Neutron Resonance in the Cuprates and its Effect on Fermionic Excitations

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We argue that the exciton scenario for the magnetic resonance in the cuprate superconductors yields a small spectral weight of the resonance, in agreement with experiment. We show that the small weight is related to its concentration in a small region of momentum and energy. Despite this, we find that a large fermionic self-energy can indeed be generated by a resonance with such properties, i.e., the scattering from the resonance substantially affects the electronic properties of the cuprates below T_c.

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The magnetic resonance observed in inelastic neutron scattering experiments in both two-layer (YBCO [1,2] and Bi2212 [3]) and single-layer (Tl2201 [4]) cuprates is one of the most striking features of high T_c superconductors. For doping concentrations, x, greater than optimal doping, a sharp peak emerges at T_c and is resolution limited in energy at low T. For x less than optimal doping, a broadened version appears at a pseudogap temperature T^*, and then narrows in energy below T_c. The energy of the peak, $\Omega_{\rm res}$, is found to scale with T_c for all dopings. The peak is centered at momentum $\mathbf{Q} = (\pi, \pi)$, and is part of a collective mode dispersion, with weaker incommensurate "side branches" extending to lower energies [5] .

One of the main issues related to the resonance is whether it can account for the measured changes in the fermionic properties of the cuprates below T_c, via a feedback effect similar to the Holstein effect in phonon mediated superconductors. It is not obvious that this effect is strong, since the total experimental spectral weight of the resonance peak, $I_0 = \int S(\mathbf{q}, \Omega) d^2q d\Omega/(8\pi^3)$, is only a few percent of the local moment sum rule [6], $S(S+1)/3 = 1/4$.

In this paper, we address the issue of whether the smallness of the integrated intensity of the peak precludes strong effects on the fermions. Our main result is that the fermionic self-energy due to scattering from the resonance is strong and unrelated to the small integrated intensity of the peak. We also discuss the relation between the resonance peak and the condensation energy

The origin of the resonance has been the subject of intense debate in recent years. Most theories find that the resonance is a spin exciton that does not exist in the normal state, but emerges in the superconducting state (or, more accurately, when electrons acquire a gap) due to a feedback from the pairing on spin collective excitations. This effect is specific to $d_{x^2-y^2}$ superconductors and has no analog for s-wave superconductors [7]. Moreover, by kinematic constraints, the peak at momentum $\mathbf{Q}$ is due to fermions in the near vicinity of the "hot spots" on the Fermi surface (points separated by $\mathbf{Q}$). For a $d_{x^2-y^2}$ superconductor with a Fermi surface such as that observed experimentally, these fermions have a large gap, Δ. As a result, spin collective excitations have no damping at $T = 0$ up to an energy 2Δ. As the spin exciton is pulled below this 2Δ continuum, it has a zero linewidth unless other effects, such as impurity scattering [8] and (for $T_c < T < T^*$) the pseudogap, are incorporated. The displacement of $\Omega_{\rm res}$ to lower energies from 2Δ increases with underdoping as the spin-fermion coupling gets larger.

By analogy with the Holstein effect, the emergence of the resonance in the exciton scenario should affect the electronic properties of the cuprates: it can give rise to the peak-dip-hump features in the fermionic spectral function, most prominent near the $(\pi, 0)$ points [9] where the peak-dip separation equals the resonance energy [10,11]. It also yields the kink in the quasiparticle dispersion along the (π, π) direction [12], with the kink energy near $\Delta + \Omega_{\rm res}$ [13], the dip in the density of states at about the same energy, and the dip in the SIS tunneling conductance [14] and in the optical conductivity [15] at $2\Delta + \Omega_{\rm res}$ [16,17]. It can also cause subgap peaks in SNS junctions [18]. The issue we address here is the strength of these effects.

From an experimental perspective, the features that could be interpreted as being due to scattering from the resonance have been observed in angle resolved photoemission (ARPES) spectra, SIN and SIS tunneling spectra, and optical conductivity measurements on Bi2212 at various doping concentrations [19]. Furthermore, the resonance energies inferred from ARPES [20] and SIS [14] measurements as a function of doping match $\Omega_{\rm res}$ as measured directly by neutron scattering. The mode extracted from SIS experiments [14] is located very near 2Δ in overdoped materials, but progressively deviates to lower energies with underdoping, as would be expected of a collective excitation inside a continuum gap [14]. In addition, the real part of the fermionic self-energy at the node as a function of temperature has been shown to scale with the resonance intensity [12]. It has been claimed, however, that other effects such as bilayer splitting, particularly in the overdoped cuprates [21], and scattering from phonons [22], can also account for these data.

There are two key points to address in the analysis of the feedback effect on fermions: the values of the spin-fermion coupling g and the dimensionless coupling constant λ, and the dependence of the self-energy on the integrated intensity of the peak.

Consider first the issue of the spin-fermion coupling, g. It is defined via the spin-fermion model:

$$H = H_{\mathrm{ferm}} + H_{\mathrm{spin}} + gS\psi^{\dagger}\sigma\psi. \tag{1}$$

The most straightforward way to extract g is to fit the position of the maximum of the spin susceptibility $\chi''(\mathbf{Q}, \Omega)$ in the normal state. Experimentally, this maximum is located at 20–25 meV in optimally doped YBCO [2]. The data are consistent with a relaxational form for the susceptibility, $\chi^{-1}(\mathbf{Q}, \Omega) = \chi_Q^{-1} - i\Gamma(\Omega)$, whose imaginary part has a maximum given by $\Gamma(\Omega_{\mathrm{max}}) = \chi_Q^{-1}$. Here $\Gamma(\Omega)$ is the imaginary part of the fermionic bubble times g^2, which can be most easily seen by considering the fermionic bubble as a self-energy insertion in the bosonic (spin fluctuation) propagator (an equivalent expression is obtained in the random phase approximation). The fermionic bubble is easily calculated by linearizing the dispersion about the hot spots ($\epsilon_{\mathbf{k}} = v_x k_x + v_y k_y$, $\epsilon_{\mathbf{k}+\mathbf{Q}} = v_x k_x - v_y k_y$) and summing over all 8 hot spots. The result is [11,23]

$$\Gamma(\Omega) = 2g^2\Omega/(\pi v_x v_y). \tag{2}$$

At the hot spots, $v_x \approx v_y \approx v_F/\sqrt{2}$, where v_F is the Fermi velocity at the hot spots. Using the experimental $\chi_Q \sim 13$ states/eV [24], $\Omega_{\mathrm{max}} = 20$ meV, and $v_F \sim 0.4$ eV [25] (in units where the lattice constant is 1) we then obtain $g \sim 1.75 v_F \sim 0.7$ eV.

The dimensionless coupling λ can be extracted from the fermionic self-energy at the lowest ω: $\mathrm{Re}\Sigma(\omega) = -\lambda\omega$. At the same level of approximation as Eq. (2), $\Sigma(\mathbf{k}, \omega)$ is determined as $3g^2$ times a convolution of $\chi(\mathbf{q}, \Omega)$ with $G_0(\mathbf{k}+\mathbf{q}, \omega+\Omega)$ (G_0 is the fermion Green's function, and the factor of 3 is due to spin summation). Again, linearizing the fermionic dispersion about the hot spots, and expanding χ quadratically about Q with a correlation length ξ, we obtain [23]

$$\lambda = 3g^2\chi_Q/(4\pi v_F \xi) = 3v_F/(16\Omega_{\mathrm{max}}\xi). \tag{3}$$

Substituting the above numbers and $\xi \sim 2$, we find $\lambda \sim 2$. We note that λ by definition refers to fermions near the hot spots, and is obtained by coupling to the entire spin fluctuation spectrum.

Our value of g is consistent with fitting resistivity data to spin fluctuation scattering [26] and with Eliashberg calculations of Δ and Ω_{res} [19]. Such a large value of g is also expected on microscopic grounds: in the Hubbard model, the effective g is expected to be of the order of the fermionic bandwidth W [27] which is 1 eV for the cuprates. Our estimate $\lambda \sim 2$ is consistent with the velocity renormalization estimated from normal state ARPES experiments [28]. Moreover, the specific heat: $C = \gamma T$ with experimental $\gamma \simeq 2\frac{\mathrm{mJ}}{\mathrm{g-atK^2}}$ (Ref. [29]) yields in a two-layer system $N_0 \sim \frac{2.8}{1+\lambda}$ eV$^{-1} \sim 1$ eV^{-1}, where N_0 is the (bare) density of states per spin. Again, this N_0 is close to our value $N_0 \sim 1/(\pi v_F) \sim 1$ eV^{-1} (using the previously mentioned number for v_F).

The result that $\lambda > 1$ might question the validity of Eqs. (2) and (3). In general, a Migdal theorem does not exist for spin fluctuations, since spin fluctuations are made out of fermions, and hence the bosonic energy scale is comparable to the (renormalized) Fermi energy for general $\mathbf{q}$. Our theory, though, is based on an expansion of fermionic degrees of freedom about the hot spots, and bosonic degress of freedom about $\mathbf{Q}$. That is, high energy excitation processes have been integrated out, and are absorbed into the definition of χ_Q. This means that in the context of our theory, only low energy vertex corrections are relevant, and they are unimportant for the same reason as in the electron-phonon problem, that is spin fluctuations are slow compared to fermions [23]. For this reason, an "effective" Migdal theorem exists, and justifies Eqs. (2) and (3).

We next discuss the spectral weight of the resonance, and how this affects the fermionic self-energy in the superconducting state. We begin by noting that since the resonance peak is strong at $\mathbf{Q}$, if it were present for all momenta, the total integrated intensity would be $O(1)$. However, the peak exists only in a momentum range between $\mathbf{Q}$ and $\mathbf{Q}_{\mathrm{min}}$, where $\mathbf{Q}_{\mathrm{min}}$ is the momentum connecting the nodal points at the Fermi surface. This occurs since the particle-hole continuum extends to zero frequency at $\mathbf{Q}_{\mathrm{min}}$, and the resonance ceases to exist there. As $\mathbf{q}$ approaches $\mathbf{Q}_{\mathrm{min}}$, both the energy and the intensity of the resonance peak vanish (that is, the incommensurate side branches). This behavior is consistent with the observed "negative" curvature of the resonance dispersion and the progressive reduction of the peak intensity as $\mathbf{q}$ deviates from $\mathbf{Q}$ [30]. The ARPES measurements of the Fermi surface all show that near optimal doping, $\mathbf{Q}$–$\mathbf{Q}_{\mathrm{min}} \approx 0.2(\pi, \pi)$, i.e., the resonance peak exists in a momentum range which constitutes only 6% of the area of the Brillouin zone. This smallness of the momentum range gives rise to the smallness of I_0.

The real issue, though, is whether a small I_0 implies a small fermionic self-energy. We argue that it does not. As just stated, the resonance peak is strong, but exists only in a limited momentum range, which is why I_0 is small. Whether or not the small momentum integrated intensity of the peak matters then depends on whether or not typical bosonic momenta that contribute to the fermionic $\Sigma(\mathrm{k},\omega)$ are within the allowed $\mathbf{q}$ range of the peak. If they are not, then the smallness of I_0 matters. If they are, then it does not. These typical $\mathbf{q}$ can be easily estimated from an analysis of the fermionic self-energy ($\Sigma \sim \int G_0\chi$) discussed above, and for $\omega \leq 100$ meV at which the resonance mode affects the self-energy, are well within the range between $\mathbf{Q}$ and $\mathbf{Q}_{\min}$ for fermions near the hot spots: $|\mathbf{Q} - \mathbf{q}| \sim \omega/v_F \approx 0.08\pi \ll \sqrt{2}(0.2\pi)$. Thus, although the resonance peak occupies only a small portion of the Brillouin zone, it is actually broader than the typical momentum scale for fermions. In this situation, in the calculations of the fermionic self-energy, one can approximate $S(\mathbf{q}, \Omega)$ by its large value in the near vicinity of $\mathbf{Q}$, and neglect the dispersion of the peak. This in turn implies that the small I_0 *does not* matter for the self-energy. We note again in this regard that experimentally [24] $\int d\Omega S(\mathbf{Q}, \Omega) \sim 1.6$ is indeed not small.

We next discuss the relation between the resonance peak and the condensation energy. The issue is whether the resonance peak contribution to the condensation energy is consistent with experiment. This issue is somewhat nontrivial as the internal energy is the sum of the kinetic and the potential energies. The exchange part of the potential energy is related to the difference between the integrated $S(\mathbf{q}, \Omega)$ in the normal and the superconducting states [31]: $E_p = (3J/16\pi^3)\sum_i \int d^2q d\Omega[S_n^{(i)}(\mathbf{q}, \Omega) - S_{\rm sc}^{(i)}(\mathbf{q}, \Omega)](\cos q_x + \cos q_y)$ (the summation over $i = o, e$ goes over odd and even channels in two-layer systems). If we assume that $S^{(e)}$ and $S_n^{(o)}$ are negligible, and approximate $S_{\rm sc}^{(o)}(\mathbf{q}, \Omega)$ by $S_{\rm sc}^{(o)}(\mathbf{q}, \Omega) = \pi\chi_Q\Omega_{\rm res}\delta(\Omega - \Omega_{\rm res})$ for $|\mathbf{Q} - \mathbf{q}| < |\mathbf{Q} - \mathbf{Q}_{\min}|$, and $S_{\rm sc}^{(o)}(\mathbf{q}, \Omega) = 0$ elsewhere, we find $E_p = 3J(2\pi\chi_Q\Omega_{\rm res})(|\mathbf{Q} - \mathbf{Q}_{\min}|/4\pi)^2 \approx 0.05J$. Similar values are found from explicit calculations using the random phase approximation [32]. This energy savings is already a small number. The actual value of the potential energy is, however, even smaller due to compensation from S_n and other nonexchange terms in the Hamiltonian. Eliashberg-type computations of the potential energy including the normal S_n part but without taking into account the restriction on $\mathbf{q}$ found [33] $E_p \sim 0.008J \sim 10$ K. The restriction on $\mathbf{q}$ further reduces this energy. The condensation energy E_c extracted from the specific heat measurements is $E_c \sim 10$ K. This condensation energy is about E_p. In reality, E_c should be greater than E_p since at strong coupling, the kinetic energy decreases in the superconducting state as the fermionic excitations become less diffusive in the superconducting state due to feedback effects again associated with the resonance [34]. In any event, we clearly see that the resonance viewed as a spin exciton for which the intensity at $\mathbf{Q}$ is not small yields a small value of E_c, in agreement with the data.

It is also essential to point out an important difference between the coupling of fermions to the resonance mode in a d-wave superconductor and the coupling of fermions to antiferromagnetic magnons. In the latter case, the spin mode couples to fermions only through gradients, i.e., the renormalized coupling $g_{\rm eff}$ is much smaller than g. This reduction from g to $g_{\rm eff}$ is the result of strong vertex corrections if antiferromagnetic magnons are present in the normal state [35], and occurs because antiferromagnetic magnons are compatible only with a small Fermi surface (hole pockets), in which case g has been absorbed into the definition of renormalized fermions with an SDW energy gap [36]. However, we are treating the metallic phase near optimal doping where a large Fermi surface exists, the normal state spin dynamics is purely relaxational, and the resonance peak appears *only* when fermions acquire a d-wave superconducting gap. Thus, g is the appropriate coupling to use, not $g_{\rm eff}$. The crossover between these two regimes should occur in the low doping regime where the Fermi surface evolves towards small hole pockets. (Note in passing that for these reasons, the resonance mode is not the "glue" for the magnetically mediated pairing theory near optimal doping—this pairing is produced by *overdamped* spin excitations.)

The above picture of the spin resonance and its effect on fermions has been challenged by a number of authors. Perhaps the work which best summarizes these objections is that of Ref. [37]. They argued that $g \sim 14$ meV and $\lambda \sim 10^{-3}$, 2 and 3 orders of magnitude smaller than our values, respectively. The large difference in g is the combination of several factors. First, the value of Γ that we extracted from the data is about 8 times larger than theirs. This is because they equated Eq. (2) with the half-width of the resonance, without taking into account the fact that the resonance width is strongly reduced compared to the normal state because of gapping of the particle-hole continuum. Moreover, from Eq. (2), we see that the full width of the normal state (relaxational) χ is not 2Γ, but rather $2\sqrt{3}\Omega_{\max}$ where $\Gamma(\Omega_{\max}) = \chi_Q^{-1}$. Second, they assumed $\Omega_{\max}$ was the resonance mode energy (40 meV), whereas we used the normal state maximum (20 meV). Third, they assumed an $N_0 \sim J^{-1} \sim 10$ eV^{-1}, i.e., their v_F is about 12.5 times smaller than ours. The combination of these three factors accounts for the factor of 50 difference in g. The even larger discrepancy in λ is due to their coupling only to the resonance (which they treat as an Einstein mode), and not to the entire spin fluctuation spectrum as we have done.

Moreover, they approximated the resonance peak as a product of two δ functions: $S(\mathbf{q}, \Omega) = (2\pi)^3 I_0 \delta(\mathbf{q} - \mathbf{Q})\delta(\Omega - \Omega_{\rm res}) + \ldots$ where dots stand for the nonresonance part. Using this approximation, the estimated fermionic self-energy due to spin-fermion scattering scales as $I_0(g/\Omega_{\rm res})^2$. By their estimates, $g \sim 0.35\Omega_{\rm res}$, $I_0 \ll 1$, and hence the effect on the fermionic self-energy is negligible. As demonstrated above, our estimate for g: $g \sim 0.7$eV $\sim 17\Omega_{\rm res}$ is very different from theirs. This is the primary reason we get a large self-energy, and they get a small one. We emphasize, however, that the approximation that $S(\mathbf{q}, \Omega)$ is a δ function in momentum space leads to a qualitatively incorrect fermionic self-energy, in that, as stated earlier, the typical fermionic momentum scale is actually smaller than the resonance width. Furthermore, in such an approximation, the imaginary part of the self-energy is simply a δ function in energy, since only one bosonic momentum contributes. This is clearly not consistent with experiment. The aspect which is completely missed by using the δ function approximation in $\mathbf{q}$ is that as soon as the resonance has a finite width in momentum space, the internal momentum sum in the Feynman diagram for the self-energy is dominated by the flat fermionic dispersion in the vicinity of the $(\pi, 0)$ points [13]. This is why the self-energy effects are so large for momenta near $(\pi, 0)$, and also why the energy scale at which structure appears in the spectral function (spectral dips and kink energies) is independent of momentum [12].

To summarize, we demonstrated in this paper that the large intensity of the resonance at $\mathbf{Q} = (\pi, \pi)$ is consistent with the small value of the total momentum and frequency integrated intensity of the resonance peak, and with the fact that the magnetic part of the condensation energy is only a small fraction of J. We found that the spin-fermion coupling g is of the order of 1 eV and argued that this value of g is consistent with experiment. This g is sufficiently large that scattering from the resonance can substantially affect the electronic properties of the cuprates below T_c.

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