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Variations of T_c for changes in the spin-fluctuation spectral weight

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We consider a two-dimensional Hubbard model within a conserving spin-fluctuation exchange approximation and determine the change in the $d_{x^2-y^2}$ superconducting transition temperature T_c produced by variations in the spin-fluctuation spectral weight. We find that T_c is increased when spectral weight is shifted to large momentum transfers and frequencies greater than T_c with an optimal frequency for T_c enhancement of order $10T_c$.

For the traditional low-temperature superconductors, the transition temperature depends upon the spectral function $\alpha^2F(\omega)$, which characterizes the effective electron-electron interaction due to phonon exchange.[1] In order to understand how different frequency regions of $\alpha^2F(\omega)$ contributed to T_c, Bergmann and Rainer[2] calculated the sensitivity of their transition temperature to variations in $\alpha^2F(\omega)$. In this manner, they were able to learn for a given $\alpha^2F(\omega)$ what type of shift in spectral weight would be optimal for achieving a higher transition temperature. Here we seek similar information for the case of $d_{x^2-y^2}$-wave superconductivity mediated by the exchange of paraantiferromagnetic spin fluctuations. In contrast to the electron-phonon problem, where the interaction is retarded but local in space, the spatial dependence of the spin-fluctuation-induced interaction is essential. Thus while only variations in the frequency dependence of the phonon spectral weight needed to be considered, one must consider variations in the momentum as well as the frequency dependence of the spin-fluctuation spectral weight.

We consider a two-dimensional Hubbard model within a conserving spin-fluctuation exchange approximation[3-5] and study the change in T_c produced by small changes in the spin-fluctuation spectral weight at various frequency and momentum transfers. Within the conserving fluctuation exchange approximation, the interactions associated with the spin- and charge-fluctuation exchanges are

$$V_s=\frac{3}{2}U^2\frac{\chi_0}{1-U\chi_0}-\frac{1}{2}U^2\chi_0 \tag{1}$$

and

$$V_c=\frac{U^2}{2}\frac{\chi_0}{1+U\chi_0}-\frac{1}{2}U^2\chi_0\ , \tag{2}$$

respectively, with

$$\chi_0(q,\omega_m)=-\frac{T}{N}\sum_{p,n}G(p+q,\omega_n+\omega_m)G(p,\omega_n)\ . \tag{3}$$

Here G is the dressed single-particle Green's function

$$G(p,\omega_n)=\frac{1}{i\omega_nZ(p,i\omega_n)-[\varepsilon_p+X(p,\omega_n)]}\ , \tag{4}$$

with $\varepsilon_p=-2t(\cos p_x+\cos p_y)-\mu$ for the case of a simple near-neighbor hopping t. Z and X are calculated from the following self-energy equations with V_s and V_c determined self-consistently from Eqs. (1), (2), and (3):

$$[1-Z(p,\omega_n)]i\omega_n=\frac{T}{N}\sum_{p',n'}\frac{[V_c(p-p',\omega_n-\omega_{n'})+V_s(p-p',\omega_n-\omega_{n'})]i\omega_{n'}Z(p',\omega_{n'})}{[i\omega_{n'}Z(p',\omega_{n'})]^2-[\varepsilon_{p'}+X(p',\omega_{n'})]^2}\ , \tag{5}$$

$$X(p,\omega_n)=\frac{T}{N}\sum_{p'n'}\frac{V_c(p-p',\omega_n-\omega_{n'})+V_s(p-p',\omega_n-\omega_{n'})[\varepsilon_{p'}+X(p',\omega_{n'})]}{[i\omega_{n'}Z(p',\omega_{n'})]^2-[\varepsilon_{p'}+X(p',\omega_{n'})]^2}\ . \tag{6}$$

The transition temperature T_c is given by the temperature for which the eigenvalue λ of the linearized gap equation is equal to unity:

$$\frac{-T}{N}\sum_{p'n'}\frac{[V_c(p-p',\omega_n-\omega_{n'})-V_s(p-p',\omega_n-\omega_{n'})+U]\phi(p',\omega_{n'})}{[i\omega_{n'}Z(p',\omega_{n'})]^2-[\varepsilon_{p'}+X(p',\omega_{n'})]^2}=\lambda\phi(p,\omega_n)\ . \tag{7}$$

We will work in units where the energy and transition temperature are measured in units of the near-neighbor hopping t and take $U=4$ with a site filling $\langle n_{i\uparrow}+n_{i\downarrow}\rangle=0.875$. In this case, the transition temperature for $d_{x^2-y^2}$ superconductivity is $T_{c0}=0.022$. The calculations were done on a 64×64 lattice with a frequency cutoff of five times the bandwidth.

Now suppose that some extra, infinitesimal spin-fluctuation spectral weight is added to V_s at a frequency ω_0 and a wave vector q^* so that for $\omega>0$,

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$$\mathrm{Im}\,\delta V_s(q,\omega)=\eta\frac{3}{2}\pi U^2\delta(\omega-\omega_0)\frac{N}{N_{q^*}}\sum_{q_i^*}\delta_{q,q_i^*}\ . \tag{8}$$

Here η is an infinitesimal dimensionless parameter. The sum over q_i^* includes q^* and the wave vectors related to it by symmetry operations of the square lattice. N_{q^*} is the number of these equivalent wave vectors and N is the total number of wave vectors in the Brillouin zone. Writing out the extra spectral weight in δV_s, Eq. (8), in terms of Matsubara frequencies,

$$\delta V_s(q,\omega_m)=\eta\frac{3}{2}U^2\frac{2\omega_0}{\omega_0^2+\omega_m^2}\frac{N}{N_{q^*}}\sum_{q_i^*}\delta_{q,q_i^*}\ . \tag{9}$$

Now $\delta V_s(q,\omega_m)$ is added to V_s in Eqs. (5)–(7), and the change δT_c of T_c is calculated:

$$\delta T_c=\frac{dT_c}{d\eta}\eta+0(\eta^2)\ . \tag{10}$$

In practice, it is easier to work at a fixed temperature and vary η. Then, for example, if the added spectral weight increases T_c, one would choose a temperature $T=T_{c0}+0.001t$ slightly above the transition temperature of the unperturbed equations ($\eta=0$). Then η is increased until the largest eigenvalue of the linearized gap equation (7) is equal to 1. Then $dT_c/d\eta$ is evaluated from $10^{-3}/\eta$. If alternatively ω_0 and q^* are such that the added spectral weight decreases T_c, one should pick a temperature slightly below T_{c0} ($T=T_{c0}-0.001$) and adjust η in the same fashion.

Note that for each value of η, the perturbed equations, namely Eqs. (5)–(7), with $V_s\to V_s+\delta V_s$, are iterated to self-consistency. That is, we let the equations adjust to the perturbed interaction. Since we are interested in the first order in η correction, one could be tempted to iterate the equations only once. This would be incorrect, however, since to first order in η one has contributions from both the first-order changes in Z, X and the first-order changes in V_s and V_c induced by the first-order changes in Z and X. If we were to iterate the equations only once, we would only pick up the first order in η changes in Z and X. In these calculations δT_c was chosen such that η was less than or of order 10^{-2} so that the η^2 corrections were negligible.

In Fig. 1 we have plotted $dT_c/d\eta$ versus ω_0/T_{c0} for several values of momentum transfer. As expected for $d_{x^2-y^2}$ pairing, increasing the spectral weight at large momentum transfer enhances the transition temperature over most of the frequency range. The peak spectral response occurs for a frequency ω_0/T_{c0} of order 10. Note that it was previously found[4,5] that $2\Delta(0)/T_{c0}\simeq 10$. For ω_0/T_{c0} less than of order 1, the transition temperature even for large momentum transfer is depressed. This reflects the fact that even at low frequency, δV_s acts as a pair breaker.[6]

For $\omega=0.2t\approx 9T_c$, we have plotted $dT_c/d\eta$ in Fig. 2 of various values of momentum. It is clear from Fig. 2 that the important momentum transfers are for q near (π,π). Physically, additional spectral weight for momentum transfers near (π,π) increases the attractive pairing

TABLE I. Tabulation of $\delta\lambda_z/\alpha$ and $\delta\lambda_d/\alpha$ for different values of q^* computed from Eqs. (14) and (15).

q^*	$\delta\lambda_z/\alpha$	$\delta\lambda_d/\alpha$
$\pi(0,0)$	0.79	−0.27
$\pi(\frac{1}{2},0)$	0.26	−0.13
$\pi(1,0)$	0.14	0.00
$\pi(1,\frac{1}{2})$	0.27	0.13
$\pi(1,0.875)$	0.81	0.24
$\pi(1,1)$	1.74	0.26
$\pi(\frac{1}{2},\frac{1}{2})$	0.57	0.00

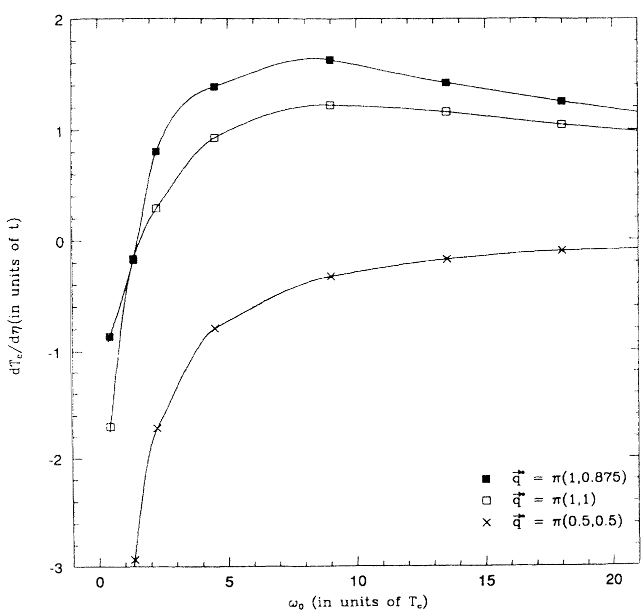

FIG. 1. Plot of $dT_c/d\eta$ versus ω_0/T_{c0} for different values of the momentum transfer q.

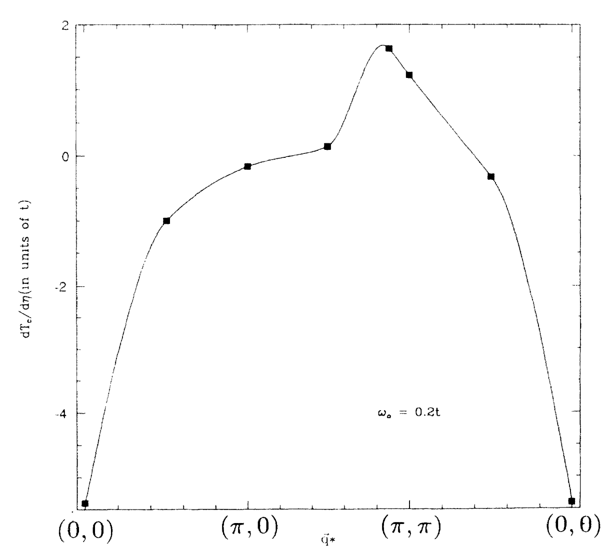

FIG. 2. Plot of $dT_c/d\eta$ versus q^* for $\omega_0=0.2t\approx 9T_c$.

interaction between electrons on near-neighbor sites.[7] In order to understand qualitatively the results of Fig. 2, it is instructive to compute the change in the coupling constants in the normal self-energy $\delta\lambda_z$ and in the pairing $\delta\lambda_d$, produced by the added spectral weight. If $N(0)$ denotes the density of states at the Fermi surface, by analogy to the electron phonon problem, the coupling constants are defined as

$$\delta\lambda_z = 2N(0)\int_0^\infty \frac{d\omega}{\pi}\frac{1}{\omega}\frac{\langle \mathrm{Im}\,\delta V_s(p-p',\omega)\rangle_{\mathrm{FS}}}{\langle 1\rangle_{\mathrm{FS}}} \tag{11}$$

and

$$\delta\lambda_d = -2N(0)\int_0^\infty \frac{d\omega}{\pi}\frac{1}{\omega}\frac{\langle (\cos p_x - \cos p_y)\mathrm{Im}\,\delta V_s(p-p',\omega)(\cos p_x' - \cos p_y')\rangle_{\mathrm{FS}}}{\langle (\cos p_x - \cos p_y)^2\rangle_{\mathrm{FS}}} . \tag{12}$$

In the numerator of the expression for $\delta\lambda$ the Fermi-surface average is taken over both p and p'. The different sign in front of the expression for $\delta\lambda_d$ is due to the fact that the spin-fluctuation interaction enters with the opposite sign in the gap equation. We have chosen to define the Fermi-surface average as

$$\langle F(p)\rangle_{\mathrm{FS}} = \int_{\mathrm{BZ}} \frac{d^2p}{(2\pi)^2}\frac{\gamma}{(\varepsilon_p-\mu)^2+\gamma^2}F(p) . \tag{13}$$

Here we will set $\gamma = 0.2t$, but the qualitative results are not dependent on the precise value of γ. Using our expression for $\delta\,\mathrm{Im}\,V_s$, Eq. (8), one finds

$$\delta\lambda_z = \alpha\frac{\left\langle (1/N_{q^*})\sum_{q_i^*}\delta_{q,q_i^*}\right\rangle_{\mathrm{FS}}}{\langle 1\rangle_{\mathrm{FS}}} \tag{14}$$

and

$$\delta\lambda_d = -\alpha\frac{\left\langle (\cos p_x - \cos p_y)(1/N_{q^*})\sum_{q_i^*}\delta_{p-p',q_i^*}(\cos p_x' - \cos p_y')\right\rangle_{\mathrm{FS}}}{\langle (\cos p_x - \cos p_y)^2\rangle_{\mathrm{FS}}} , \tag{15}$$

where $\alpha = 3N(0)U^2\eta N/\omega_0$. Table I shows the values of $\delta\lambda_z/\alpha$ and $\delta\lambda_d/\alpha$ that are obtained for different values of q^*. By comparing Fig. 2 and Table I, one sees that the wave vectors for which $dT_c/d\eta$ is negative are those for which $\delta\lambda_d \leq 0$, namely the momentum transfers for which the spin-fluctuation interaction connects predominantly regions of the Fermi surface where the gap has the same sign. The most repulsive momentum transfer is $p-p'=q^*=0$, since the gap at p and p' then always has the same sign. One also sees that in this model it is preferable to put the extra spectral weight at the nesting vector $\pi(1,0.875)$ rather than $\pi(1,1)$, and from Table I one notices that it is the renormalization factor Z more than the spectral weight at $\pi(1,0.875)$ which affects $dT_c/d\eta$.

From this analysis, we conclude that the transition temperature for $d_{x^2-y^2}$ pairing due to spin-fluctuation exchange is increased when spectral weight is shifted to large momentum transfers and frequencies greater than T_c with the optimal frequency being of order $10T_c$. In this respect, it is interesting to note that below T_c, at temperatures where the gap is well formed, the superconducting gap itself provides just this type of shift of the spectral weight of the spin fluctuations. This is in fact the reason[4,5] one finds such an anomalously large $2\Delta(0)/kT_c$ for this type of pairing mechanism. If a spin gap could be opened above T_c, without at the same time suppressing the strength of the interaction, one would find that T_c increased.[8]

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[8]Of course there are physical limits which must be kept in mind, for example, if we were to approximate the spin-fluctuation interaction by $V_s \simeq \frac{3}{2}U^2\chi(q,\omega)$. Then we know that the spectral weight $\mathrm{Im}\chi(q,\omega)$ is limited by the sum rule bound $\int d\omega \sum_q \mathrm{Im}\chi(q,\omega)n(\omega) = \langle (n_{i\uparrow}+n_{i\downarrow})^2\rangle \leq 1$.