Vertex corrections in antiferromagnetic spin fluctuation theories

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Abstract

We calculate the first vertex correction $\delta \Lambda_k$ to the bare vertex $\Lambda_0$ in the nearly antiferromagnetic spin fluctuation Fermi liquid theory of the cuprate superconductor $\text{YBa}_2\text{Cu}_3\text{O}_7$. It is calculated for $k$ on the Fermi surface, and $Q = (\pm \frac{\pi}{a}, \pm \frac{\pi}{a})$. We find that the dimensionless ratio $|\delta \Lambda_k|/\Lambda_0$, which parametrizes the vertex correction, is not small. It is a maximum for $k = k_h$, where $k_h$ is a “hot spot” on the Fermi surface. This makes large quantitative corrections to the theory.

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Most theories of the cuprate superconductors are either (i) phenomenological attempts to tie together many different experiments, or (ii) attempts at a “microscopic” derivation, beginning from models such as the Hubbard or t-J Hamiltonians.

Of the variety of phenomenological theories, one of the most widely-discussed is that involving antiferromagnetic (AFM) spin fluctuations in a random-phase approximation (RPA) model of a nearly AFM Fermi liquid, in the optimally-doped regime [1–3]. For weak doping a Non-Linear Sigma (NLσ) model is used [4–6], but no attempt is made to deal with the intervening metal-insulator transition. This transition plays a central role in the more microscopic theories, many of which do not yield a Fermi liquid state except at high T and/or rather large doping; instead one finds that “singular interactions” are generated [7–9], and these inevitably give a non-Fermi liquid normal state [7–10], even at optimal doping. However they also yield strong AFM spin fluctuations [10,11], as do some other microscopic approaches; a wide variety of phenomenological approaches involving AFM spin fluctuation is possible.

To decide between competing theories it is useful to check their internal consistency. Several analyses have been made of the critical properties of AFM spin fluctuations [11–13], but here we wish to focus specifically on the Fermi liquid model [1–3]. We find, in agreement with earlier work [12,13], that once the nearly AFM form of the spin fluctuation spectrum,

\[ \chi(q,\omega) = \frac{\chi_Q}{1 + \xi^2 (q - Q)^2 - i\omega/\omega_{SF}} \]  

has been assumed for \( q \) near \( Q = (\pm\pi a, \pm\pi a) \), and provided we assume from the outset a Fermi liquid model, then no singularities strong enough to destroy Fermi liquid behavior emerge in the fermion spectrum, provided \( \xi \) and \( \omega_{SF} \) are finite. However we also find that a detailed quantitative determination of vertex corrections shows that previous estimates of these have been over-optimistic - they are not small. This has important quantitative repercussions for the theory.

We start from a model Hamiltonian
\[ \mathcal{H} = \sum_{p, \sigma} \epsilon_p \psi_{p\sigma}^\dagger \psi_{p\sigma} + \frac{\bar{g}}{2} \sum_{q, k, \alpha, \beta} \psi_{k+q\alpha}^\dagger \psi_{k\beta} \sigma_{\alpha\beta} S(-\mathbf{q}) \] (2)

where

\[ \epsilon_p = -2t [\cos(p_x a) + \cos(p_y a)] - 4t' \cos(p_x a) \cos(p_y a) - \mu \] (3)

is the quasiparticle dispersion relation [3,4], with \( t = 0.25 \text{eV} \) and \( t' = -0.45t \). The presence of \( t' \) allows “hot spots” on the Fermi surface \( S_F \) (FIG. 1) which can be connected by \( \mathbf{Q} \); this leads to singular behavior when the gap in (1) disappears [13,15]. \( S(\mathbf{r}) \) is the spin fluctuation density operator; use of (2), with a bosonic spin fluctuation propagator (1) and a phenomenological interaction \( \bar{g} \), with a bosonic spin fluctuation propagator [11] and a phenomenological interaction \( \bar{g} \), allows one to develop the usual “paramagnon” effective field theory [10]. The first vertex correction can be calculated for general external momenta [17]; here we concentrate on the interaction between a Fermi surface electron and a spin fluctuation with \( \mathbf{q} = \mathbf{Q} \) (FIG. 2) for which the lowest vertex correction is

\[
\frac{\delta \Lambda_k}{\Lambda_o} = -\frac{\bar{g}}{4V} \sum_{\mathbf{Q}'} \int \frac{d^2q}{(2\pi)^2} \frac{d\omega}{2\pi} \chi'(\mathbf{Q}' + \mathbf{q}, \omega) G(k + \mathbf{Q}' + \mathbf{q}, \omega) G(k + \mathbf{Q}'' + \mathbf{q}, \omega)
\] (4)

where \( \delta \Lambda_k = \delta \Lambda(k, \epsilon = 0; \mathbf{q} = \mathbf{Q}, \Omega = 0) \) and \( \mathbf{Q}'' = \mathbf{Q} + \mathbf{Q}' \); the sum over \( \mathbf{Q}' \) takes care of Umklapp processes. In the reduced Brillouin zone \( \mathbf{Q}'' = (0,0) \). Note that the overall sign of the graph in FIG. 2 is negative, i.e., eqtn. (4) is negative; the bare vertex \( \Lambda_o = \frac{\pi}{2} \) in eqtn. (4) is positive.

We concentrate on \( \delta \Lambda_k \), with \( k \in S_F \) (here \( S_F \) is the Fermi surface) because it gives an indication of the size of vertex corrections. This is because in general \( |\delta \Lambda(k, \epsilon; \mathbf{q}, \Omega)| \) exceeds \( |\delta \Lambda_k| \) (in fact it diverges along a surface in k-space, for given values of \( \mathbf{q}, \Omega \) and \( \epsilon \)); thus one cannot argue, even after integrating over one or more of its arguments, that \( |\delta \Lambda(k, \epsilon; \mathbf{q}, \Omega)| \) will lead to corrections smaller than one would get from just using \( \delta \Lambda_k \) (our argument here parallels Migdal’s [18]). More generally one finds that if \( \Omega \ll q_{vF}, \Delta \), where \( \Delta \) is the spin gap, then \( \delta \Lambda_k \) is a good approximation to \( \delta \Lambda(k, \epsilon; \mathbf{q}, \Omega) \). Writing (4) as

\[
\frac{\delta \Lambda_k}{\Lambda_o} = -\frac{\bar{g}}{4V} \sum_{\mathbf{Q}'} \int \frac{d^2q}{(2\pi)^2} \frac{d\omega}{2\pi} \frac{\chi''(\mathbf{Q}' + \mathbf{q}, \omega)}{\epsilon_{k+\mathbf{Q}'+\mathbf{q}} - \epsilon_{k+\mathbf{Q}'+\mathbf{q}} - \omega} \frac{\epsilon_{k+\mathbf{Q}'+\mathbf{q}} - \omega}{2} - \frac{\epsilon_{k+\mathbf{Q}'+\mathbf{q}} - \omega}{\epsilon_{k+\mathbf{Q}'+\mathbf{q}} + \omega} = -\frac{g^2}{12\pi^3} \frac{\chi Q}{\omega_{SF}^2} \left( \frac{\omega_{SF}}{\mu} \right)^2 T_k
\] (5)
where $g^2 = \frac{3}{4} \bar{g}^2$ and $\mathcal{I}_k$ is dimensionless; we define $g$ to correspond directly with the coupling constant $g$ used in Monthoux and Pines [3]. At zero temperature one has

$$
\mathcal{I}_k = \int_{-2\pi}^{2\pi} d\bar{q}_x \int_{-2\pi}^{2\pi} d\bar{q}_y \frac{1}{\bar{\epsilon}_1 - \bar{\epsilon}_2} \left[ \text{Sgn}(\bar{\epsilon}_1) G_1(\bar{q}, \bar{\epsilon}_1) - \text{Sgn}(\bar{\epsilon}_2) G_1(\bar{q}, \bar{\epsilon}_2) - G_2(\bar{q}, \bar{\epsilon}_1) + G_2(\bar{q}, \bar{\epsilon}_2) \right]
$$

(6)

where $\bar{q}_x = q_x a$, etc.; $\bar{\epsilon}_1 = \epsilon_{k+Q+q}/\mu$ and $\bar{\epsilon}_2 = \epsilon_{k+Q''+q}/\mu = \epsilon_{k+q}/\mu$. $G_1$ and $G_2$ are defined by

$$
G_1(\bar{q}, \bar{\epsilon}) = \frac{\pi X}{2(\bar{\epsilon}^2 + X^2)}
$$

(7)

$$
G_2(\bar{q}, \bar{\epsilon}) = \frac{\bar{\epsilon} \ln(X/|\bar{\epsilon}|)}{\bar{\epsilon}^2 + X^2}
$$

(8)

with $X = [1 + (\xi a)^2 (\bar{q}_x^2 + \bar{q}_y^2)] (\omega_{SF}/|\mu|)$.

$\mathcal{I}_k$ can be investigated both analytically and numerically. Here we calculate it for two different points in k-space, both on the Fermi surface (see FIG. 1); $k_1$ makes a $45^\circ$ angle with $k_x$, and $k_h$ is a “hot spot” wave vector.

In order to obtain a value for $\delta \Lambda_k$, we need values for the spin fluctuation energy $\omega_{SF}$, the correlation length $\xi$, the susceptibility $\chi_Q$, the coupling constant $g$, and the chemical potential $\mu$ (which is determined by the electron filling factor $n$). There are different values reported in the references [3,19,20]. We have evaluated $\delta \Lambda_k$ for $k = k_1, k_h$, in two ways, viz. (a) by assuming various published values for the different parameters, and (b) by making the simple assumption that one is very close to an AFM instability, and then, in the spirit of RPA, imposing the condition $|\langle \bar{g}/2 \rangle \Pi^{(1)}(Q,0)| = 1$ where $\Pi^{(1)}(Q,\omega)$ is the electron-hole bubble. Numerical calculation gives $|\Pi^{(1)}(Q,0)| = 2.6(eV)^{-1}$ and thereby $g = 0.67$ eV, assuming $n=0.75$ and the band structure in (3). Since $\omega_{SF}/|\mu| \ll 1$, this value of $g$ should be a very good guess, within a naive RPA scheme.

The results are summarized in Table I. We use two different values for $\omega_{SF}$; these are the two different values quoted by Monthoux and Pines et al. [3]. We also use two different values for the coupling constant $g$, quoted from MPI and MPII (see ref. [3] again). We use
values of $\xi = 2.5a$, $\chi_Q = 80$ states/eV (from [3]) and $n=0.75$, appropriate to YBa$_2$Cu$_3$O$_7$ (again quoted from [3]). This value of $n$ corresponds, with the band structure in (4), to a value of $|\mu| \sim 1.46t \equiv 0.365$ eV.

We see that even the values for the vertex correction calculated from the simple RPA model (b) are not small; as in the standard discussion of Migdal’s theorem, the importance of vertex corrections appears in the ratio $|\delta\Lambda_k|/\Lambda_\circ$. If one takes values of $g$ from the literature [3], this ratio is quite unreasonably large (as large as 2.43 for the hot spots in the model used by MPI). Thus vertex corrections are clearly very important. The values we quote for $|\delta\Lambda_k|/\Lambda_\circ$ are considerably larger than previous estimates [3,22,23]. The reason for this difference with previous work can be tracked back to the factor $I_k$, which is impossible to guess from purely dimensional arguments. In fact if we drop the factor $I_k$ from $\delta\Lambda_k$, we get an order of magnitude estimate for $\delta\Lambda_k$ given by

$$\frac{|\delta\Lambda_k|}{\Lambda_\circ} \sim O\left[\frac{g^2}{4\pi^3}\frac{\chi_Q^4}{|\mu|\omega_{SF}}\right] \ll 1$$

which is broadly in agreement with previous estimates (see eg. Millis [22]); $\chi_Q$, $\omega_{SF}$ and $g$ must be redefined to conform with the parametrizations in this paper).

In fact however $I_k$ is surprisingly large, and also shows a significant variation around the Fermi surface, with a maximum at the hot spots, and a minimum at intermediate wave-vector like $k_1$. We should emphasize here that analytic calculations of $\delta\Lambda_k$ have to be approximated rather carefully in order to give reasonable agreement with the numerical results in Table I. Approximations such as those of Hertz et al. [24] (see also [23]), which try to separate off a rapidly-varying (in $q$-space) contribution from $\chi''(q, \omega)$, give quantitatively incorrect results (including a completely unphysical $\ln[(k - k_h)a]$ divergence as one approaches the hot spot). A more detailed discussion of the behavior of $I_k$ is given in ref. [17].

One might suppose that $I_k$ is large simply because of the band structure (ie., because of van Hove singularities, or the hot spots). If this were true one could argue that the quasiparticle weight ought to be renormalised down near these singular points in the Brillouin zone, and that this would considerably reduce the vertex correction. In fact however we find
this is not the case; this can be checked analytically by suppressing the regions immediately around the hot spots in the integral for $I_k$, or by simply redoing the numerical calculation for a slightly different band structure. We find that suppressing the hot spots entirely, reduces the vertex correction by a factor which is everywhere less than 2 (and which differs very little from unity when $k$ is far from a hot spot). Thus we do not believe that incorporating self-energy corrections near the hot spots would significantly reduce the vertex correction.

We re-emphasize here that these results do not necessarily invalidate the internal consistency of the Fermi liquid starting point, in this theory. However they do show that the theory cannot be trusted quantitatively, at least in the usual RPA form. As is well known the RPA is not a “conserving approximation”, and for spin fluctuation theories this makes it unreliable (cf. ref. [16], especially section 3). It is useful to compare the case of nearly ferromagnetic $^3$He liquid, where vertex corrections are also quite large, and where use of the paramagnon model yields values for $m^*/m$ which are off by a large factor [21]. Thus if we use melting curve Landau parameters, $F_0^A \sim 0.75$ and $F_1^S \sim 15$, we infer a value for the Stoner factor $S \sim 24$ which yields $m^*/m = \frac{9}{2} \ln S \sim 15$, in the paramagnon model. This is roughly 2.5 times the correct value of $\sim 6$ (note that the first vertex correction is $\delta \Lambda/\bar{I} \sim \ln S \sim 3$ in this model), and no amount of self-consistent summing of diagrams can cure this numerical problem.

Similar problems can clearly occur in the present AFM spin fluctuation model. We believe this is the main reason for the difficulty one encounters in the MP models, in determining a value for $g$ that (a) gives the correct superconducting $T_c$, and (b) is consistent with the observed spin susceptibility.

To check the structure at higher order, we have also estimated the contributions from the graphs containing 2 spin fluctuation lines (there are actually 7 distinct graphs at this level), and found that some of them are also large for the values of $g$ used above [17]. Thus, just as for the case of nearly ferromagnetic $^3$He, we see no reason to believe, for the values of the parameters given in the table, that performing infinite graphical sums will lead to results which are numerically more reliable, even if they do converge to some smaller renormalised
vertex-there will always be other diagrams with large values, which will in general give uncontrolled contributions.

It is interesting to compare these results with some other recent investigations. In the weak-coupling limit, Chubukov [13] has calculated the leading vertex corrections to $g$, concentrating on the gapless case; in the case where there is a gap, he finds that the renormalised coupling is also small (for realistic values of the gap). On the other hand Schrieffer [25] has argued that a correct formulation of the theory, even in the weak-coupling limit, must take account of the short-range local antiferromagnetic order even in the normal state-if this done, he finds that a weak-coupling calculation shows very strong suppression of the vertex when one is close to the antiferromagnetic transition. This theory seems rather interesting-note that a related calculation by Vilk and Tremblay [26] finds that the existence of such a short-range antiferromagnetic order will cause a breakdown of the Fermi-liquid starting point itself! Thus the question of what is the correct theory itself is rather confused, even in the weak-coupling regime. It is certainly not clear how any of these arguments will work in the regime discussed in this paper, when $g$ is not small enough to control the magnitude of the vertex corrections.

It is of course crucial that these higher-order corrections also be included in any version of this theory that tries to reconcile different experiments - as emphasized by Pines [20], the justification of the theory stands or falls on its ability to do this quantitatively. It is possible that such a programme might succeed if one can show that the actual parameters $g$, $\omega_{SF}$, and $\chi_Q$ are such that $|\delta \Lambda_k|/\Lambda_o$ is considerably less than one (ie., if one is genuinely in the weak-coupling regime). This would also be true of versions of the theory in which $\omega_{SF}$ depends on $g$, whilst the spin gap becomes an independent parameter [13]; or of the theory of Schrieffer cited above [25]. On the other hand if $|\delta \Lambda_k|/\Lambda_o > O(1)$, we see no hope that such a scheme could succeed quantitatively (in., eg., the calculation of $T_c$), since the vertex corrections become large.

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Canada, and by the CIAR.
TABLE I. Calculated values of the vertex correction $\delta \Lambda_k$ for two different wave-vectors $k_1$ and $k_h$ on the Fermi surface (columns 4 and 6 in the table). The papers MPI and MPII (ref. 3) give different values for $g$, and different values for $\omega_{SF}$. From the values for these two models one calculates $I_k$ in equation (6), and thence $\delta \Lambda_k / \Lambda_\circ$. The third model is the naive “RPA” model described in the text, for which $g$ is determined; we have calculated $I_k$ and $\delta \Lambda_k / \Lambda_\circ$ for two values of $\omega_{SF}$ given in MPI and MPII respectively.

|       | $g$ (eV) | $\omega_{SF}$ (meV) | $I_{k_1}$ | $\delta \Lambda_{k_1} / \Lambda_\circ$ | $I_{k_h}$ | $\delta \Lambda_{k_h} / \Lambda_\circ$ |
|-------|----------|---------------------|-----------|----------------------------------------|-----------|---------------------------------------|
| MPI   | 1.36     | 7.7                 | 78.6      | -1.81                                  | 105.6     | -2.43                                 |
| MPII  | 0.64     | 14                  | 49.6      | -0.46                                  | 73.4      | -0.68                                 |
| “RPA” | 0.67     | 7.7                 | 78.6      | -0.44                                  | 105.6     | -0.59                                 |

Table continues...
FIG. 1. Fermi surface in the first Brillouin zone, with the value for $t$ and $t'$ given in the text; and we assume $n=0.75$. Calculations are presented here for the wave vectors $k_1$ and $k_h$. 
FIG. 2. First correction $\delta \Lambda_k$ to the bare vertex, for an incoming fermion with momentum $k$ and energy 0 (relative to the Fermi energy), interacting with a fluctuation of wave-vector $Q$ and zero energy.
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