Influence of vortices on the magnetic resonance in cuprate superconductors

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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\textsubscript{2}Cu\textsubscript{3}O\textsubscript{6}\textsubscript{4.8}. 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. We demonstrate that an even simpler description of the data can be achieved by assuming that the resonance is not supported within an effective radius \(\xi_{eff}\) around each vortex, where \(\xi_{eff}\) is the sum of the superconducting and spin-spin correlation lengths. We use this simple idea 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 of a magnetic field dependent magnetic resonance.\textsuperscript{1} Recently, it was found that a c-axis magnetic field suppressed the intensity of this resonance,\textsuperscript{1,2} as predicted from an analysis of specific heat data.\textsuperscript{3} Since the same effect was not observed in in-plane fields,\textsuperscript{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 (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 \(\langle \Delta_k \Delta_{k+Q} \rangle\) correlator which enters the coherence factors of the spin susceptibility (where \(Q\) 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.\textsuperscript{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 case (c) 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, \(p_s\), is proportional to the gradient of the phase, \(p_s = \hbar \text{e}_\phi/2r\). 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 scale large 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,

\[
\chi(\omega, Q, p_s) = \frac{\chi_0(\omega, Q, p_s)}{1 - J_\Omega \chi_0(\omega, Q, p_s)}.
\] (1)

The bare susceptibility \(\chi_0(\omega, Q, p_s)\), is determined as

\[
\chi_0(\omega, Q, p_s) = - \sum_{k} \sum_{\mu,\nu=\pm} \frac{A^\mu_k A^\nu_{k+Q}}{\omega + E^\mu_k - E^\nu_{k+Q} + i\Gamma} \times (f(E^\mu_k) - f(E^\nu_{k+Q}))
\] (2)

where the excitation spectrum in the presence of a superflow with momentum \(p_s\) is given by

\[
E^\pm_k = \pm \sqrt{\xi^2_k + |\Delta_k|^2 + \delta \xi_k}
\] (3)
with $\delta \xi_k = (\xi_{k+p} - \xi_{k-p})/2$, $\tilde{\xi}_k = (\xi_{k+p} + \xi_{k-p})/2$, and
\[ A^\pm_k = \frac{1}{2} \pm \frac{\tilde{\xi}_k}{E^+_k - E^-_k}, \quad C^\pm_k = \pm \frac{\Delta_k}{E^+_k - E^-_k} \] as coherence factors. The factor $\alpha$ (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, $\chi(\omega, \mathbf{Q}) = \langle \chi(\omega, \mathbf{Q}, \mathbf{p}_s(\mathbf{R})) \rangle$. We evaluated Eq. (4) for a $512 \times 512$ grid of $k$-points and performed the spatial average over 320 $\mathbf{R}$-points. Note 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.

Calculations were performed using a model quasiparticle dispersion in the superconducting state motivated by photoemission measurements. Similar dispersions were found to give a good description of the zero field INS data, including the incommensurate structure observed at energies below resonance. 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 STM measurements. A broadening factor, $\Gamma$, of 2 meV was employed, and a temperature of 13 K.

In Fig. 2 we show our results for the influence of Doppler shifts due to supercurrents on the susceptibility. The exchange coupling, $J_0$, 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 $k = 2a$ (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. 2 shows, the supercurrent has three effects: (a) it shifts the position of the resonance to 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 $\sim 2\Delta$ 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, and a variety of assumed values for $\Delta$ 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. 2 where we find virtually no effect of the Doppler shift on the susceptibility.

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. 2 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 $\langle \Delta_k \Delta_{k+\mathbf{Q}} \rangle$ correlator in the $C_kC_{k+\mathbf{Q}}$ coherence factors (by reducing $\alpha$ to less than 1 in Eq. 3). 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 $k_x = \pi/d$, where $d$ is the separation of nearest neighbor CuO layers). The observed deconvolution inferred from the field dependence of the Josephson plasmon [though, is probably due to the weaker bilayer-bilayer coupling, which is also consistent with small mesa experiments]. 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 feature is seen attributed to an optical Josephson plasmon). For now, though, we will assume that this is a possibility, and test its consequences.

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. 3, we plot the integrated weight versus $\alpha$). We note that the
exponential suppression goes like $1 - H/H^*$, where $H^*$ is a number not much lower than $H_{c2}$, the upper critical field. 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 $\alpha$. This suppression is in good agreement with the calculation, as can be seen in Fig. 3. 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. Therefore, we assume that the resonance is not supported in the region of the vortex core. This assumption is based on five facts: a) the considerable momentum width of the resonance shows that the corresponding spin excitations have a decay length of only two lattice constants, which 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; this would modify the $2\Delta$-edge in $\chi''_\omega$ (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; e) the dip feature in the tunneling density

\[ \chi(\omega) \]

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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. While this conjecture is at this stage admittedly speculative, we believe it deserves further experimental and theoretical investigation.

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