Vertex corrections in antiferromagnetic spin-fluctuation theories

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(Received 21 January 1997)

We clarify the physical origin of the discrepancy between recent purely perturbative and self-consistent calculations of the vertex correction in the spin-fermion model for cuprates. We argue that perturbative calculations substantially overestimate the strength of the vertex corrections at moderate couplings.

More recently, Amin and Stamp computed the lowest-order vertex corrections numerically, without assuming that the correlation length is large. They found a much larger, negative value of the correction for the same g and argued that the origin of the discrepancy between their and earlier results lies in their more accurate evaluation of the logarithmic approximation. We will argue in this paper that the reason for the discrepancy in fact has a physical rather than a numerical origin. To demonstrate this, we will first compute the vertex corrections analytically, and include terms beyond the logarithmic approximation. We will show that both our present and earlier results in fact yield roughly the same vertex correction (apart from the sign difference) as Amin and Stamp obtained provided we use the same values for both the coupling constant and the spin damping which they used. We will further argue that in optimally doped cuprates, the damping of spin fluctuations is predominantly due to the interaction between spins and low-energy fermionic excitations. In this situation, the actual spin damping has to be computed within the spin-fermion model, as was done in Refs. 4, 5. We will show that in order to obtain the experimentally measured value of the damping, one should either use a much smaller value of the coupling constant g or assume that even without spin-fermion interaction, the fermionic residue Z is smaller than one. Specifically, we will show that g_{eff}=gZ has to be reduced by a factor of 0.28 to reproduce the measured damping rate. This in turn reduces the vertex correction Δg ∝ (g_{eff})^2 by an order of magnitude and brings it in agreement with earlier results.

The spin-fermion model describes fermions coupled to spin fluctuations by

\[ \mathcal{H}_{s-f} = g \sum c_{k,\sigma}^\dagger \tilde{\sigma}_{\alpha,\beta} c_{k+q,\beta} \tilde{S}_{-q}. \]

Here g is the coupling constant, and \( \sigma_i \) are the Pauli matrices. This model neglects the direct fermion-fermion interaction, which can be quite strong, and therefore is valid only near the Fermi surface where the electronic Green’s function...
at $g=0$ possesses the Fermi-liquid form $G(k, \omega_n) = Z/(i\omega_n - \epsilon_k)$, where $\epsilon_k = \epsilon_k - \mu$, and $Z\leq 1$ is a positive constant. The dispersion near the Fermi surface in optimally doped cuprates is assumed to be well described by $\epsilon_k = -2t'\cos k_x \cos k_y - 4t'' \cos k_x \cos k_y$. The fermionic $Z$ factor can be formally eliminated by introducing a new coupling constant $g_{\text{eff}} = gZ$. Clearly, the reduction of $Z$ just implies a reduction of the effective bare spin-fermion vertex which should still be considered as an input parameter for the spin-fermion model.

Further, we need the Hamiltonian for the localized spins. In general, it should have the form of some Heisenberg model from which one can extract the dynamical spin susceptibility $\chi(q, \omega_n)$. The exact form of this Hamiltonian is however not known except very close to half-filling, where it reduces to a nearest-neighbor Heisenberg model. Away from half-filling, one can rely on a less justified but still physically plausible phenomenological approach in which one just assumes that the dynamical spin susceptibility is strongly peaked near the antiferromagnetic momentum $Q = (\pi, \pi)$ and behaves at low energies as $\chi(q, \omega_n) = \chi_0/(1 + \xi^2 q^2 + i |\omega_n|/\omega_d)$. Here $\xi = q - Q$, $\xi$ is the magnetic correlation length, and $\omega_d \propto \xi^{-2} / \gamma$ is a typical spin-fluctuation frequency which is much smaller than any other energy scales in the problem due to the proximity to the antiferromagnetic instability.

The amplitude of the vertex correction depends on the value of the incoming and outgoing fermionic momentum. For the pairing mechanism in high $T_c$, the most relevant interaction is between $k$ points located such that both $k$ and $k + Q$ are near the Fermi surface in which case both fermions have low energies. The points on the Fermi surface which are connected by $Q$ are called “hot spots.” In our further considerations, we will focus on vertex corrections at these points. Monthoux$^5$ as well as Amin and Stamp$^7$ considered vertex corrections for other $k$ points and found that the relative correction is the largest at the hot spots.

The second-order vertex correction is presented in Fig. 1. The computation of the correction is tedious but straightforward: we expand the fermionic energies near hot spots as $\epsilon_k - \mu = \nu \cos \phi_i$ $\epsilon_{k+Q} - \nu = \nu \cos (\phi + \phi_0)$ where $\nu = k + k_0$ measures the deviation from a hot spot, $\nu = (u_x^2 + u_y^2)^{1/2}$, $\phi_i = \partial \epsilon_i / \partial k_{i|\gamma}$, and $\phi_0$ is the angle between the normals to the Fermi surface at the hot spots (see Fig. 2). For $u_x > u_y > 0$, $\phi_0$ is given by $\phi_0 = \pi/2 + 2 \tan^{-1} u_x / u_y$. Substituting the expansion for the energies into the vertex correction and performing the integration over $k$ and $\phi$, we obtain

$$\Delta g = g^2 Z^2 \chi_0 \omega_d \left[ \frac{\ln(\sin(\phi/2))}{\cos \phi + \cos \phi_0} \right] \times \ln \frac{\sin(\phi/2)}{\delta^2} + O(\delta^2),$$

where $\delta = \xi \omega_d / \nu \approx \xi^{-1} \ll 1$. Notice that not only the term $-\ln \xi$ but also the $\xi$-independent contribution to $\Delta g$ is universal in the sense that they do not depend on the upper cutoff in the integration over $\vec{k}$. Previous analytical calculations of the vertex correction$^4$ restricted with the $|\ln \delta|$ term only. We will see, however, that for the range of parameters relevant to cuprates both terms almost equally contribute to the vertex renormalization.

We now evaluate the vertex correction for the same experimentally motivated set of parameters as was used in Ref. 7, namely $t = 0.25$ eV, $t' = 0.45t$, $|\mu| = 1.46t$, $\omega_d = 14$ meV, $\xi = 2.5a$, $g = 0.64$ eV, $\chi_0 = 80$ states/eV, and $Z = 1$. For this set of parameters we obtain $\phi_0 = 1.78$ and $\delta = 0.27$. Evaluating the integral over $\phi$, we find $\Delta g / g \approx 0.55$ which is close to $\Delta g / g \approx -0.7$ obtained by Amin and Stamp apart from the different overall sign which we discuss later. We see therefore that the discrepancy between Amin and Stamp and others is not associated with the accuracy of the calculations. In fact, if we computed $\Delta g$ only with logarithmic accuracy, as was done in Refs. 4, 5, we would obtain an even larger value for $\Delta g / g$.

We now argue that the above results should be substantially scaled down. The point is that one has to carefully examine the physical origin of the spin damping. The damping which appears in Eq. (1) as an input parameter, is the bare damping due to a direct spin-spin interaction. It does not include the contribution from the interaction with low-energy fermions. This last contribution should be computed within the spin-fermion model of Eq. (1) by evaluating the imaginary part of the self-energy for the spin propagator shown in Fig. 3. It is essential that this calculation does not take us outside the range of applicability of the spin-fermion model since the imaginary part of the self-energy is confined to fermionic excitations in the vicinity of the Fermi surface, where the spin-fermion model is valid.

In any case, near optimal doping, the damping due to the direct spin exchange is rather weak and is very likely to be
overshadowed by the damping produced by the interaction with fermions. In other words, $\omega_{vd}$ inferred from experiments is not the same as $\omega_{sf}$ in the bare spin susceptibility. Indeed, one can include the renormalization of the damping into the vertex correction diagram of Fig. 1 by assuming that the wavy line already contains the full $\omega_{sf}$. This was actually assumed in earlier studies. However, in adopting this approach, we still have to compute $\omega_{sf}$ explicitly and see whether it agrees with the value inferred from experiment.

The computation of $\omega_{sf}$ proceeds along the same line as the computation of the vertex corrections. We first observe that since $\omega_{sf}$ is related to the damping at momentum transfer $Q$, the fermions in the particle-hole bubble are located near the hot spots, since otherwise they cannot simultaneously be close to the Fermi surface. We therefore can use the same expansion in $\mathbf{k}$ in the computations of $\omega_{vd}$ as was used in the calculation of the vertex correction. We first compute the lowest-order self-energy diagram for the spin susceptibility. Evaluating the imaginary part of the diagram in Fig. 3, we obtain

$$\omega_{sf} = \frac{\pi}{4} \left| \sin \phi_0 \right| \frac{v^2}{g^2 Z^2 \chi_0}.$$  

Using the same parameters as above, we obtain $\omega_{sf} \approx 1.06$ meV which is more than ten times less than $\omega_{vd} = 14$ meV used in the above calculations of $\Delta g/g$. Let us suppose now that higher-order diagrams are irrelevant. In this situation, a way to restore the experimentally inferred value of $\omega_{sf}$ is to assume that $g_{\text{eff}}$ is in fact different from $g$ either because the actual interaction is weaker or because the fermions are not free particles, i.e., $Z < 1$. Specifically, we need $g_{\text{eff}} = 0.28g$ to obtain the correct value of $\omega_{sf}$. In other words, the set $g = 0.64$ eV and $Z = 1$ is incompatible with the experimental value of $\omega_{sf}$.

We now observe that the same $g_{\text{eff}}$ also governs the strength of the vertex correction. Substituting $g_{\text{eff}} = 0.28g$ into Eq. (2), we immediately obtain $\Delta g/g \approx 0.04$ for the same set of parameters as we used above. This value is indeed very small. Moreover, Eq. (2) is actually somewhat misleading as one could infer from it that the vertex correction scales with $g_{\text{eff}}$. This is in fact true only for very small couplings when the damping due to the spin-fermion interaction is actually smaller than the one due to the direct spin-spin exchange. At larger $g_{\text{eff}}$, the dependence of the coupling constant in Eq. (2) is in fact eliminated since $\omega_{vd}$ itself scales as $(g_{\text{eff}})^{-2}$. Substituting Eq. (3) into Eq. (2), we obtain neglecting terms of $O(\delta^2)$

$$\frac{\Delta g}{g} = -\frac{\left| \sin \phi_0 \right|}{4 \pi^2} \text{Re} \int_0^\pi d \phi \frac{\ln(\sin(\phi/2))}{\cos \phi + \cos \phi_0} \ln \frac{\sin(\phi/2)}{\delta^2}.$$  

Notice that the correction is nearly universal—it depends only on $\phi_0$, but not on the fermionic velocity and the parameters of the spin susceptibility. Evaluating the vertex correction using Eq. (4), we indeed recover the same very small vertex correction as above. Note in passing that the very fact that the lowest-order vertex correction is small justifies, at least partly, the restriction with the lowest-order diagrams in the calculations of both $\Delta g/g$ and $\omega_{sf}$ as higher-order diagrams most probably contain higher powers of small $\Delta g/g$ from Eq. (4).

The earlier analytical calculations of the vertex correction assumed that the system is at the edge of the antiferromagnetic instability, i.e., the correlation length is very large. It follows from Eq. (4) that since $\Delta g \omega_{sf} \approx \xi^{-1}$ tends to zero, $\Delta g$ diverges logarithmically. In this situation, higher-order corrections are indeed relevant. The higher-order vertex corrections were studied in Refs. 4, 5. It was found that the logarithms sum up to a power law, and the full vertex takes the form

$$g_{\text{full}} = g_{\text{eff}} \left( \frac{\xi}{a} \right)^\beta,$$

where

$$\beta = \frac{\left| \sin \phi_0 \right|}{2 \pi^2} \text{Re} \int_0^\pi d \phi \frac{\ln(\sin(\phi/2))}{\cos \phi + \cos \phi_0}.$$  

We see that the full vertex diverges when the correlation length becomes infinite. However, $\beta$ is numerically quite small for all $\phi_0$ (it varies between 1/16 and 1/8 for $\phi_0$ between $\pi/2$ and $\pi$) such that one needs to be very close to the transition point to observe the enhancement of the vertex. Besides, Eq. (5) is valid, for $\xi \rightarrow \infty$, only if the antiferromagnetic transition occurs at small to moderate $g$, before self-energy corrections produce any changes in the Fermi surface geometry. This last assumption is probably not satisfied in cuprates where the antiferromagnetic transition occurs very close to half-filling where $g$ is already large and comparable to the Hubbard $U$.

A somewhat different though conceptually similar calculation of the vertex correction was performed numerically by one of us. In this approach, the bare fermions are considered as free particles, but the internal fermionic lines in Fig. 1 include self-energy corrections. For the above set of parameters, these self-energy corrections reduce the quasiparticle residue at the Fermi surface which in turn reduces the total vertex correction to $\Delta g/g \sim 0.04$ consistent with our analytical results. Note in passing that the reduction of $Z$ is consistent with photoemission data which show that even at optimal doping, the spectral area of the quasiparticle peak is substantially reduced compared to the one for noninteracting electrons.

Finally, we want to discuss the overall sign of the vertex correction. We have already mentioned that the sign obtained in earlier calculations and confirmed in this work is opposite to the one obtained by Amin and Stamp. Actually, a
simple way to check the sign of the correction is to consider the limit where the coupling constant is much larger than the fermionic bandwidth, $W$. In this limit, the electronic structure develops precursors of the spin-density-wave (SDW) state, as two of us have recently demonstrated explicitly. This process is accompanied by a splitting of a single quasiparticle peak in the spectral function into two peaks (precursors of the valence and conduction band), separated by the gap $g$. The chemical potential $\mu$ remains in the lower band, and to first approximation we then have $\mu = -g/2$. Further, in the true SDW state, the Ward identity implies that the fully renormalized spin-fermion vertex vanishes for magnon momentum $q = Q$. The mean-field SDW calculations confirm this result and also show that the full vertex is substantially suppressed from $U$ to $O(W)$ for all momenta. In the disordered state but with strong precursors of the SDW state, the vertex indeed does not vanish at $Q$, but it should be much smaller than the bare one (our argument here parallels the one recently displayed by Schrieffer). In other words, for large $g$, the vertex correction should be negative and nearly cancel the bare vertex. Meanwhile, a simple examination of Eq. (6) in Ref. 7 shows that for large negative $\mu$, the vertex correction is positive, i.e., $\Delta g/g \to +1$ rather than tending to $-1$ which is necessary to obtain the physically motivated strong reduction of the vertex. We therefore believe that the sign of the vertex correction reported in Ref. 7 is incorrect.

We thank D. Pines and P. C. E. Stamp for useful conversations. The work by A.Ch. and D.M. has been supported by the NSF Grant No. DMR 9629839. P.M. acknowledges support from the National High Magnetic Field Laboratory and the State of Florida. A. Ch. acknowledges support from the A. P. Sloan Foundation.

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4 A. Chubukov, Phys. Rev. B 52, R3840 (1995). The expression for the vertex correction in this paper should contain $0.5 \ln \sin \phi/2$ instead of $\ln \cos \phi/2$.
7 M. H. S. Amin and P. C. E. Stamp, Phys. Rev. Lett. 77, 3011 (1996). Notice that their definition of $g$ is by a factor of $\sqrt{3}$ larger than ours.
8 Diagrammatically, this implies that each wavy line includes a set of bubbles made of two fermions.