max principle (Theorem 2.1.27) to obtain

$$k_{0,N}^2 \leq k_0^2 \leq k_{0,D}^2 \tag{6.3.5}$$

where the index N indicates Neumann boundary condition whereas the index D indicates Dirichlet boundary conditions. Now, since $k_{0,D}^2$ and $k_{0,N}^2$ converge to zero

in the limit $\mathcal{L} \to \infty$, we readily obtain

$$\lim_{\mathcal{L}\to\infty} k_0^2 = 0. \tag{6.3.6}$$

□

As a next step, we consider realisations $(-\Delta_N, \mathcal{D}_N^{\alpha=0}(P,L))$, i.e. systems where the particles interact via (repulsive) singular interactions located at the vertices of the graph. However, we do neglect contact interactions by setting $\alpha = 0$.

Corollary 6.3.4. *Let $(-\Delta_N, \mathcal{D}_N^{\alpha=0}(P,L))$ be a self-adjoint realisation of the N-particle Laplacian on the Hilbert space $\mathcal{H}_N^{*B}$ with $\alpha = 0$. Assuming that the N-particle map L is negative definite, we have*

$$e_0^\infty(\rho) = 0 \ . \tag{6.3.7}$$

Proof. The proof follows the same lines as the proof of Lemma 6.3.3. Since the N-particle map L is negative definite, the min-max principle (Theorem 2.1.27) directly yields

$$e_{0,N}^\infty(\rho) \leq e_0^\infty(\rho) \leq e_{0,D}^\infty(\rho), \tag{6.3.8}$$

where the indices (D,N) refer to Dirichlet or Neumann boundary conditions respectively. Furthermore, since those two cases correspond to systems of non-interacting particles, we can take Lemma 6.3.3 into account and the corollary follows. □

Note that, under the assumption that the N-particle map L is negative definite and $0 \leq \alpha(y) \leq \infty$ for all $y \in [0,1]$, an upper and a lower bound for the ground-state energy density can be established. Indeed, it is straightforward to check that $e_0^\infty(\rho) \geq 0$. Furthermore, in [LL63] an upper bound for the case $\alpha \to \infty$ was given, i.e. $e_0^\infty(\rho) = \frac{\pi^2}{3}\rho^2$. Therefore, applying the min-max principle (see Theorem 2.1.27), we readily see that $\frac{\pi^2}{3}\rho^2$ is an upper bound for all other realisations considered.

As a final result in this section, we want to show that for a system with repulsive two-particle contact interactions, the ground state energy density is strictly positive. For example, Lieb and Liniger have established this for their model using the eigenvalues which could be implicitly given [LL63]. More explicitly, they established the following result.

Proposition 6.3.5. *Consider the simplest compact graph, i.e. an interval of length l, and a system of N bosons described by the form* (5.3.13) *with maps*

$$P_{vert} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \quad \text{and} \quad L_{vert} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \tag{6.3.9}$$

as well as $\alpha(y) = \alpha$ with $\alpha > 0$ some constant. Then, one has

$$e_0^\infty(\rho) > 0 \tag{6.3.10}$$

for all values ρ of the particle density.

Our aim is now to generalise their result to more general systems on quantum graphs. To establish this result, we need the following version of Lemma 5.12 of [Dob05].

Lemma 6.3.6. *Let $\Omega \subset \mathbb{R}^N$ be an open domain and $K \subset \Omega$ a compact subset. Then there exists a real-valued function $\tau \in C_0^\infty(\Omega)$ such that $0 \leq \tau \leq 1$ and $\tau = 1$ on K. Furthermore, given the distance between K and Ω is δ, i.e.* $\operatorname{dist}(\partial K, \partial\Omega) = \delta$*, one can choose the function τ such that*

$$|\partial_j \tau| \leq \frac{c_N}{\delta}, \quad in \quad \Omega \backslash K, \quad j = 1, ..., N, \tag{6.3.11}$$

where the constant c_N depends only on N but not on Ω or K. More explicitly, one has $c_N = \left(\frac{\sqrt{\pi}}{4}\right)^N \frac{\gamma}{\Gamma(\frac{N}{2}+1)}$, where $\gamma > 0$ is some constant not depending on N.

We can now state our result.

Theorem 6.3.7. *Let $(-\Delta_N, \mathcal{D}_N^\alpha(P, L))$ be a self-adjoint realisation of the N-particle Laplacian as introduced in Chapter 5. Assume that the N-particle map L_{vert} is negative definite as well as $\alpha(y) \geq \alpha > 0$ for all $y \in [0, 1]$. Furthermore, assume that the sequence of (normalised) ground states is (in the thermodynamic limit) bounded from above, i.e. there exists a constant $c > 0$ such that*

$$|\left(\Psi_N^0\right)_{e_1 \ldots e_N}| \leq \frac{c}{\sqrt{l_{e_1}} \cdots \sqrt{l_{e_N}}}, \quad \forall N, \ \forall e_1, ..., e_N \in \mathcal{E}. \tag{6.3.12}$$

Then there exists a constant $\gamma(\rho) > 0$ such that

$$\gamma(\rho) \leq e_0^\infty(\rho). \tag{6.3.13}$$

Proof. For simplicity, we will restrict ourselves to the case of an interval of length l and, accordingly, the N-particle configuration space is $D_N = (0,l)^N$. Note that, due to the min-max principle (Theorem 2.1.27), it is enough to consider the case $P_{vert} = 0$, $L_{vert} = 0$ and constant α.
We will prove the theorem by contradiction and assume that $e_0^\infty(\rho) = 0$. On the rescaled domain $D_N^* = (0,1)^N$, we choose a symmetric test function $\tau_N \in C^\infty(D_N^*)$ such that $0 \leq \tau_N \leq 1$ and $\tau_N = 1$ on a domain $\Omega_N^* \Subset D_N^*$. Note that we denote the corresponding domain contained in D_N by Ω_N. Indeed, Ω_N^* is supposed to be a smaller hypercube such that $\operatorname{dist}(\partial D_N^*, \partial\Omega_N^*) = \delta_N$. By construction,

$$\mu\left(D_N^* \backslash \Omega_N^*\right) = 1^N - (1-2\delta_N)^N \to 0, \tag{6.3.14}$$

if $4^N\delta_N \to 0$ and we have

$$\|\Psi_N^0\|^2_{L^2(D_N\backslash\Omega_N)} \leq c^2 \cdot \mu\left(D_N^* \backslash \Omega_N^*\right) \to 0. \tag{6.3.15}$$

Furthermore,

$$\begin{aligned}\frac{\|\nabla\left(\Psi_N^0 - (\tau_N\Psi_N^0)\right)\|^2_{L^2(D_N)}}{2N} &\leq \frac{\|\nabla\Psi_N^0\|^2_{L^2(D_N)}}{N} + \frac{\|\left(\nabla\tau_N\right)\Psi_N^0\|^2_{L^2(D_N)}}{N} \\ &\leq \frac{\|\nabla\Psi_N^0\|^2_{L^2(D_N)}}{N} + \sup_j|\partial_j\tau_N|^2 \cdot \|\Psi_N^0\|^2_{L^2(D_N\backslash\Omega_N)},\end{aligned} \tag{6.3.16}$$

where $\sup_j|\partial_j\tau_N|^2$ shall denote the supremum on the rescaled domain D_N^*. Note that, since we assume $e_0^\infty(\rho) = 0$, the first term on the right-hand side of (6.3.16) vanishes in the limit $N \to \infty$. Using Lemma 6.3.6 as stated above, we can choose the test function τ_N such that

$$\sup_j|\partial_j\tau_N| \leq \frac{c_N}{\delta_N}, \tag{6.3.17}$$

with $c_N = \left(\frac{\sqrt{\pi}}{4}\right)^N \frac{\gamma}{\Gamma(\frac{N}{2}+1)}$ and $\gamma > 0$ is some constant not depending on N. Therefore also the second term in (6.3.16) vanishes in the limit $N \to \infty$. Now, for the state $\tilde{\Psi}_N = \frac{\tau_N\Psi_N^0}{\|\tau_N\Psi_N^0\|_{L^2(D_N)}}$ we obtain, using that $\|\tau_N\Psi_N^0\|_{L^2(D_N)} \geq \lambda$ for all $N > N_0$

with $1 > \lambda > 0$ some constant,

$$\begin{aligned} \frac{Q_B^{(N)}(\tilde{\Psi}_N)}{N} &\leq \frac{2}{\lambda^2}\left(\frac{\|\nabla\left(\Psi_N^0 - \tau_N\Psi_N^0\right)\|^2_{L^2(D_N)}}{N} + \frac{Q_B^{(N)}(\Psi_N^0)}{N}\right) \\ &\leq \frac{2}{\lambda^2}\left(\kappa_N + e_0^\infty(\rho)\right) \end{aligned} \tag{6.3.18}$$

for all $N > N_0$ and $\kappa_N \to 0$ as $N \to \infty$. Since $\tilde{\Psi}_N$ fulfils Dirichlet boundary conditions, $\tilde{\Psi}_N$ lies in the domain of the quadratic form considered in Proposition 6.3.5. Therefore, the left-hand side of (6.3.18) is bounded from below by the ground state energy density (6.3.10) which is larger than zero. On the other hand, by assumption we have $e_0^\infty(\rho) = 0$ and hence we conclude that the right-hand side of (6.3.18) converges to zero which yields a contradiction. □

Theorem 6.3.7 indicates, as described above, that repulsive contact interactions act against Bose-Einstein condensation. Furthermore, since the implementation of purely repulsive singular interactions does not increase the ground state energy density as established in Corollary 6.3.4, they can be considered as only a 'small perturbation'.

6.3.2 Fermi-Bose mapping on general quantum graphs

In this subsection, we generalise the Fermi-Bose mapping introduced by M. Girardeau [Gir60, VIY05] to general quantum graphs. This will then allow us to establish results concerning Bose-Einstein condensation in a system of particles interacting via repulsive hard-core interactions. Note that we use the results established in part A of the appendix. To construct the Fermi-Bose mapping, we define a map

$$\sigma : H_F^1(\Gamma_N) \to H_{0,B}^1(\Gamma_N^*) \tag{6.3.19}$$

as follows: Let $\Phi_F \in H_F^1(\Gamma_N)$ be any state with components $(\Phi_F)_{e_1\ldots e_N} = \varphi^F_{e_1\ldots e_N}$. For a given component $\varphi^F_{e_1\ldots e_N}$, we form a set that contains $\varphi^F_{e_1\ldots e_N}$ as well as all other components whose edge indices are a permutation of $e_1\ldots e_N$ and choose one representative of this set, denoted as $\varphi^F_{\tilde{e}_1\ldots\tilde{e}_N}$. Now, for each component $\varphi^F_{\tilde{e}_1\ldots\tilde{e}_N}$, $n(j)$ shall denote the number of particles on edge $j \in \mathcal{E}$. We then define a subdo-

main $\tilde{\Omega} \subset D_{\tilde{e}_1 \dots \tilde{e}_N}$ such that all $x \in \tilde{\Omega}$ fulfil

$$x_j^{\zeta(1)} < \dots < x_j^{\zeta(n_j)}, \quad \forall j \in \{1, \dots, E\}, \tag{6.3.20}$$

where the map ζ associates the particle label to the coordinate. Based on this, we can define a bosonic component $\varphi^B_{\tilde{e}_1 \dots \tilde{e}_N}$ on $D_{\tilde{e}_1 \dots \tilde{e}_N}$. To this end, we set

$$\varphi^B_{\tilde{e}_1 \dots \tilde{e}_N}(x) := \varphi^F_{\tilde{e}_1 \dots \tilde{e}_N}(x) \tag{6.3.21}$$

for $x \in \tilde{\Omega}$ and, by symmetric continuation, we extend $\varphi^B_{\tilde{e}_1 \dots \tilde{e}_N}$ to all of $D_{\tilde{e}_1 \dots \tilde{e}_N}$. Finally, by permuting the edge indices of $\varphi^B_{\tilde{e}_1 \dots \tilde{e}_N}$ and setting

$$\varphi^B_{\pi(\tilde{e}_1 \dots \tilde{e}_N)} := \varphi^B_{\tilde{e}_1 \dots \tilde{e}_N}, \tag{6.3.22}$$

we obtain all other components, defining a symmetric function $\Phi_B \in H^1_{0,B}(\Gamma_N^*)$. Based on the map σ, we can introduce a diagonal matrix $\Sigma(\boldsymbol{y})$ whose entries $\Sigma_{ii}(\boldsymbol{y}) \in \{1, -1\}$ account for the possible sign changes. More explicitly, if $\Phi \in \mathcal{D}_{Q_F^{(N)}}$ is a function with boundary values Φ_{bv}, the function $\Phi^\sigma := \sigma(\Phi)$ has boundary values

$$\Phi^\sigma_{bv}(\boldsymbol{y}) = \Sigma(\boldsymbol{y}) \Phi_{bv}(\boldsymbol{y}). \tag{6.3.23}$$

Furthermore, we set

$$\begin{aligned} P_\sigma(\boldsymbol{y}) &= \Sigma(\boldsymbol{y}) P(\boldsymbol{y}) \Sigma(\boldsymbol{y}), \\ L_\sigma(\boldsymbol{y}) &= \Sigma(\boldsymbol{y}) L(\boldsymbol{y}) \Sigma(\boldsymbol{y}). \end{aligned} \tag{6.3.24}$$

Note that we associate, in the same way as in (A.0.8) and (A.0.7), bounded and self-adjoint operators Λ^σ and Π^σ with $L_\sigma(\boldsymbol{y})$ and $P_\sigma(\boldsymbol{y})$, respectively.

Theorem 6.3.8. *Let $Q_F^{(N)}[\cdot]$ be a quadratic form on the (fermionic) Hilbert Space $\mathcal{H}_N^F$ with corresponding maps P and L. Then there exists a mapping*

$$\sigma : H^1_F(\Gamma_N) \to H^1_{0,B}(\Gamma_N^*) \tag{6.3.25}$$

such that the form $Q_B^{(N)}[\cdot]$ with maps P_σ and L_σ, defined on the dissected Hilbert space $\mathcal{H}_N^{B*}$, is symmetric, closed and semi-bounded. Furthermore, the spectrum of the corresponding self-adjoint operators is discrete and identical.

Proof. We note that the map σ applied to $\mathcal{D}_{Q_F^{(N)}}$ yields the domain

$$\mathcal{D}_\sigma = \{\Phi^\sigma \in H^1_{0,B}(\Gamma_N^*);\ P_\sigma(\boldsymbol{y})\Phi^\sigma_{bv}(\boldsymbol{y}) = 0 \text{ for a.e. } \boldsymbol{y} \in [0,1]^{N-1}\}. \tag{6.3.26}$$

Furthermore, we have

$$\begin{aligned} Q_F^{(N)}[\Phi] &= \sum_{e_1\dots e_N} \int_0^{l_{e_1}} \dots \int_0^{l_{e_N}} |\nabla \varphi_{e_1\dots e_N}|^2 \ \mathrm{d}x^1_{e_1}\dots \mathrm{d}x^N_{e_N} \\ &\quad - N \int_{[0,1]^{N-1}} \langle \Phi_{bv}, L(\boldsymbol{y})\Phi_{bv}\rangle_{\mathbb{C}^{2E^N}} \ \mathrm{d}\boldsymbol{y} \\ &= \sum_{e_1\dots e_N} \int_0^{l_{e_1}} \dots \int_0^{l_{e_N}} |\nabla \varphi^\sigma_{e_1\dots e_N}|^2 \ \mathrm{d}x^1_{e_1}\dots \mathrm{d}x^N_{e_N} \\ &\quad - N \int_{[0,1]^{N-1}} \langle \Phi^\sigma_{bv}, L_\sigma(\boldsymbol{y})\Phi^\sigma_{bv}\rangle_{\mathbb{C}^{2E^N}} \ \mathrm{d}\boldsymbol{y} \\ &= Q_B^{(N)}[\Phi^\sigma]. \end{aligned} \tag{6.3.27}$$

Since P_σ is bounded and L_σ is self-adjoint, we can reformulate the proof of Theorem A.0.16 to show that $Q_B^{(N)}[\cdot]$ with domain $\mathcal{D}_\sigma$ is a densely defined, closed, symmetric and semi-bounded form. Furthermore, taking into account that $L_\sigma(\boldsymbol{y}) = L(\boldsymbol{y})$ whenever $L(\boldsymbol{y})$ is a diagonal matrix and applying the min-max principle (Theorem 2.1.27), we readily see that the inequality

$$\mu_n^R \leq \mu_n \leq \mu_n^D \tag{6.3.28}$$

holds for all $n \in \mathbb{N}$ (see also proof of Theorem 4.3.3). Here the index R refers to the form with maps $P_\sigma = 0$ and $L_\sigma = \mathbb{1}\|\Lambda\|_{op}$, whereas the index D refers to the form with maps $P_\sigma = \mathbb{1}$ and $L_\sigma = 0$. Since the spectrum of the two corresponding fermionic operators is known to be discrete (see Lemma A.0.21), we conclude that $\mu_n^R, \mu_n^D \to \infty$. Hence, employing Theorem XIII.64 of [RS78], we see that the self-adjoint operator corresponding to the form $Q_B^{(N)}[\cdot]$ has purely discrete spectrum since $\mu_n \to \infty$. Finally, due to (6.3.27) we see that the spectrum of this operator is identical to the spectrum of the corresponding fermionic operator. □

As a consequence of Theorem 6.3.8, we can associate with any fermionic operator $(-\Delta_N, \mathcal{D}_F^N(P, L))$ the bosonic operator $(-\Delta_N, \mathcal{D}_B^N(P_\sigma, L_\sigma))$ whose spectrum is identical. Also, since the map σ is invertible, we can assign to any bosonic

operator with hard-core interactions, $(-\Delta_N, \mathcal{D}_N^\infty(P,L))$, a fermionic operator with identical spectrum, i.e. $(-\Delta_N, \mathcal{D}_F^N(P_\sigma, L_\sigma))$.

6.3.3 Bose-Einstein condensation in a gas of bosons interacting via repulsive hard-core interactions

In this final subsection, we use the Fermi-Bose mapping established in Theorem 6.3.8 in order to discuss Bose-Einstein condensation for a system of interacting particles on general quantum graphs. In particular, the particles shall be interacting via repulsive hard-core interactions.

Remark 6.3.9. Condensation in a Bose gas on an interval, with bosons interacting via repulsive hard-core interactions, was rigorously investigated in [Sch63, Len64, Len66] showing that no condensation in the sense of Definition 6.1.10 is present at zero temperature.

In the following, we will work in the grand-canonical ensemble. Hence, the free energy density of a system at finite volume is given by

$$f_{\mathcal{L}}(\beta,\mu) = -\frac{1}{\beta\mathcal{L}} \ln Z_{\mathcal{L}}(\beta,\mu), \tag{6.3.29}$$

where

$$Z_{\mathcal{L}}(\beta,\mu) = \sum_{N=0}^{\infty} z^N Z_N^{\mathcal{L}}(\beta) \tag{6.3.30}$$

is the partition function and $Z_N^{\mathcal{L}}(\beta)$ (see (6.1.32)) the partition function in the canonical ensemble [Sch06]. Note that $z = e^{\beta\mu}$ is the fugacity. In a first step, we consider fermionic operators of the form $(-\Delta_N, \mathcal{D}_F^N(P,L))$. We will show that the free energy densities of such systems are identical in the thermodynamic limit. As a reference model, consider the realisation $(-\Delta_N, \mathcal{D}_F^N(P,L))$ with $P = \mathbb{1}_{2E^N}$ and $L = 0$. This realisation corresponds to a free gas of fermions with Dirichlet boundary conditions in the vertices. Its free energy density (6.3.29) can be calculated using basic techniques of statistical mechanics [Sch06], i.e.

$$f_{F,D}(\beta,\mu) = -\lim_{\mathcal{L}\to\infty} \frac{1}{\beta\mathcal{L}} \sum_{n=0}^{\infty} \ln\left(1 + e^{-\beta(k_n^2-\mu)}\right), \tag{6.3.31}$$

where $\{k_n^2\}_{n\in\mathbb{N}_0}$ are the eigenvalues of the one-particle realisation $(-\Delta_1, \mathcal{D}(P,L))$

with $P = \mathbb{1}_{2E}$ and $L = 0$.

Remark 6.3.10. Note that the free energy density $f_{F,D}(\beta,\mu)$ is infinitely differentiable, i.e. $f_{F,D}(\beta,\mu) \in C^\infty((0,\infty)\times\mathbb{R})$. Indeed, a direct calculation yields

$$f_{F,D}(\beta,\mu) = -\frac{1}{\pi\beta}\int_0^\infty \ln\left(1+e^{-\beta(k^2-\mu)}\right)\,\mathrm{d}k \tag{6.3.32}$$

from which the statement follows by standard arguments.

Proposition 6.3.11. *For each $N\in\mathbb{N}$, let $(-\Delta_N, \mathcal{D}_F^N(P_N,L_N))$ be a self-adjoint realisation of the N-particle Laplacian $-\Delta_N$ as introduced above. Assume that there exists $M\in\mathbb{R}^+$ such that*

$$\|\Lambda_N\|_{op} \leq M, \quad \forall N. \tag{6.3.33}$$

Then, denoting the corresponding free energy density by $f_F(\beta,\mu)$, we have

$$f_F(\beta,\mu) = f_{F,D}(\beta,\mu), \quad \forall\beta\in(0,\infty),\ \forall\mu\in\mathbb{R}. \tag{6.3.34}$$

Proof. As a first step, we use the min-max principle (see Theorem 2.1.27) to conclude that the inequality

$$f_{F,R}^{\mathcal{L}}(\beta,\mu) \leq f_F^{\mathcal{L}}(\beta,\mu) \leq f_{F,D}^{\mathcal{L}}(\beta,\mu) \tag{6.3.35}$$

holds. Here R refers to the realisation with maps $P_N = 0$ and $L_N = M\mathbb{1}_{2E^N}$. Furthermore, since $f_{F,R}^{\mathcal{L}}(\beta,\mu)$ is the free energy density of a free gas whose corresponding one-particle Laplacian is described by the one-particle maps $P=0$ and $L = M\mathbb{1}_{2E}$, we have

$$f_{F,R}^{\mathcal{L}}(\beta,\mu) = -\frac{1}{\beta\mathcal{L}}\sum_{k_n^2\leq 0}\ln\left(1+e^{-\beta(k_n^2-\mu)}\right) - \frac{1}{\beta\mathcal{L}}\sum_{k_n^2>0}\ln\left(1+e^{-\beta(k_n^2-\mu)}\right). \tag{6.3.36}$$

Here we have split up the sum into two parts. Since the number of negative eigenvalues is bounded (see Lemma 6.2.5), the first term does not contribute in the thermodynamic limit. Furthermore, the second term in (6.3.36) can be evaluated using the trace formula as demonstrated in the proof of Theorem 6.2.7. In

particular, we arrive at

$$\lim_{\mathcal{L}\to\infty} f_{F,R}^{\mathcal{L}}(\beta,\mu) = f_{F,D}(\beta,\mu) \tag{6.3.37}$$

which completes the proof. □

Remark 6.3.12. Note that condition (6.3.33) can be understood as a stability condition for the interaction potential as commonly required in statistical mechanics [Rue68]. More precisely, for a self-adjoint N-particle Hamiltonian $\hat{H}_N$ one requires the lower bound to be $-NB$ where $B \geq 0$ is some constant (see (A.0.12) and (A.0.13)).

Finally, we can state the main results of this section.

Theorem 6.3.13. *For each $N \in \mathbb{N}$, let $(-\Delta_N, \mathcal{D}_N^\infty(P_N, L_N))$ be a self-adjoint realisation of the bosonic N-particle Laplacian as described above. Assume that there exists $M \in \mathbb{R}^+$ such that*

$$\|\Lambda_N\|_{op} \leq M, \quad \forall N. \tag{6.3.38}$$

Then, denoting the corresponding free energy density in the thermodynamic limit by $f_B(\beta,\mu)$, we have

$$f_B(\beta,\mu) = f_{F,D}(\beta,\mu), \quad \forall \beta \in (0,\infty),\ \forall \mu \in \mathbb{R}. \tag{6.3.39}$$

In particular, $f_B(\beta,\mu)$ is infinitely differentiable, i.e. $f_B(\beta,\mu) \in C^\infty((0,\infty)\times\mathbb{R})$.

Proof. Theorem 6.3.8 implies that the spectrum of $(-\Delta_N, \mathcal{D}_N^\infty(P,L))$ is identical to the spectrum of $(-\Delta_N, \mathcal{D}_F^N(P_\sigma, L_\sigma))$. Hence we can apply Proposition 6.3.11 and the Theorem follows. □

Theorem 6.3.13 shows that no phase transition in the free energy density is present in a system of interacting bosons on a general quantum graph, given the particles interact via repulsive hard-core interactions. Most importantly, this holds *independently* of the singular interactions in the vertices.

Remark 6.3.14. Note that Theorem 6.3.13 can be regarded as a quantum statistical version of a famous theorem by van Hove, see Theorem 5.6.7 of [Rue68]. In this theorem, a classical continuous one-dimensional system of particles with hard-cores

and short-range two-particle interactions is considered. More precisely, the (continuous) two-particle potential $V(x,y)$ is such that $V(x,y) = \infty$ for $0 < |x-y| < R$ and $V = 0$ for $|x-y| \geq R_0$. As a result, it is proved that no phase transitions occur in such a system, i.e. the free energy density is analytical in z (see also [Gal99, GGR68]).

Theorem 6.3.13 also shows that Bose-Einstein condensation, present for systems characterised in Theorem 6.2.7, is destroyed as soon as repulsive hard-core interactions are switched on. To illustrate this, we consider a simple quantum graph, i.e. an interval $(0,L)$ with the one-particle Laplacian $-\Delta_1$ defined on

$$\mathcal{D}(-\Delta_1) = \{\varphi \in H^2(0,L) |\ \varphi'(0) = \kappa\varphi(0) \text{ and } \varphi'(L) = \kappa\varphi(L)\}, \tag{6.3.40}$$

where $\kappa > 0$ is some parameter. Note that the operator $(-\Delta_1, \mathcal{D}(-\Delta_1))$ has exactly one negative eigenvalue [BP85] and hence, due to the gap in the one-particle spectrum, condensation occurs in the non-interacting many-particle system (see Theorem 6.2.7). Most importantly, however, there exists a phase transition in the free energy density, i.e. the function $f(\rho) = \lim_{L\to\infty} f(\beta, \mu_L(\rho))$ is not differentiable at some critical density $\rho = \rho_{crit}$ (see (6.2.25)). Note that, in order to derive $f(\rho)$, one has to choose a volume-dependent sequence of chemical potentials as mentioned in Remark 6.1.3, see [LW79]. However, as a consequence of Theorem 6.3.13, we see that this phase transition is destroyed by switching on repulsive hard-core interactions.

Remark 6.3.15. Note that the domain (6.3.40) can be expressed in the form $\mathcal{D}_1(P,L)$ by setting $P_\kappa = 0$ and $L_\kappa = \mathrm{diag}\,(-\kappa,\kappa)$. Consequently, we can describe (see Remark A.0.20) the (non-interacting) many-particle system of this model by a self-adjoint realisation $(-\Delta_N, \mathcal{D}_B^N(P_\kappa^N, L_\kappa^N))$ with N-particle maps

$$P_\kappa^N = \bigoplus P_\kappa \quad \text{and} \quad L_\kappa^N = \bigoplus L_\kappa. \tag{6.3.41}$$

Repulsive hard-core interactions are then implemented by considering the self-adjoint realisation $(-\Delta_N, \mathcal{D}_N^\infty(P_\kappa^N, L_\kappa^N))$.

7. SUMMARY AND OUTLOOK

In this thesis, we have developed models of interacting many-particle systems on general compact quantum graphs. In a first step, we have introduced singular two-particle interactions localised at the vertices of the graph. In a second step, we have introduced additional contact interactions between the particles which are present whenever (at least) two particles are situated at the same position. This means, in particular, that contact interactions are present also along the edges. Finally, we have discussed Bose-Einstein condensation for many-particle systems on general quantum graphs. We have identified non-interacting many-particle systems which display condensation and others which do not, depending on the nature of the interactions with external potentials in the vertices. As a final result, we have shown that no Bose-Einstein condensation is present (in the sense of phase transitions) in a system where the particles are interacting via repulsive hard-core interactions.

Based on the results obtained, there are various possibilities for future research. Regarding many-particle quantum chaos, it would be of great interest to establish a trace formula analogous to (1.0.8) for a two-particle systems interacting via singular interactions and (or) contact interactions. Unfortunately, compared to the one-particle case, there is no secular equation as (3.2.5) for the two-particle problem. To construct such an equation, one could regard the system of two-particles (e.g. on an interval) as a two-dimensional billiard and employ semiclassical methods as described in [DS92]. However, the resulting secular equation would only be valid in a semiclassical limit. Also, it would be interesting to calculate numerically the nearest-neighbour level spacing distribution (1.0.5) for the developed models in order to establish a connection with the Bohigas-Gianonni-Schmit conjecture [BGS84]. This would, in particular, be interesting with respect to the results mentioned in the introduction of Chapter 5. Regarding the theory of phase transitions, there exists a very interesting connection between quantum graphs and lattice systems. Lattice systems have a long history in statistical mechanics since they are

models for which rigorous results, e.g. regarding phase transitions, can be obtained [Rue68, GMS67]. In a d-dimensional lattice $\Lambda \subset \mathbb{Z}^d$, particles are situated at the lattice points whereas particles on a graph are situated on the edges. One could therefore relate quantum graphs to lattices in two different ways. One could either associate the edges of a graph with the lattice points or, alternatively, consider the vertices of a graph as the lattice points. In the latter case, one would introduce potentials along the edges of the graph that confine the particles to the vicinity of the vertices. In general, using the tools available for quantum graphs, it would be very interesting to derive rigorous results and compare them to results established for lattice systems.

APPENDIX

A. SINGULAR INTERACTIONS IN MANY-PARTICLE SYSTEMS ON GENERAL COMPACT QUANTUM GRAPHS

In this part of the appendix, we will generalise the methods of Chapter 4 and 5 in order to describe a system of N fermions or bosons on a general compact graph interacting via singular interactions. Although we have already discussed the more general case of combined singular and contact interactions for a system of N bosons, it is convenient to formulate the following results for both types of particles. Note that the main motivation of this appendix is to provide the necessary results for the discussion of Bose-Einstein condensation in the last chapter of the thesis. The bosonic/fermionic N-particle Hilbert space is given by

$$\begin{aligned} \mathcal{H}_N^{B/F} &= \Pi_{B/F}(\underbrace{\mathcal{H}_1 \otimes ... \otimes \mathcal{H}_1}_{N-\text{times}}), \\ &= \Pi_{B/F}\mathcal{H}_N, \end{aligned} \tag{A.0.1}$$

where $\Pi_{B/F} : \mathcal{H}_N \to \mathcal{H}_N^{B/F}$ is the projector onto the subspace of (anti-)symmetric functions. On a graph, the N-particle Hilbert space $\mathcal{H}_N^{B/F}$ can be represented as

$$L^2_{B/F}(\Gamma_N) = \Pi_{B/F}L^2(\Gamma_N), \tag{A.0.2}$$

where

$$L^2(\Gamma_N) = \bigoplus_{e_1...e_N} L^2(D_{e_1...e_N}) \tag{A.0.3}$$

and $D_{e_1...e_N} = (0, l_{e_1}) \times ... \times (0, l_{e_N})$. Given a function $\Psi \in \mathcal{H}_N$, the projection operators act via

$$(\Pi_{B/F}\Psi)_{e_1...e_N} = \frac{1}{N!}\sum_{\pi \in S_N} (-1)^{\operatorname{sgn}\pi}\psi_{\pi(e_1)...\pi(e_N)}(x^{\pi(1)}_{\pi(e_1)}...x^{\pi(N)}_{\pi(e_N)}), \tag{A.0.4}$$

where, for fermions, $(-1)^{\operatorname{sgn}\pi} = 1$ for an even permutation and $(-1)^{\operatorname{sgn}\pi} = -1$ for an odd permutation. For bosons we set $(-1)^{\operatorname{sgn}\pi} = 1$ for all permutations. Note that Sobolev spaces are introduced in the same manner. In order to characterise self-adjoint realisations of the N-particle Laplacian that incorporate singular interactions in the vertices, we will construct suitable quadratic forms. However, before we have to introduce some notation. As a first step, we define the vector

$$\Psi_{bv}(\boldsymbol{y}) = \begin{pmatrix} \sqrt{l_{e_2}\dots l_{e_N}}\psi_{e_1\dots e_N}(0, l_{e_2}y_1, \dots, l_{e_N}y_{N-1}) \\ \sqrt{l_{e_2}\dots l_{e_N}}\psi_{e_1\dots e_N}(l_{e_1}, l_{e_2}y_1, \dots, l_{e_N}y_{N-1}) \end{pmatrix}, \tag{A.0.5}$$

for $\Psi \in H^1(\Gamma_N)$ and if $\Psi \in H^2(\Gamma_N)$, we define in addition

$$\Psi'_{bv}(\boldsymbol{y}) = \begin{pmatrix} \sqrt{l_{e_2}\dots l_{e_N}}\psi_{e_1\dots e_N, x^1_{e_1}}(0, l_{e_2}y_1, \dots, l_{e_N}y_{N-1}) \\ -\sqrt{l_{e_2}\dots l_{e_N}}\psi_{e_1\dots e_N, x^1_{e_1}}(l_{e_1}, l_{e_2}y_1, \dots, l_{e_N}y_{N-1}) \end{pmatrix}, \tag{A.0.6}$$

for $\boldsymbol{y} \in [0,1]^{N-1}$. As a next step, we introduce two bounded and measurable maps $P, L : [0,1]^{N-1} \to \mathrm{M}(2E^N, \mathbb{C})$ such that

1. P is an orthogonal projector,

2. L is a self-adjoint endomorphism on $\ker P$,

for a.e. $\boldsymbol{y} \in [0,1]^{N-1}$. Moreover, we set $Q(\boldsymbol{y}) = \mathbb{1}_{2E^N} - P(\boldsymbol{y})$ and we will associate two bounded and self-adjoint multiplication operators with the maps P and L on the Hilbert space $L^2(0,1)^{N-1} \otimes \mathbb{C}^{2E^N}$, i.e.

$$\Pi : L^2(0,1)^{N-1} \otimes \mathbb{C}^{2E^N} \to L^2(0,1)^{N-1} \otimes \mathbb{C}^{2E^N}, \quad (\Pi\Psi_{bv})(\boldsymbol{y}) = P(\boldsymbol{y})\Psi_{bv}(\boldsymbol{y}), \tag{A.0.7}$$

and

$$\Lambda : L^2(0,1)^{N-1} \otimes \mathbb{C}^{2E^N} \to L^2(0,1)^{N-1} \otimes \mathbb{C}^{2E^N}, \quad (\Lambda\Psi_{bv})(\boldsymbol{y}) = L(\boldsymbol{y})\Psi_{bv}(\boldsymbol{y}). \tag{A.0.8}$$

Theorem A.0.16. *Let the maps $P, L : [0,1]^{N-1} \to \mathrm{M}(2E^N, \mathbb{C})$ be bounded and*

measurable. Then the quadratic form

$$\begin{aligned} Q^{(N)}_{B/F}[\Psi] = N \sum_{e_1 \dots e_N} \int_0^{l_{e_1}} \dots \int_0^{l_{e_N}} |\psi_{e_1 \dots e_N, x^1_{e_1}}(x^1_{e_1}, \dots, x^N_{e_N})|^2 \, \mathrm{d}x^1_{e_1} \dots \mathrm{d}x^N_{e_N} \\ - N \int_{[0,1]^{N-1}} \langle \Psi_{bv}, L(\boldsymbol{y}) \Psi_{bv} \rangle_{\mathbb{C}^{2E^N}} \, \mathrm{d}\boldsymbol{y} \end{aligned} \tag{A.0.9}$$

defined on the domain

$$\mathcal{D}_{Q^{(N)}_{B/F}} = \{\Psi \in H^1_{B/F}(\Gamma_N); \; P(\boldsymbol{y})\Psi_{bv}(\boldsymbol{y}) = 0 \text{ for a.e. } \boldsymbol{y} \in [0,1]^{N-1}\}, \tag{A.0.10}$$

is closed and semi-bounded.

Proof. Since $\Pi_{B/F} C_0^\infty(\Gamma_N) \subset \mathcal{D}_{Q^{(N)}_{B/F}}$ is dense in $L^2_{B/F}(\Gamma_N)$, the form is densely defined. Also, from (5.3.13) we can readily see that the form is symmetric. Furthermore, as a consequence of Lemma 8 in [Kuc04] (which is a variation of Theorem 2.2.13), we have the estimate

$$\|\Psi_{bv}\|^2_{L^2(0,1)^{N-1} \otimes \mathbb{C}^{2E^N}} \leq 2 \left(\delta \|\Psi_{x^1_{e_1}}\|^2_{L^2(\Gamma_N)} + \frac{2}{\delta} \|\Psi\|^2_{L^2(\Gamma_N)} \right) \tag{A.0.11}$$

which holds for all $\delta \leq 1$. Setting

$$A = N \left| \int_{[0,1]^{N-1}} \langle \Psi_{bv}, L(\boldsymbol{y}) \Psi_{bv} \rangle_{\mathbb{C}^{2E^N}} \, \mathrm{d}\boldsymbol{y} \right|, \tag{A.0.12}$$

we arrive at

$$A \leq K \left(\delta \|\nabla \Psi\|^2_{L^2(\Gamma_N)} + \frac{2}{\delta} \|\Psi\|^2_{L^2(\Gamma_N)} \right), \tag{A.0.13}$$

with $K \in \mathbb{R}_+$ some constant. Now, choosing δ small enough, we see that there exists $\lambda \in \mathbb{R}_+$ such that

$$Q^{(N)}_{B/F}[\Psi] \geq -\lambda \|\Psi\|^2_{L^2(\Gamma_N)}, \quad \forall \Psi \in \mathcal{D}_{Q^{(N)}_{B/F}}. \tag{A.0.14}$$

Hence the form is semi-bounded. Again using (A.0.13) we see that the form norm

$$\|\cdot\|^2_{Q^{(N)}_{B/F}} = Q^{(N)}_{B/F}[\cdot] + (1+\lambda)\|\cdot\|^2_{L^2(\Gamma_N)} \tag{A.0.15}$$

is equivalent to the H^1-norm. Now, let $\{\Psi_n\}_{n \in \mathbb{N}} \in \mathcal{D}_{Q^{(N)}_{B/F}}$ be a Cauchy-sequence

with respect to the form norm. By the completeness of H^1, there exists a function $\Psi \in H^1_{B/F}(\Gamma_N)$ such that

$$\|\Psi - \Psi_n\|_{H^1_{B/F}(\Gamma_N)} \leq \epsilon_1, \quad \forall n \geq n_0. \tag{A.0.16}$$

Finally, since

$$\begin{aligned} \|P\Psi_{bv}\|_{L^2(0,1)^{N-1}\otimes\mathbb{C}^{2E^N}} &\leq \|P\|_{op}\|\Psi_{bv} - \Psi_{bv;n}\|_{L^2(0,1)^{N-1}\otimes\mathbb{C}^{2E^N}}, \\ &\leq \epsilon_2 \end{aligned} \tag{A.0.17}$$

for an arbitrarily small $\epsilon_2 > 0$, we conclude that $\Psi \in \mathcal{D}_{Q^{(N)}_{B/F}}$. □

Remark A.0.17. According to the representation theorem of quadratic forms [Kat66], we conclude that each form $Q^{(N)}_{B/F}$ corresponds to a unique self-adjoint operator which will be denoted by $(-\Delta_N, \mathcal{D}^N_{B/F}(P, L))$.

Definition A.0.18. Let $Q^{(N)}_{B/F}$ be a quadratic form as described in Theorem A.0.16. We call the form *regular* iff the corresponding self-adjoint operator has domain $\mathcal{D}^N_{B/F}(P, L) \subset H^2_{B/F}(\Gamma_N)$.

For regular forms, it is then possible to give an explicit characterisation of the domain $\mathcal{D}^N_{B/F}(P, L)$.

Theorem A.0.19. *Let $Q^{(N)}_{B/F}$ be a regular quadratic form as characterised in Theorem A.0.16. Then the corresponding self-adjoint operator is the N-particle Laplacian $-\Delta_N$ with domain*

$$\begin{aligned} \mathcal{D}^N_{B/F}(P, L) = \{\Psi \in H^2_{B/F}(\Gamma_N); P(\boldsymbol{y})\Psi_{bv}(\boldsymbol{y}) = 0 \text{ and} \\ Q(\boldsymbol{y})\Psi'_{bv}(\boldsymbol{y}) + L(\boldsymbol{y})Q(\boldsymbol{y})\Psi_{bv}(\boldsymbol{y}) = 0 \text{ for a.e. } \boldsymbol{y} \in [0,1]^{N-1}\}, \end{aligned} \tag{A.0.18}$$

with $Q(\boldsymbol{y}) = \mathbb{1}_{2E^N} - P(\boldsymbol{y})$.

Remark A.0.20. Let $(-\Delta_1, \mathcal{D}_1(P, L))$ be a self-adjoint realisation of the one-particle Laplacian. With respect to (A.0.5) and (A.0.6), define the N-particle maps

$$P_N = \bigoplus P \quad \text{and} \quad L_N = \bigoplus L, \tag{A.0.19}$$

ordered according to the second edge index e_2 as in (4.2.11). Then the self-adjoint operator $(-\Delta_N, \mathcal{D}^N_{B/F}(P, L))$ corresponds to a system of non-interacting particles,

i.e. it equals the closure of the operator $(-\Delta_N, \mathcal{D}_N(-\Delta_1))$ as described in Lemma 6.2.2. See also Proposition 4.1.19.

Finally, we want to discuss spectral properties of $(-\Delta_N, \mathcal{D}^N_{B/F}(P,L))$. Since we are dealing with a self-adjoint realisation of the N-dimensional Laplacian on a bounded domain, we expect the spectrum to be purely discrete. Furthermore, we expect Weyl asymptotics for the eigenvalue count.

Lemma A.0.21. *Let $(-\Delta_N, \mathcal{D}^N_{B/F}(P,L))$ be a self-adjoint operator associated with the (not necessarily regular) form $Q^{(N)}_{B/F}$ as characterised in Theorem A.0.16. Then its spectrum is purely discrete and the counting function*

$$N(\lambda) = \#\{n; \lambda_n \leq \lambda\}, \tag{A.0.20}$$

where the eigenvalues are counted according to their multiplicities, obeys the Weyl law

$$N(\lambda) \sim \frac{\mathcal{L}^N}{N!(4\pi)^{\frac{N}{2}}\Gamma(1+\frac{N}{2})}\lambda^{\frac{N}{2}}, \quad \lambda \to \infty. \tag{A.0.21}$$

B. A REGULARITY THEOREM

In this part of the appendix, we prove Theorem 4.1.16. Given a quadratic form as described in Theorem 4.1.7 or 4.1.21, it is our goal to establish regularity in the sense of Definition 4.1.10. To achieve this, we use an effective cut-off of the corners in combination with the standard *difference quotient technique* as described in Chapter 2. Also, we use some obvious properties of difference quotients, i.e. the 'product rule'

$$D_n^{\pm h}(\phi\,\psi)(x) = (D_n^{\pm h}\phi)(x)\,\psi(x) + \phi(x \pm he_n)\,D_n^{\pm h}\psi(x)\ , \tag{B.0.1}$$

where e_n is the unit vector in the direction of x_n and an 'integration by parts', i.e.

$$\int_a^b \big(D_x^{+h}\phi(x)\big)\,\psi(x)\ \mathrm{d}x = -\int_a^b \phi(x)\,D_x^{-h}\psi(x)\ \mathrm{d}x\ , \tag{B.0.2}$$

where either ψ or ϕ is compactly supported (a, b) (see Lemma 2.3.5). For convenience, we state here the result (Theorem 4.1.16) that we wish to prove.

Theorem B.0.22. *Let L be Lipschitz continuous on $[0, l]$ and let P be of the block-diagonal form (4.1.43). Assume that the matrix entries of $\tilde{P}$ are in $C^3(0, l)$. Moreover, when $y \in [0, \varepsilon_1] \cup [l - \varepsilon_2, l]$ with some $\varepsilon_1, \epsilon_2 > 0$, suppose that $L(y) = 0$ and that $\tilde{P}(y)$ is diagonal with diagonal entries that are either zero or one. Then the quadratic form $Q_{P,L}^{(2)}$ is regular.*

Proof. [BK13b] We first show regularity on any subdomain of the form $D' = [0, l] \times [\epsilon, l - \epsilon]$ with $\epsilon > 0$, leaving the discussion of regularity in the corners of the domain D until the end. Our first tool is the double difference quotient

$$\begin{aligned} D_y^{-h}\tau^2 D_y^{+h}\phi(x, y) =& \frac{1}{h^2}\big(\tau^2(y)\phi(x, y + h) - \tau^2(y)\phi(x, y) \\ &- \tau^2(y - h)\phi(x, y) + \tau^2(y - h)\phi(x, y - h)\big)\ , \end{aligned} \tag{B.0.3}$$

where $\phi \in \mathcal{D}(H) \subset \mathcal{D}_{Q^{(2)}}$ and $\tau \in C_0^\infty(\mathbb{R})$ is a test function with support in

$(0,l)$ such that $\tau|_{[\epsilon,l-\epsilon]} = 1$ and $\tau \leq 1$ elsewhere. Even though ϕ satisfies the boundary condition $P(y)\phi_{bv}(y) = 0$, (B.0.3) does in general not. This is due to the dependence of the matrix P on y. We therefore introduce a correction function $\kappa \in H^1(D)$ such that

$$D_y^{-h}\tau^2 D_y^{+h}\phi + \kappa \in \mathcal{D}_{Q^{(2)}} \ . \tag{B.0.4}$$

We now determine and estimate κ and, to this end, insert (B.0.4) for ψ into (4.1.24), i.e.

$$\begin{aligned}\langle \nabla\phi, \nabla(D_y^{-h}\tau^2 D_y^{+h}\phi)\rangle_{L^2(D)} + \langle \nabla\phi, \nabla\kappa\rangle_{L^2(D)} - \langle \phi_{bv}, \Lambda\big(D_y^{-h}\tau^2 D_y^{+h}\phi\big)_{bv}\rangle_{L^2(0,l)\otimes\mathbb{C}^4} \\ - \langle \phi_{bv}, \Lambda\kappa_{bv}\rangle_{L^2(0,l)\otimes\mathbb{C}^4} = \langle \chi, D_y^{-h}\tau^2 D_y^{+h}\phi\rangle_{L^2(D)} + \langle \chi, \kappa\rangle_{L^2(D)} \ .\end{aligned} \tag{B.0.5}$$

Employing the integration by parts (B.0.2) while taking into account that τ is compactly supported in $(0,l)$ and choosing h to be sufficiently small, the first term of (B.0.5) can be re-written as

$$\begin{aligned}\int_0^l\int_0^l \nabla\bar{\phi}\nabla\big(D_y^{-h}\tau^2 D_y^{+h}\phi\big)\,\mathrm{d}x\,\mathrm{d}y = &- \int_0^l\int_0^l \tau^2 |D_y^{+h}\nabla\phi|^2\,\mathrm{d}x\,\mathrm{d}y \\ &- \int_0^l\int_0^l (\nabla D_y^{+h}\bar{\phi})(\partial_y\tau^2)(D_y^{+h}\phi)\,\mathrm{d}x\,\mathrm{d}y \ .\end{aligned} \tag{B.0.6}$$

Hence, (B.0.5) yields

$$\begin{aligned}\|\tau D_y^{+h}\nabla\phi\|^2_{L^2(D)} = &- \langle \nabla D_y^{+h}\phi, \partial_y(\tau^2) D_y^{+h}\phi\rangle_{L^2(D)} + \langle \nabla\phi, \nabla\kappa\rangle_{L^2(D)} \\ &- \langle \phi_{bv}, \Lambda\big(D_y^{-h}\tau^2 D_y^{+h}\phi\big)_{bv}\rangle_{L^2(0,l)\otimes\mathbb{C}^4} - \langle \phi_{bv}, \Lambda\kappa_{bv}\rangle_{L^2(0,l)\otimes\mathbb{C}^4} \\ &- \langle \chi, D_y^{-h}\tau^2 D_y^{+h}\phi\rangle_{L^2(D)} - \langle \chi, \kappa\rangle_{L^2(D)} \ ,\end{aligned} \tag{B.0.7}$$

which allows the estimate

$$\begin{aligned}\|\tau D_y^{+h}\nabla\phi\|^2_{L^2(D)} \leq &\ \|\tau D_y^{+h}\nabla\phi\|_{L^2(D)}\,\|2(\partial_y\tau) D_y^{+h}\phi\|_{L^2(D)} + \|\nabla\phi\|_{L^2(D)}\,\|\nabla\kappa\|_{L^2(D)} \\ &+ \big|\langle \phi_{bv}, \Lambda\big(D_y^{-h}\tau^2 D_y^{+h}\phi\big)_{bv}\rangle_{L^2(0,l)\otimes\mathbb{C}^4}\big| + \big|\langle \phi_{bv}, \Lambda\kappa_{bv}\rangle_{L^2(0,l)\otimes\mathbb{C}^4}\big| \\ &+ \|\chi\|_{L^2(D)}\,\|D_y^{-h}\tau^2 D_y^{+h}\phi\|_{L^2(D)} + \|\chi\|_{L^2(D)}\,\|\kappa\|_{L^2(D)} \ .\end{aligned} \tag{B.0.8}$$

We now use estimate (2.2.10) from the trace theorem to conclude that

$$\left|\langle \phi_{bv}, \Lambda\kappa_{bv}\rangle_{L^2(0,l)\otimes\mathbb{C}^4}\right| \leq \tilde{c}\,\|\phi\|_{H^1(D)}\,\|\kappa\|_{H^1(D)}\ , \tag{B.0.9}$$

where the constant $\tilde{c} > 0$ incorporates the constant c from (2.2.10) as well as the norm of the bounded map Λ. Furthermore, using the Cauchy-inequality

$$|ab| < \epsilon a^2 + \frac{b^2}{4\epsilon}\ , \qquad \forall a, b \in \mathbb{R}\ ,\ \epsilon > 0\ , \tag{B.0.10}$$

in the first, second and fourth term on the right-hand side of (B.0.8) we arrive at

$$\begin{aligned}\|\tau D_y^{+h}\nabla\phi\|^2_{L^2(D)} \leq\ & c_1(\epsilon_1) + \epsilon_1\,\|\tau\nabla D_y^{+h}\phi\|^2_{L^2(D)} + c_2(\epsilon_2) + \epsilon_2\,\|\nabla\kappa\|^2_{L^2(D)} \\ & + \left|\langle \phi_{bv}, \Lambda\big(D_y^{-h}\tau^2 D_y^{+h}\phi\big)_{bv}\rangle_{L^2(0,l)\otimes\mathbb{C}^4}\right| \\ & + c_3(\epsilon_3) + \epsilon_3\left(\|\kappa\|^2_{L^2(D)} + \|\nabla\kappa\|^2_{L^2(D)}\right) \\ & + \|\chi\|_{L^2(D)}\,\|D_y^{-h}\tau^2 D_y^{+h}\phi\|_{L^2(D)} + \|\chi\|_{L^2(D)}\,\|\kappa\|_{L^2(D)}\ .\end{aligned} \tag{B.0.11}$$

Here we kept all terms containing the still unknown function κ or difference quotients of $\nabla\phi$ explicitly, as these are the quantities we want to estimate; all other terms are absorbed in the quantities $c_j(\epsilon_j)$. Now, in order to estimate the fourth, the seventh and the last term on the right-hand side of (B.0.11), we need to determine a suitable function κ and, in particular, establish the bounds

$$\|\kappa\|_{L^2(D)} \leq K_1 \quad \text{and} \quad \|\nabla\kappa\|^2_{L^2(D)} \leq K_2 + K_3\,\|\tau D_y^{+h}\nabla\phi\|^2_{L^2(D)} \tag{B.0.12}$$

hold, where $K_j > 0$ are some constants not depending on h.
To characterise κ, we infer from (B.0.4) that its boundary values have to be such that

$$P(y)\big((D_y^{-h}\tau^2 D_y^{+h}\phi)_{bv}(y) + \kappa_{bv}(y)\big) = 0\ . \tag{B.0.13}$$

Expanding the double difference quotient and using $P(y)\phi_{bv}(y) = 0$, we obtain a condition of which the upper two components read, i.e.

$$\tilde{P}(y)\big(\tau^2(y)\tilde{\phi}_{bv}(y+h) + \tau^2(y-h)\tilde{\phi}_{bv}(y-h)\big) + h^2\tilde{P}(y)\tilde{\kappa}_{bv}(y) = 0. \tag{B.0.14}$$

Here we employed the notation $\tilde{\phi}_{bv}(y) = (\phi(0,y), \phi(l,y))^T$ as well as the block-

structure (4.2.4) of P. Since $\tilde{P}(y)$ is a projector, this condition is solved by

$$\tilde{\kappa}_{bv}(y) = -\frac{1}{h^2}\tilde{P}(y)\big(\tau^2(y)\tilde{\phi}_{bv}(y+h) + \tau^2(y-h)\tilde{\phi}_{bv}(y-h)\big) \ . \tag{B.0.15}$$

This, however, only yields the boundary values of the function we wish to find. An extension of κ_{bv} into the interior of the rectangle D can be achieved by making use of the particular structure (4.1.43), required for the projectors $P(y)$ as well as the assumed regularity of its matrix entries. This allows us to find functions $a, b \in C^3(D_0)$, where D_0 is an open domain containing $\bar{D}$, and define

$$\tilde{\mathcal{P}}(x,y) = \begin{pmatrix} a(x,y) & b(x,y) \\ b(l-x,y) & a(l-x,y) \end{pmatrix} \ , \tag{B.0.16}$$

in such a way that $\tilde{P}(y) = \tilde{\mathcal{P}}(0,y)$. Due to the required regularity of the respective functions, the Taylor expansions

$$\tilde{\mathcal{P}}(x, y \pm h) = \tilde{\mathcal{P}}(x,y) \pm h\, \tilde{\mathcal{P}}_y(x,y) + h^2\, \tilde{\mathcal{P}}^{\pm}_{R_2}(x,y;h) \tag{B.0.17}$$

and

$$\tau^2(y-h) = \tau^2(y) - h\, \tau^2_{R_1}(y;h) \tag{B.0.18}$$

hold with remainder terms that are of class C^1 in the variable y and are bounded in h. Using these expansions in (B.0.15) yields

$$\begin{aligned} \tilde{\kappa}_{bv}(y) = \tau^2(y)\, \tilde{P}_y(y)\Big(\frac{\tilde{\phi}_{bv}(y+h) - \tilde{\phi}_{bv}(y-h)}{h}\Big) + \tau^2_{R_1}(y;h)\tilde{P}_y(y)\tilde{\phi}_{bv}(y-h) \\ + \tau^2(y)\tilde{P}^{+}_{R_2}(y;h)\tilde{\phi}_{bv}(y+h) + \tau^2(y-h)\tilde{P}^{-}_{R_2}(y;h)\tilde{\phi}_{bv}(y-h) \ . \end{aligned} \tag{B.0.19}$$

We then define the function

$$\begin{aligned}\kappa(x,y) = \tau^2(y)\Big(a_y(x,y)\,\frac{\phi(x,y+h)-\phi(x,y-h)}{h} \\ + b_y(x,y)\,\frac{\phi(l-x,y+h)-\phi(l-x,y-h)}{h}\Big) \\ + \tau_{R_1}^2(y;h)\big(a_y(x,y)\phi(x,y-h) + b_y(x,y)\phi(l-x,y-h)\big) \\ + \tau^2(y)\big(a_{R_2}^+(x,y;h)\phi(x,y+h) + b_{R_2}^+(x,y;h)\phi(l-x,y+h)\big) \\ + \tau^2(y-h)\big(a_{R_2}^-(x,y;h)\phi(x,y-h) + b_{R_2}^-(x,y;h)\phi(l-x,y-h)\big)\ ,\end{aligned} \tag{B.0.20}$$

whose boundary values indeed satisfy (B.0.13). The regularity of the functions involved implies that $\kappa \in H^1(D)$ and, thus, $\|\kappa\|_{L^2(D)}$ and $\|\kappa\|_{H^1(D)}$ are finite. Moreover, since $\phi \in H^1(D)$ and

$$\frac{\phi(x,y+h)-\phi(x,y-h)}{h} = D_y^{+h}\phi(x,y) + D_y^{-h}\phi(x,y)\ , \tag{B.0.21}$$

Theorem 2.3.6 implies that $\|\kappa\|_{L^2(D)}$ has an h-independent upper bound. In the same way, the second bound in (B.0.12) follows from (B.0.20) and (B.0.21).
As a next step, we estimate the fifth term on the right-hand side of (B.0.11). We use the self-adjointness of Λ and perform an integration by parts (B.0.2) as well as employing the product rule (B.0.1) to obtain

$$\begin{aligned}\langle\phi_{bv}, \Lambda\big(D_y^{-h}\tau^2 D_y^{+h}\phi\big)_{bv}\rangle_{L^2(0,l)\otimes\mathbb{C}^4} = &-\int_0^l \langle L(y+h)(\tau D_y^{+h}\phi_{bv})(y), (\tau D_y^{+h}\phi_{bv})(y)\rangle_{\mathbb{C}^4}\ \mathrm{d}y \\ &-\int_0^l \langle(\tau(D_y^{+h}L)\phi_{bv})(y), (\tau D_y^{+h}\phi_{bv})(y)\rangle_{\mathbb{C}^4}\ \mathrm{d}y\ .\end{aligned} \tag{B.0.22}$$

Noting that L is supposed to be bounded and Lipschitz continuous, the right hand side can be estimated from above in absolute value by

$$d_1\,\|\tau D_y^{+h}\phi_{bv}\|^2_{L^2(0,l)\otimes\mathbb{C}^4} + d_2\,\|\phi_{bv}\|_{L^2(0,l)\otimes\mathbb{C}^4}\,\|\tau D_y^{+h}\phi_{bv}\|_{L^2(0,l)\otimes\mathbb{C}^4}\ , \tag{B.0.23}$$

with suitable constants $d_j > 0$. Estimating further, we apply (4.1.20) to the first

term and (2.2.10) to the second and obtain the bound

$$4\,d_1\,\left(\frac{2}{\epsilon_4}\|\tau D_y^{+h}\phi\|^2_{L^2(D)}+\epsilon_4\|\nabla(\tau D_y^{+h}\phi)\|^2_{L^2(D)}\right)+d_3\,\|\phi_{bv}\|_{L^2(0,l)\otimes\mathbb{C}^4}\,\|\tau D_y^{+h}\phi\|_{H^1(D)}\,, \tag{B.0.24}$$

where $\epsilon_4 > 0$ is sufficiently small. Eventually, again using (4.1.20), this can be further bounded by

$$d_4+d_5\,\epsilon_5\,\|\tau D_y^{+h}\nabla\phi\|^2_{L^2(D)}\,,\quad \text{where } d_j>0\,. \tag{B.0.25}$$

It remains to estimate the last-but-one term on the right-hand side of (B.0.11),

$$\|D_y^{-h}\tau^2 D_y^{+h}\phi\|_{L^2(D)}\le\|\partial_y(\tau^2 D_y^{+h}\phi)\|_{L^2(D)}\le d_6+d_7\,\|\tau^2 D_y^{+h}\nabla\phi\|_{L^2(D)}\,. \tag{B.0.26}$$

The last term on the right-hand side can be estimated with the help of (B.0.10), and using that $\tau^2\le 1$,

$$\|D_y^{-h}\tau^2 D_y^{+h}\phi\|_{L^2(D)}\le c_6(\epsilon_6)+d_8\,\epsilon_6\|\tau D_y^{+h}\nabla\phi\|^2_{L^2(D)}\,. \tag{B.0.27}$$

Finally, we collect all bounds for the terms on the right-hand side of (B.0.11) and subtract all contributions of the form $\epsilon_j\|\tau D_y^{+h}\nabla\phi\|^2_{L^2(D)}$. By choosing $\epsilon_1,\dots,\epsilon_6$ sufficiently small we obtain the bound

$$\|\tau D_y^{h}\nabla\phi\|_{L^2(D)}\le K, \tag{B.0.28}$$

for $h\le h_0$.

Hence, by applying Theorem 2.3.6 to $\nabla\phi$ on the domain $D'=[0,l]\times[\epsilon,l-\epsilon]$, we conclude that ϕ_{xy} and ϕ_{yy} are in $H^2(D')$. Since $\phi_{xx}+\phi_{yy}=\Delta_2\phi$ is known to be in $L^2(D)$, we conclude that $\phi\in H^2(D')$. The same argument can now be repeated on a domain $D''=[\epsilon,l-\epsilon]\times[0,l]$ so that, indeed, ϕ has H^2-regularity away from small neighbourhoods of the corners of the rectangle D.

Finally, as the condition imposed on P implies that close to the corners either Dirichlet or Neumann or mixed Dirichlet-Neumann boundary conditions are imposed, regularity of ϕ in neighbourhoods of the corners follows from standard results (see, e.g., [Neč67, Dau88]). □

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