Influence of vortices on the magnetic resonance in cuprate superconductors

M. Eschrig,[1] M. R. Norman,[1] and B. Jankó[1,2]
[1]*Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439*
[2]*Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556*
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We investigate several theoretical possibilities for the suppression in a c-axis magnetic field of the magnetic resonance recently observed in inelastic neutron scattering experiments on $YBa_2Cu_3O_{6.6}$. We find that neither the Doppler shift of the quasiparticle states caused by supercurrents outside the vortex core, nor an assumed spatially uniform suppression of the coherence factors or spectral gap due to the applied field, can account for the observed effect. In contrast, suppressing the gap or the coherence factors in the vortex core to zero is consistent with the data, and an even simpler description of the data can be achieved by assuming that the resonance is not supported within the core. These three models can then be used to estimate the effective radius ξ_{eff} around each vortex, which we find to be larger than ξ_{sc} but smaller than $\xi_{sc}+\xi_{mag}$, where ξ_{sc} and ξ_{mag} are respectively the superconducting and spin-spin correlation lengths. We use this observation to predict the doping dependence of the field suppression.

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One of the more intriguing developments in the field of high-temperature cuprate superconductivity has been the observation by inelastic neutron scattering (INS) experiments of a sharp magnetic resonance in the superconducting state.[1] Recently, it was found that a *c* axis magnetic field suppressed the intensity of this resonance,[2] as predicted from an analysis of specific-heat data.[3] Since the same effect was not observed for in-plane fields,[4] this indicates that the resonance is sensitive to the presence of Abrikosov vortices, and thus intimately connected to the nature of the superconducting ground state. This has obvious implications for microscopic theories of the resonance.

In this paper, we consider a model where the resonance is treated as a particle-hole bound state in a *d*-wave superconductor, with calculations performed within linear response theory (random-phase approximation, RPA). Several effects of the vortices are considered. First, we calculate the influence of the supercurrents circulating around the vortices on the resonance. We find that this only leads to a broadening of the resonance in energy; the integrated weight remains the same, in conflict with experiment. Second, we study the effect of a spatially uniform suppression of the $\langle \Delta_{\mathbf{k}} \Delta_{\mathbf{k+Q}} \rangle$ correlator that enters the coherence factors of the spin susceptibility (where $\mathbf{Q}$ is the antiferromagnetic wave vector at which the resonance is peaked). Such a suppression is speculative, but could be a result of dephasing of the pairing in a *c* axis field due to the vortices, as observed in Josephson plasma resonance experiments.[5] We find that although this does lead to a suppression of the integrated weight as observed experimentally, the effect causes the resonance to shift to higher energy, in conflict with experiment. Third, an assumed (field induced) spatially uniform suppression of the gap magnitude causes the resonance to shift to lower energy, also in conflict with experiment.

This leads us to consider the effect of the vortex cores themselves. We observe that if the resonance is not supported in the vortex cores, then the resulting field dependence is in reasonable agreement with experiment. We consider three possibilities for the suppression of the resonance in the vortex core regions: (a) the suppression of the gap magnitude in the core, (b) the suppression of the $\langle \Delta\Delta \rangle$ correlator in the core, and (c) the absence of quasiparticles in the core. Any of these three possibilities give a good account of the data. We use this to estimate the doping dependence of the field-suppression effect.

To calculate the influence of the supercurrents around the vortices on the resonance in the spin-spin correlation function, we approximate the superflow by a circular flow around the vortex center. The corresponding local supermomentum $\mathbf{p}_s$ is proportional to the gradient of the phase, $\mathbf{p}_s = \hbar \mathbf{e}_\phi / 2r$. This is a good approximation for the experiments considered here, where the intervortex spacing is smaller than the penetration depth and large compared to the coherence length.

In the intervortex regions, the variation of the order parameter and of the superflow occurs on a large scale as compared to the spin-spin correlation length, which amounts to only a few lattice constants as determined from the momentum width of the resonance. Consequently, we determine the RPA susceptibility in the intervortex region at each point of the unit cell of the vortex lattice in the presence of the *local* superflow,

$$\chi(\omega,\mathbf{Q},\mathbf{p}_s) = \frac{\chi_0(\omega,\mathbf{Q},\mathbf{p}_s)}{1 - J_{\mathbf{Q}} \chi_0(\omega,\mathbf{Q},\mathbf{p}_s)}. \quad (1)$$

The bare susceptibility $\chi_0(\omega,\mathbf{Q},\mathbf{p}_s)$, is determined as

$$\chi_0(\omega,\mathbf{Q},\mathbf{p}_s) = -\sum_{\mathbf{k}} \sum_{\mu,\nu=\{\pm\}} \frac{A^\mu_{\mathbf{k}} A^\nu_{\mathbf{k+Q}} + \alpha C^\mu_{\mathbf{k}} C^\nu_{\mathbf{k+Q}}}{\omega + E^\mu_{\mathbf{k}} - E^\nu_{\mathbf{k+Q}} + i\Gamma} \times [f(E^\mu_{\mathbf{k}}) - f(E^\nu_{\mathbf{k+Q}})], \quad (2)$$

where the excitation spectrum in the presence of a superflow with momentum $\mathbf{p}_s$ is given by[6]

$$E^\pm_{\mathbf{k}} = \pm \sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2} + \delta\xi_{\mathbf{k}} \quad (3)$$

with

$$\delta\xi_{\mathbf{k}}=(\xi_{\mathbf{k}+\mathbf{p}_s}-\xi_{\mathbf{k}-\mathbf{p}_s})/2, \overline{\xi_{\mathbf{k}}}=(\xi_{\mathbf{k}+\mathbf{p}_s}+\xi_{\mathbf{k}-\mathbf{p}_s})/2,$$

and

$$A_{\mathbf{k}}^{\pm}=\frac{1}{2}\pm\frac{\overline{\xi_{\mathbf{k}}}}{E_{\mathbf{k}}^{+}-E_{\mathbf{k}}^{-}}, \quad C_{\mathbf{k}}^{\pm}=\pm\frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}}^{+}-E_{\mathbf{k}}^{-}} \tag{4}$$

as coherence factors. The factor α (1 in the current case) will be discussed later. The spatial average of the Doppler shifted susceptibility over the intervortex region of the vortex lattice unit cell is then calculated, $\chi(\omega,\mathbf{Q})=\langle\chi(\omega,\mathbf{Q},\mathbf{p}_s(\mathbf{R}))\rangle_{\mathbf{R}}$. We evaluated Eq. (2) for a 512×512 grid of **k** points and performed the spatial average over 320 **R** points. Note that we use a normalization equal to the intervortex area, not the total area. The contribution from the vortex cores will be discussed later in the paper.

For small Doppler shifts, the spectrum is approximated by $\pm E_{\mathbf{k}}+\mathbf{v}_{\mathbf{k}_F}\mathbf{p}_s$, and the coherence factors are unaffected to first order. The main effect of the Doppler shift is the term $\delta\xi_{\mathbf{k}}-\delta\xi_{\mathbf{k+Q}}\approx(\mathbf{v}_{\mathbf{k}}-\mathbf{v}_{\mathbf{k+Q}})\mathbf{p}_s$ in the energy denominators of Eq. (2). As shown in the appendix, this "linearized" approximation can be exploited to perform the spatial average of Eq. (2) analytically. This can then be inserted into Eq. (1). The advantage of this approximation is that the resulting expressions are no more difficult to calculate than for the zero-field case. Although we do not present results in the present paper for this approximation, we have found that it gives results nearly equivalent to the exact expression if the hot spots at position $\mathbf{p}_0$ are not too close to the nodes of the order parameter, and if the normal state dispersion is to a good approximation linear in a region $\delta p=\Delta(\mathbf{p}_0)/v_F(\mathbf{p}_0)$ around the hot spots.

Calculations were performed using a model quasiparticle dispersion in the superconducting state motivated by photoemission measurements.[7] Similar dispersions were found to give a good description of the zero-field INS data, including the incommensurate structure observed at energies below resonance.[8] A d-wave superconducting gap proportional to $\cos(k_xa)-\cos(k_ya)$ was assumed, with a maximum value of $\Delta=29$ meV as determined from recent scanning tunnel microscope (STM) measurements.[9] A broadening factor Γ of 2 meV was employed, and a temperature of 13 K.

In Fig. 1 we show our results for the effect of the circulating supercurrents on the resonance. The exchange coupling $J_{\mathbf{Q}}$ is fixed to give a resonance at 34 meV for zero magnetic field. For the spatial average we assumed a lower cutoff at the value $\xi=2a$ (vortex core radius) and an upper cutoff at the value $R=25a$ (radius for enclosing one flux quantum at 7 T), where a is the Cu-Cu distance. The results are insensitive to the lower cutoff. As Fig. 1 shows, the supercurrent has three effects: (a) it shifts the position of the resonance to a slightly lower energy, (b) it broadens the resonance, and (c) it reduces the magnitude of the resonance at the peak energy. Also shown are the energy-integrated susceptibilities, which demonstrate that the integrated weight between 0 and $\approx 2\Delta$ is conserved. These findings are in apparent contradiction with the experimental facts, which are that the resonance does not shift, nor broaden, and that the integrated weight is reduced by about 15% at 7 T [Ref. 2]. We have also tested a number of other dispersions,[8] and a variety of assumed values for Δ and J. Although the amount of broadening is somewhat sensitive to these details, we find that the integrated weight is always approximately conserved. An example is given in the right panel of Fig. 1, where we find virtually no effect of the Doppler shift on the susceptibility.

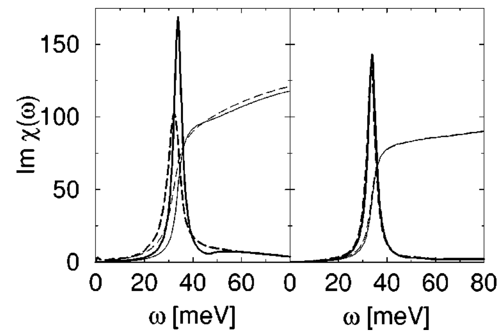

FIG. 1. Influence of Doppler shifts due to supercurrents on Im $\chi(\omega,\mathbf{Q})$. The full lines correspond to zero magnetic field, the dashed ones to a field of 7 T. The thin lines are the energy-integrated susceptibilities (scaled by a constant so that they could be plotted on the same graph). Although the magnitude of the resonance at the peak energy is suppressed, its integrated weight is not. The parameters employed were $\Delta=29$ meV, $\Gamma=2$ meV, and $T=13$ K. In the left panel we use $J=357$ meV, and the dispersion taken from Ref. 7. In the right panel we use $J=142$ meV and the dispersion $tb2$ taken from Ref. 8; for this case, the Doppler shift has virtually no effect.

We also checked if an assumed field-induced (spatially uniform) reduction of the gap magnitude accounts for the observed effect. Our result is shown as the dotted line in Fig. 2 compared to the zero-field result (full line). The integrated weight is suppressed in this case [the left panel of Fig. 4 shows the reduction of the integrated weight versus $\Delta^2(H)/\Delta^2(0)$]. To obtain the observed 15% reduction in weight at 7 T would require reducing the gap from 29 to 20 meV. This reduction is substantially larger than would be indicated by the upper critical field (45 T), and the reduction appears to have the wrong functional dependence on H. Moreover, this gap reduction shifts the resonance to considerably lower energy, in contradiction with experiment.

As a third mechanism, we studied a (spatially uniform) suppression of the $\langle\Delta_{\mathbf{k}}\Delta_{\mathbf{k+Q}}\rangle$ correlator in the $C_{\mathbf{k}}C_{\mathbf{k+Q}}$ coherence factors [by reducing α to less than 1 in Eq. (2)]. The motivation for this is that phase fluctuations induced by the vortices are known to lead to a dephasing of the layers, and the resonance will be sensitive to this since it involves c-axis coupling (it is peaked at $k_z=\pi/d$, where d is the separation of nearest neighbor CuO layers). The observed decoupling inferred from the field dependence of the Josephson plasmon,[5] though, is probably due to the weaker bilayer-bilayer coupling, which is also consistent with small mesa experiments.[10] Therefore at the current time, it is not known whether the two layers within a bilayer are dephased or not (though this could be determined from the field dependence of c-axis infrared conductivity measurements, where a fea-

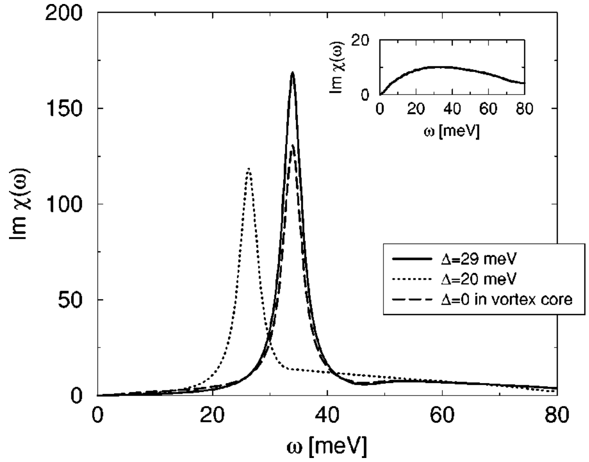

FIG. 2. Comparison of zero-field susceptibility with the same susceptibility, but with reduced gap magnitude Δ. Dotted line: assuming a spatially uniform reduction from 29 meV to 20 meV; dashed line: assuming a reduction to zero in 24% of the vortex unit cell area representing the cores (the uniform zero gap response is shown in the inset). In both cases the weight of the resonance is reduced, but for the spatially uniform case, the resonance is shifted considerably downwards in energy. The parameters used are the same as in Fig. 1.

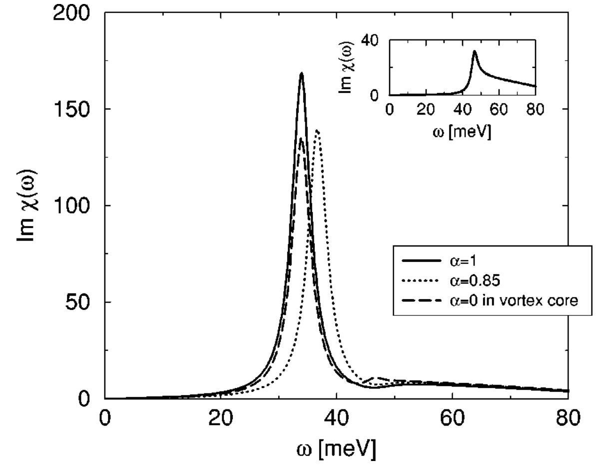

FIG. 3. Comparison of zero-field susceptibility with the same susceptibility, but with the $\langle\Delta\Delta\rangle$ correlator in the numerator of Eq. (2) reduced $(\alpha<1)$. Dotted line: assuming a spatially uniform reduction by 15%; dashed line: assuming a reduction to zero in 20% of the vortex unit cell area representing the cores (the uniform zero α response is shown in the inset). In both cases the weight of the resonance is reduced, but for the spatially uniform case, the resonance is shifted considerably upwards in energy. The parameters used are the same as in Fig. 1.

ture is seen attributed to an optical Josephson plasmon[11]). For now, though, we will assume that this is a possibility, and test its consequences.[12]

In Fig. 3, we compare the zero-field result to the same result, but with the correlator reduced by 15% $(\alpha=0.85)$. This leads to a large reduction of the integrated weight, as seen experimentally (in Fig. 4, we plot the integrated weight vs α). We note that the experimental suppression goes like $1-H/H^*$, where H^* is a number not much lower than H_{c2}, the upper critical field.[2] Based on quantum Ginzburg-Landau theory, a reduction of the $\langle\Delta\Delta\rangle$ correlator proportional to $1-H/H_{c2}$ is expected. Therefore it is reasonable to suppose that the relative experimental suppression goes like α. This suppression is in good agreement with the calculation, as can be seen in Fig. 4. We note, however, that the position of the resonance shifts to higher energies, in disagreement with the data. It would be coincidental if this energy shift was exactly canceled by an assumed shift of the superconducting gap to lower energies by the field.

Let us now consider the effect of the vortex cores. The fact that the experimental suppression goes like $1-H/H^*$ is highly suggestive of a vortex core effect, as originally noted by Dai *et al.*[2] This implies that the resonance is not supported in the region of the vortex core. This implication is additionally supported by five facts: (a) the considerable momentum width of the resonance shows that the corresponding spin excitations have a decay length that is smaller than the coherence length; thus the resonance will be sensitive to variations of the order parameter on the coherence length scale; (b) the resonance at zero field only exists in the superconducting state, and disappears in the normal state; (c) coherence peaks in the single-particle density of states at the gap edge were not found in the core region in STM measurements;[13] this would modify the 2Δ edge in χ_0'' [Eq. (2)] and suppress the resonance; (d) in underdoped materials, missing subgap states point towards a loss of quasiparticle weight due to a pseudogap in the vortex core;[13] (e) the dip feature in the tunneling density of states, thought to be due to the coupling of quasiparticles to the resonance,[7] is not observed in the vortex core region.[13]

In Figs. 2 and 3, we show in the insets the susceptibility for zero Δ, and for zero $\langle\Delta\Delta\rangle$ correlator. In both cases, the resonance is strongly suppressed. In the main panels, we show as dashed curves the results for the case when we use the curves in the insets for the vortex core regions, and the full curves (zero-field results) for the intervortex regions. The latter is justified since we found above that the Doppler shift has a negligible effect on the integrated intensity. In both cases, the resulting curves, calculated for a 15% reduction in total integrated weight, reproduce very well the ex-

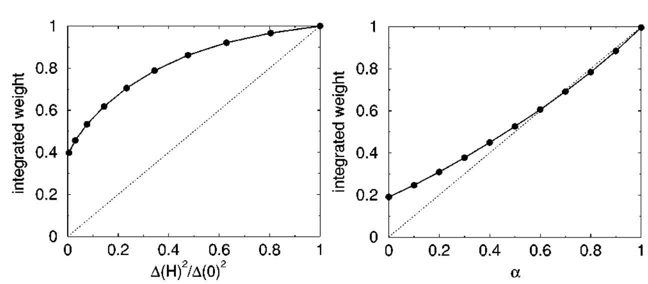

FIG. 4. Energy-integrated weight (from $\omega=0$ to $\omega=50$ meV, normalized to the zero-field value) from Figs. 2 and 3. Left: versus $\Delta^2(H)/\Delta^2(0)$, where Δ is the maximal *d*-wave gap magnitude. Right: versus α, where α is the prefactor in front of the $\langle\Delta\Delta\rangle$ correlator in the numerator of Eq. (2). The dotted lines are the expected behavior if the normalized weight was equal to $(1-H/H_{c2})$.

perimental finding of no shift or broadening of the resonance. One problem is that the observed weight suppression would require a vortex core region filling 24% of the total area for the first case, and 20% for the second case. Both values are somewhat larger than what one might expect at 7 T, as discussed below, especially for the first case.

There is a way of testing whether either of these two scenarios is correct. In the case where the gap is reduced in the cores, then extra weight would show up at lower energies, whereas for the case where the correlator is reduced in the cores, extra weight would show up at higher energies. Although our calculations indicate that the corresponding changes between 0 and 7 T are perhaps within experimental error bars, we encourage experimentalists to look for extra weight, both in the region around 20 meV and around 50 meV.

We note that our formalism assumes the presence of quasiparticle states, and thus we do not expect a resonance to exist if quasiparticles do not exist. A simpler idea to those discussed in the previous two paragraphs is to assume that the weight is zero in the considered energy range, consistent with a spin gap of ~ 50 meV inside the cores. From this, we can estimate the effective radius of the core ξ_{eff} from the ratio of the INS weight to that at zero field. Since the ratio of the vortex core area to the total area is equal to $B\pi\xi_{eff}^2/\Phi_0$,[14] to obtain an effect of 15% at 7 T in underdoped $YBa_2Cu_3O_{7-\delta}$, we estimate a ξ_{eff} of 38 Å for the no resonance in the core model. This is larger than the estimated superconducting coherence length of 27 Å (H_{c2} of 45 T), but is smaller than 55 Å, the sum of the superconducting (27) and magnetic (28) (Ref. 15) correlation lengths. The latter quantity (55) should represent an upper bound on the size of the effective core radius. We note that in the other models, the effective core radius would be 48 Å for the zero gap in the core case, and 43 Å for the zero correlator in the core case.

It is interesting to remark that the sample studied experimentally had an anomalously long magnetic correlation length. Other samples studied by neutron scattering have a significantly smaller correlation length.[15] This implies that the resonance suppression effect will be weaker in other samples. In addition, as the doping increases towards optimal doping, the superconducting correlation length becomes shorter. Assuming $\xi_{eff} \approx 20$–24 Å for an optimally doped compound, our prediction for this case is that the suppression of the total weight at 7 T will only be 4–6%. Going further to the overdoped regime, the superconducting coherence length increases, leading to an increase of the sensitivity of the resonance with magnetic field again. Further underdoping, though, should lead to an even more dramatic reduction, as both coherence lengths are expected to increase as the doping is reduced. In fact, we would argue that the field dependence of the resonance at various dopings would be a good measure of the doping dependence of the superconducting coherence length, and it would be of great interest to correlate STM and INS measurements on the same samples.

We wish to conclude this paper with the following speculation, motivated by the above results. As documented by angle-resolved photoemission measurements,[16] quasiparticle-like peaks in the spectral functions are present only below T_c, the onset temperature of phase coherence. The superconducting phase is singular at the vortex core, and therefore the phase correlations are strongly suppressed between points close to the core region (this was a motivation for the $\alpha < 1$ calculations). We suggest that this may lead to a destruction of quasiparticle excitations in the vortex core region similar to what happens in the pseudogap state. The absence of quasiparticle peaks as well as the neutron resonance in the core region is consistent with the notion that *both* these spectral features require substantial local-phase correlations.[3] While this conjecture is at this stage admittedly speculative, we believe it deserves further experimental and theoretical investigation.

ACKNOWLEDGMENTS

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APPENDIX

In the following, we give an analytic expression for the spatial average of Eq. (2) in the linearized approximation, which works well as long as the Fermi velocity near the M point of the Brillouin zone is not smaller than approximately 0.5 eV Å. For low temperatures we can neglect the Doppler shifts in the distribution functions, as they are always smaller than the excitation energies near the hot spots (if the hot spots are not too close to the nodes). As a function of $R = \sqrt{\Phi_0/\pi H}$, the spin susceptibility averaged over the vortex unit cell is given by

$$\overline{\chi_0(\omega,\mathbf{Q})} = -\sum_{\mathbf{k}} \sum_{\mu,\nu=\{\pm\}} \frac{A^\mu_{\mathbf{k}} A^\nu_{\mathbf{k+Q}} + C^\mu_{\mathbf{k}} C^\nu_{\mathbf{k+Q}}}{\omega + E^\mu_{\mathbf{k}} - E^\nu_{\mathbf{k+Q}} + i\Gamma} \times [f(E^\mu_{\mathbf{k}}) - f(E^\nu_{\mathbf{k+Q}})] \left[I\left(\frac{\hbar V}{WR}\right) - \frac{\xi^2}{R^2} I\left(\frac{\hbar V}{W\xi}\right)\right], \tag{A1}$$

where the abbreviations

$$I(x) = \sqrt{1-x^2} + x^2[\ln(1+\sqrt{1-x^2}) - \ln(ix)], \tag{A2}$$

$$W = \omega + E^\mu_{\mathbf{k}} - E^\nu_{\mathbf{k+Q}} + i\Gamma, \quad V = \tfrac{1}{2}|\mathbf{v_k} - \mathbf{v_{k+Q}}| \tag{A3}$$

are used. The lower cutoff ξ is introduced to account for the vortex core regions. The modification due to the Doppler shifts are contained in the function $I(x)$ [note that $I(0)=1$].

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