Vertex Corrections in the Spin-fluctuation-induced Superconductivity

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We evaluate vertex corrections to \( T_c \) on the basis of the antiferromagnetic spin-fluctuation model of the high-\( T_c \) superconductivity. It is found that the corrections are attractive in the \( a_x^+a_y^2 \) channel, and they become appreciable as we go through an intermediate-coupling regime of \( T_c \approx 100K \), the maximum \( T_c \) attainable in the one-loop Eliashberg calculation.

KEYWORDS: high-\( T_c \) superconductor, antiferromagnetic spin fluctuation, vertex correction

As a model for the high-\( T_c \) superconductivity, the spin fluctuation mechanism has been one of the most widely discussed\(^{1,2} \). The model assumes that quasiparticle is coupled with antiferromagnetic spin fluctuation, represented by a peculiar low-energy expression for the magnetic susceptibility\(^{3} \). The phenomenological coupling constant to fit the transition temperature \( T_c \) is used to explain, among others, the anomalous transport properties consistently with the formal perturbation theory\(^{1,2,3} \). On the other side, from a microscopic point of view, numerical studies based on the fluctuation exchange (FLEX) approximation\(^{14} \) have been carried out by many authors to estimate \( T_c \) as well as to explain the deviations from the normal Fermi liquid behavior\(^{15,16,17} \). Computational feasibility of these strong coupling theories rests on the effective use of a fast Fourier transform (FFT) algorithm. To ascertain the quantitative aspect of the theories, corrections coming from higher-order terms are investigated for the vertex function at some fixed external momenta, e.g., on the basis of the spin-fluctuation model, and the qualitative features of the effect are emerging to some extent\(^{18,19,20,21,22,23,24} \). However, the total effect of the vertex corrections on the physical observables is yet to be estimated numerically. Indeed to do this is generally formidable because of the inapplicability of the FFT to a required additional sum on internal frequency and momentum. In this paper, we manage to evaluate the vertex corrections to \( T_c \), and discuss questions of convergence of the formal perturbation theory with respect to the coupling constant.

To put it concretely, the following investigation is based on the model of Monthoux and Pines (MP)\(^{25} \), in which the self-energy \( \Sigma(p, i\omega_n) \) is determined as a self-consistent solution of the equations,

\[
\Sigma(p, i\omega_n) = g^2 T \sum_{q,m} \chi(q, i\nu_m) G(p - q, i\omega_n - i\nu_m),
\]

and

\[
G(p, i\omega_n)^{-1} = G^{(0)}(p, i\omega_n)^{-1} - \Sigma(p, i\omega_n) + \delta \mu,
\]

where

\[
G^{(0)}(p, i\omega_n) = \frac{1}{i\omega_n - \varepsilon_p + \mu^{(0)}},
\]

and

\[
\varepsilon_p = -2t(\cos p_x + \cos p_y) - 4t' \cos p_x \cos p_y.
\]

In eq. (\( \Box \)), \( \chi(q, i\nu_m) \) as a function of the Matsubara frequency \( \nu_m = 2m\pi T \) is inferred from the low-energy form of the magnetic susceptibility\(^{25} \)

\[
\chi(q, \omega) = \frac{\chi_q \omega_A}{\omega_A - i\omega},
\]

where

\[
\omega_A \equiv \omega_A(1 + \xi^2(q - Q)^2), \quad Q = (\pi, \pi),
\]

for \( q_x > 0 \) and \( q_y > 0 \). We assume

\[
\chi(q, i\nu_n) = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\Im \chi(q, \omega)}{i\nu - \omega} d\omega
\]

\[
= \frac{2}{\pi} \int_{0}^{\infty} \frac{\omega \Im \chi(q, \omega)}{\nu^2 + \omega^2} d\omega \quad (n \neq 0)
\]

\[
= \chi(q, \omega = 0) \quad (n = 0)
\]

Here it is noted that a cutoff \( \omega_0 \) has to be artificially introduced so as to meet the condition \( \chi(q, i\nu_n) \rightarrow 1/\nu_n \) as \( |\nu_n| \rightarrow \infty \). For eq. (\( \Box \)), the integral in eq. (7) is analytically evaluated:

\[
\chi(q, i\nu_n) = \frac{2\chi_q \omega_A}{\nu^2 - \omega_q^2} \left( |\nu_n| \tan^{-1} \frac{\omega_q}{|\nu_n|} - \omega_q \tan^{-1} \frac{\omega_n}{\omega_q} \right).
\]

To estimate the critical temperature \( T_c \), the linearized gap equation is used,

\[
\Phi(p, i\omega_n) = -\frac{T}{\Omega} \sum_{p', \nu_n'} V(p, i\omega_n; p', i\nu_n') \times \left| G(p', i\nu_n') \right|^2 \Phi(p', i\nu_n'),
\]

where \( \Phi(p, i\omega_n) \) is the anomalous self-energy. The pairing potential \( V(p, i\omega_n; p', i\nu_n') \) reads

\[
\begin{align*}
V(p, i\omega_n; p', i\nu_n') &= V^{(1)}(p - p', i\omega_n - i\nu_n) \\
+ V^{(2)}(p, i\omega_n; p', i\nu_n) + V^{(2)}(p, i\omega_n; p', i\nu_n'),
\end{align*}
\]

\( \Box \)

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where
\[ V^{(1)}(\mathbf{p} - \mathbf{p}', \mathbf{i} \omega_n - \mathbf{i} \omega_{n'}) = g^2 \chi(\mathbf{p} - \mathbf{p}', \mathbf{i} \omega_n - \mathbf{i} \omega_{n'}). \]
The second and third terms in eq. (10) originate from the vertex corrections that we discuss below.
As we are concerned about the \(d\)-wave instability, introducing a notation
\[ \langle f(\mathbf{p}) \rangle_p = \frac{1}{\Omega} \sum_{\mathbf{p}} (\cos(p_x) - \cos(p_y)) f(\mathbf{p}), \]
we put eq. (9) into
\[ \Phi(\mathbf{i} \omega_n) = \sum_{\mathbf{n'}} K(\mathbf{i} \omega_n, \mathbf{i} \omega_{n'}) \Phi(\mathbf{i} \omega_{n'}), \]
where
\[ \Phi(\mathbf{i} \omega_n) = \langle \Phi(\mathbf{p}, \mathbf{i} \omega_n) \rangle_p, \]
\[ K(\mathbf{i} \omega_n, \mathbf{i} \omega_{n'}) = K^{(1)} + K^{(2)} + K^{(2)}, \]
and
\[ K^{(1,2)} = -T \left\langle V^{(1,2)} \right\rangle \frac{|G(\mathbf{p}', \mathbf{i} \omega_{n'})|^2}{p, p'}. \]
Here \( K^{(2)}(\mathbf{i} \omega_n, \mathbf{i} \omega_{n'}) \) \((i = v, c)\) come from the vertex corrections. As is clear from eq. (13), the condition that the largest eigenvalue of \( K(\mathbf{i} \omega_n, \mathbf{i} \omega_{n'}) \) reaches unity provides a nonzero solution \( \Phi(\mathbf{i} \omega_n) \), thus defines \( T_c \). Below we look for a real solution \( \bar{\Phi}(\mathbf{i} \omega_n) \), for which the imaginary part of \( K(\mathbf{i} \omega_n, \mathbf{i} \omega_{n'}) \), namely, \( \text{Im} V(\mathbf{p}, \mathbf{i} \omega_n; \mathbf{p}', \mathbf{i} \omega_{n'}) \), is neglected.
As for the parameters, we assume \( t = 0.25 \text{eV} \) and \( t' = -0.45t \) for eq. (4), and we take
\[ \xi = 2.3, \quad \chi_0 = 75/\text{eV}, \quad \omega_{sf} = 14 \text{meV}, \]
to describe \( \chi(\mathbf{q}, \omega) \) of YBa\(_2\)Cu\(_3\)O\(_7\) at \( T_c = 90\text{K} \), according to MP. The chemical potential \( \mu^{(0)} \) is fixed by
\[ n = \frac{2T}{\Omega} \sum_{\mathbf{p}, \mathbf{n}} G^{(0)}(\mathbf{p}, \mathbf{i} \omega_n) e^{\mathbf{i} \mathbf{p} \cdot \mathbf{n}} = \frac{2}{\Omega} \sum_{\mathbf{p}} \frac{1}{e^{(e_p - \mu^{(0)})/T} + 1}, \]
in which we assume \( n = 0.75 \) throughout this paper. The shift \( \delta \mu \) in eq. (2) is adjusted in every iteration to assure
\[ \delta n = \frac{2T}{\Omega} \sum_{\mathbf{p}, \mathbf{n}} \left( G(\mathbf{p}, \mathbf{i} \omega_n) - G^{(0)}(\mathbf{p}, \mathbf{i} \omega_n) \right) = 0, \]
as this is easier to handle than the formally divergent sum, \( n = (2T/\Omega) \sum_{\mathbf{p}, \mathbf{n}} G(\mathbf{p}, \mathbf{i} \omega_n) \).

Fig. 1. The coupling constant \( g^2 \) to account for \( T_c = 90\text{K} \) as a function of the cutoff \( \omega_0 \), calculated on a 16\( \times \)16 lattice with periodic boundary conditions.

Fig. 2. Critical temperature \( T_c \) is shown as a function of \( g^2 \) for the cutoff \( \omega_0 = 0.4\text{eV} \). The other parameters are given in the text. The results are shown for a 16\( \times \)16 (circles), 32\( \times \)32 (squares), 64\( \times \)64 (diamonds) and 128\( \times \)128 (triangles) square lattice. The effect of \( \Sigma(\mathbf{p}, \mathbf{i} \omega_n) \) is not taken into account for the open symbols, while it is included for the closed symbols. A closed triangle for 128\( \times \)128 is not shown.

The above, except for the cutoff \( \omega_0 \) in eq. (7), are all the necessary ingredients to reproduce the results of MP. Nevertheless, we could not derive them precisely, though qualitative features are consistently reproduced. Let us discuss the point briefly. First we have to note the \( \omega_0 \) dependence of \( T_c \) as a function of the coupling constant \( g^2 \). In Fig. 1, \( g^2 \) to give \( T_c = 90\text{K} \) is shown as a function of \( \omega_0 \). In this result, \( K^{(1)} \) in eq. (13) is used for the eigenequation (13), i.e., the vertex correction \( K^{(2)} \) is not taken into account, but the effect of \( \Sigma(\mathbf{p}, \mathbf{i} \omega_n) \) is. As we see from the figure, we cannot fix \( g^2 \) just from \( T_c(g^2) = 90\text{K} \), excluding the knowledge of the cutoff \(\omega_0 \) in eq. (7). The strong dependence on \( \omega_0 \) in the low-energy region \(\omega_0 \leq 0.3\text{eV} \) reflects that the transition temperature \( T_c \) (unlike the transport properties controlled by the quasiparticle damping, is not determined solely from the low-energy expression, eq. (6)). Indeed, this is one of the general problems to infer the full structure of \( \chi(\mathbf{q}, \omega) \) entirely from the low-energy ‘observable’ \( \chi(\mathbf{q}, \omega) \), and to settle \( \omega_0 \) may be a key point in the discrepancy between Radtke et al. and MP. As it is not our purpose to discuss this point further, for the time being, we assume eq. (6) up to the cutoff energy \( \omega_0 \) in eq. (7), and arbitrarily set \( \omega_0 = 0.4\text{eV} \approx 4.6 \times 10^{3}\text{K} \), following MP. This value is used throughout in the following. Then we obtain \( g^2 = 0.57\text{eV}^2 \) for \( T_c = 90\text{K} \), still in disagreement
with $g^2 = 0.41eV^2$ of MP. This is not due to the size of a square lattice, as we see in Fig. 2, where $T_c$ is shown as a function of $g^2$. At $T = T_c = 90K$, the $16 \times 16$ lattice is large enough for us to conclude $g^2 = 0.57eV^2$ in the self-consistent calculation including the effect of $\Sigma(p, i\omega_n)$. A close inspection indicates that the disagreement originates in details of $\chi(q, i\nu_n)$. In fact, we find $g^2 = 0.34$, smaller than $g^2 = 0.41$ of MP, if we adopt the second line, instead of the third line, of eq. (7) for $n = 0$ too. This means that $T_c$ depends sensitively on how we prepare $\chi(q, i\nu_n)$ in the low-energy regime. This is complementary to the above remark on the high-energy contribution to $T_c$. As this quantitative difference is not of our primal concern either, deferring this problem, we choose to use our own definition, i.e., $\chi(q, i\nu_n)$ for $n = 0$ is specified separately by eq. (7). The qualitative results presented below are not affected by this choice.

Now let us discuss how we evaluate the vertex correction. The pairing potentials $\bar{V}^{(2)}_v(p, i\omega_n; p', i\omega_{n'})$ and $V^{(2)}_v(p, i\omega_n; p', i\omega_{n'})$ including the vertex correction are diagrammatically represented by Fig. 3(a) and Fig. 3(b), respectively. These potentials at low frequencies $\omega_n = \omega_{n'} = \pi T$ for $n = n' = 0$ are particularly studied by Monthoux. To see the effect on $T_c$ precisely, however, we have to evaluate the kernel $K^{(2)}(i\omega_n, i\omega_{n'})$, eq. (16), for a full set of the Matsubara frequencies $\omega_n$ and $\omega_{n'}$, then the kernel must be diagonalized. In effect, this is not practical at present. Thus, as a tractable method, we set up perturbation theory to evaluate the vertex corrections to the eigenvalue $\kappa$ of the kernel.

We shall make effective use of the results obtainable by means of the FFT. Let us introduce the eigenfunction $\Phi^{(1)}(i\omega_n)$ for the largest eigenvalue $\kappa^{(1)}$ of the kernel $K^{(1)}(i\omega_n, i\omega_{n'})$. $\Phi^{(1)}(i\omega_n) = \sum_n K^{(1)}(i\omega_n, i\omega_{n'}) \Phi^{(1)}(i\omega_{n'}) = \kappa^{(1)} \Phi^{(1)}(i\omega_n)$. Then the eigenvalue $\kappa$ including the vertex corrections is given by

$$\kappa = \kappa^{(1)} + \kappa^{(2)} + \kappa^{(3)} + \kappa^{(4)},$$

where

$$\kappa^{(2)}_v = \sum_{n, n'} \Phi^{(1)}(i\omega_n) K^{(2)}_{v}(i\omega_n, i\omega_{n'}) \Phi^{(1)}(i\omega_{n'}).$$

We assume $\Phi^{(1)}(i\omega_n)$ is normalized. On physical grounds, the norm of $\Phi^{(1)}(i\omega_n)$ decreases quite rapidly as $|\omega_n|$ increases. Therefore, the sum over the Matsubara frequencies in eq. (21) is allowed to be restricted in a narrow region around $(n, n') \sim (0, 0)$. In effect, we evaluate $K^{(2)}_v(i\omega_n, i\omega_{n'})$ for a $16 \times 16$ mesh around the Fermi energy. Moreover, in the remainder of the paper, the results are calculated on a $16 \times 16$ square lattice. Measured in terms of the weight $|\Phi^{(1)}(i\omega_n)|^2$, we find $\sum_{|i\omega_n| \leq 1.5T} |\Phi^{(1)}(i\omega_n)|^2 = 0.98, 0.91$ and $0.78$ at $T = T_c = 90K, 45K$ and $22K$, respectively. Even at low $T_c$, the error involved is not appreciable, for the coupling constant itself is small there. As Fig. 2 shows, a $16 \times 16$ mesh in the momentum space is large enough to grasp the qualitative features caused by the vertex corrections.

To prepare $V^{(2)}_v(p, i\omega_n; p', i\omega_{n'})$ is most time-consuming. Therefore, we use the bare Green’s function $G^{(0)}(p, i\omega_n)$ instead of $G(p, i\omega_n)$ to provide $V^{(2)}_v(p, i\omega_n; p', i\omega_{n'})$. With $\langle V^{(2)}_v(p, i\omega_n; p', i\omega_{n'}) \rangle_p$ thus calculated beforehand and $G(p, i\omega_n)$ of the solution of eqs. (1) and (3), we calculate $K^{(2)}(i\omega_n, i\omega_{n'})$ in eq. (16). Then, to evaluate $\kappa^{(2)}_v$, eq. (21), is straightforward, and the critical coupling $g^*$ at $T_c$ is determined. Results thus obtained are shown in Fig. 4, where the triangles (without $\Sigma(p, i\omega_n)$) and circles (with $\Sigma(p, i\omega_n)$) denote the results without the vertex corrections. (See Fig. 2). The diamonds include the vertex correction $V^{(2)}_v$ as well as $V^{(2)}_c$, while only the effect of $V^{(2)}_v$ is taken into account for the two squares at $T = 90K$ and $45K$.

Several points are noted from the figure. In the first place, both the effects of $V^{(2)}_v$ and $V^{(2)}_c$ are attractive on the whole, or enhances $T_c$ of the $d$-wave instability. The effect of $V^{(2)}_c$ (Fig. 3(b)) is, however, is negligibly small, as noted by Monthoux. On the other hand, the effect of $V^{(2)}_v$ (Fig. 3(a)) is prominent. In particular, it affects the result of MP, denoted by the circles interpolated with the solid line in Fig. 4, that the maximum transition temperature attainable in this model is about
In fact, $T_c$ as a function of $g^2$ shows no sign of saturation, and keeps increasing beyond 200K when the vertex correction $V_i^{(2)}$ is taken into account. In this regard, the vertex correction has an effect more than a mere scale-up of the effective coupling constant $g^2$.

Next, the effect of $\Sigma(p, \omega_n)$ on $V_i^{(2)}$ has to be investigated. To this end, $G(p, \omega_n)$ to meet eqs. (1) and (2) is used to evaluate $V_i^{(2)}(p, \omega_n; p', \omega_n')$. The maximum eigenvalues calculated for $T_c = 90K$ are shown in Fig. 5 as a function of $g^2$. The effect of $\Sigma(p, \omega_n)$ is to weaken the vertex corrections. The effect, however, is not appreciable for $T_c = 90K$, as we see from Fig. 5 in which we see $g^2 = 0.36$ while we have $g^2 = 0.32$ in Fig. 4 in the case including the vertex corrections. Comparing these with $g^2 = 0.57$ without the vertex corrections, we conclude that the correction due to $\Sigma(p, \omega_n)$ in $V_i^{(2)}$ is not important at least at $T_c = 90K$. In other words, if the coupling constant $g$ should be evaluated to account for $T_c$, our result is that the vertex correction is not negligibly small at this temperature, at variance with previous results.

The discrepancy may be due to a high-energy contribution included in our calculation, or it is traced back to the above finding of a slight renormalization effect on $V_i^{(2)}$. On the other hand, for $T_c = 180K$, we find that $g^2 = 0.73$ in Fig. 4 is modified to $g^2 = 1.57$. The large modification in this case is due to a large coupling constant to realize that high transition temperature. The results in this regime must be taken with care.

To the extent that the vertex corrections that we found for the pairing potentials are not negligible, the vertex corrections to eq. (1) should have to be investigated next. The latter effect on $\Sigma(p, \omega_n)$ will reduce $T_c$ somewhat particularly through the pair propagator $|G(p', \omega_n')|^2$ in eq. (4), according to the above note, as a result of enhanced quasiparticle damping. Therefore, we will be ultimately led to a convergent result of $T_c(g^2)$, somewhere in between the dashed and solid lines of Fig. 4. The results, however, would then indicate that $T_c \simeq 100K$ is on the verge of practical applicability of this kind of perturbation theory in $g^2$, as inferred from Fig. 4. Note that, for us in this context, to suffer a small correction is more important than to find out a high $T_c$.

In summary, a result of this paper is presented in Fig. 4, though the result at high temperature is somewhat modified as stated above. Applying perturbation theory to the eigenvalue of the kernel $K(\omega_n, \omega_n')$, we estimated the vertex corrections to $T_c$ as a function of the coupling constant $g^2$ on the basis of the spin-fluctuation model of the high-$T_c$ superconductivity. We found that the effect of Fig. 3(b) is numerically negligible as far as the $d_{x^2-y^2}$ pairing instability is concerned, while Fig. 3(a) enhances $T_c$ appreciably. For $T_c \sim 100K$, the effect of $\Sigma(p, \omega_n)$ mainly comes in through the pair propagator $|G(p', \omega_n')|^2$, dressing the vertex functions is not so important. In a strong-coupling regime at high temperatures, the vertex corrections become even qualitatively important, particularly in case where $T_c$ in the one-loop Eliashberg calculation is substantially suppressed by lifetime effects.

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$\omega_0 (eV)$

$g^2 (eV^2)$

$T_c = 90 \text{ K}$
\( \kappa^{(1)} \) and \( \kappa^{(1)} + \kappa^{(2)} \) vs. \( g^2 \text{ (eV}^2) \) at \( T = 90 \text{ K} \).