$d_{x^2-y^2}$ symmetry and the pairing mechanism

N. Bulut and D. J. Scalapino
Department of Physics, University of California, Santa Barbara, California 93106-9530
(Received 21 February 1995; revised manuscript received 2 August 1996)

An important question is, if the gap in the high-temperature cuprates has $d_{x^2-y^2}$ symmetry, what does that tell us about the underlying interaction responsible for pairing? Here we explore this by determining how three different types of electron-phonon interactions affect the $d_{x^2-y^2}$ pairing found within a random phase approximation treatment of the two-dimensional Hubbard model. These results imply that interactions which become more positive as the momentum transfer increases favor $d_{x^2-y^2}$ pairing in a nearly half-filled band. [S0163-1829(96)05646-9]

There has been a great deal of interest in the interpretation of recent experiments which address the question of the symmetry of the gap in the high-temperature cuprate superconductors.[1–3] If this symmetry turns out to be $d_{x^2-y^2}$, it is natural to ask what this would imply about the pairing mechanism. Here we discuss the relationship of the $d_{x^2-y^2}$ symmetry to the pairing mechanism by examining how three types of electron-phonon interactions affect $d_{x^2-y^2}$ pairing.

As discussed by a number of authors,[1–3] a $d_{x^2-y^2}$ gap naturally arises from the exchange of antiferromagnetic spin fluctuations. However, the physical picture that emerges from these calculations is more general and shows that a $d_{x^2-y^2}$ gap will occur for a nearly half-filled band when there is an effective singlet interaction which is repulsive for on-site pairing and attractive for near-neighbor pairing. This spatial structure of the interaction means that its Fourier transform becomes more positive as the momentum transfer increases towards large values. This is easily understood from the BCS gap equation

$$\Delta_{\mathbf{p}} = -\sum_{\mathbf{p}'} \frac{V(\mathbf{p}-\mathbf{p}')\Delta_{\mathbf{p}'}}{2E_{\mathbf{p}'}}. \tag{1}$$

Near half-filling of the two-dimensional (2D) system, the phase space is such that the important scattering processes take electrons from $(\mathbf{p}\uparrow,-\mathbf{p}\downarrow)$ with $\mathbf{p}$ near a corner of the Fermi surface, say, near $(\pi,0)$, to $(\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow)$ with $\mathbf{p}'$ near $(0,\pi)$ or $(0,-\pi)$. Since the interaction $V(\mathbf{p}-\mathbf{p}')$ is positive, the relative phase of the states $(\mathbf{p}\uparrow,-\mathbf{p}\downarrow)$ making up the bound Cooper pair changes sign as $\mathbf{p}$ goes from $(\pi,0)$ to $(0,\pi)$ or $(0,-\pi)$, leading to a gap with $d_{x^2-y^2}$ symmetry. This is the case within a random phase apporximation (RPA) in which the interaction is mediated by the exchange of antiferromagnetic spin fluctuations. It has also been found by Monte Carlo calculations[4] that for the Hubbard model the pairing interaction is attractive in the $d_{x^2-y^2}$ channel. In these cases the interaction is positive at all momentum transfers becoming larger in the region near (π,π) associated with the short-range antiferromagnetic correlations.

In order to explore the effect of electron-phonon interactions, we begin with a 2D Hubbard model on a square lattice:

$$H = -t\sum_{\langle i,j\rangle,s}(c_{is}^{\dagger}c_{js}+c_{js}^{\dagger}c_{is}) + U\sum_i n_{i\uparrow}n_{i\downarrow}. \tag{2}$$

Here t is a near-neighbor hopping and U is the on-site Coulomb interaction. We take a simple phenomenological RPA form[5] of the singlet pairing interaction associated with the exchange of spin fluctuations:

$$V_{\mathrm{SF}}(p'-p) = \frac{3}{2}\overline{U^2}\chi(p'-p), \tag{3}$$

with $\chi(q)=\chi_0(q)/[1-\overline{U}\chi_0(q)]$. Here $p=(\mathbf{p},i\omega_n)$, $\overline{U}$ is a renormalized Coulomb interaction, and χ_0 is the spin susceptibility:

$$\chi_0(\mathbf{q},\omega) = \frac{1}{N}\sum_{\mathbf{p}} \frac{f(\varepsilon_{\mathbf{p}+\mathbf{q}})-f(\varepsilon_{\mathbf{p}})}{\omega-(\varepsilon_{\mathbf{p}+\mathbf{q}}-\varepsilon_{\mathbf{p}})+i0^+}, \tag{4}$$

with $\varepsilon_{\mathbf{p}}=-2t(\cos p_x+\cos p_y)-\mu$. Now, in addition to V_{SF}, we will examine three model electron-phonon interactions. The first is a simple on-site Holstein coupling of the form

$$V_1 = \sum_i g x_i n_i, \tag{5}$$

with x_i the atomic displacement at site $\hat{i}$ and $n_i=n_{i\uparrow}+n_{i\downarrow}$ the on-site electron density. One could imagine this type of coupling arising from the interaction with an apical oxygen O(4). In Eq. (5) the coupling is linear in the atomic displacement rather than quadratic. This is possible since O(4) breaks the reflection symmetry with respect to a single CuO_2 layer. The second electron-phonon interaction can be viewed as arising from the in-plane breathing motion[10] of an O(2) oxygen:

$$V_2 = \sum_i g[x_i(n_i-n_{i+x})+y_i(n_i-n_{i+y})]. \tag{6}$$

Here x_i describes the displacement of the O(2) along the $\mathbf{x}$ axis between the Cu sites at $\hat{i}$ and $\hat{i}+\hat{\mathbf{x}}$ and y_i the $\mathbf{y}$-axis displacement of an O(2) along the $\mathbf{y}$ axis between the Cu sites at $\hat{i}$ and $\hat{i}+\hat{\mathbf{y}}$. The third interaction involves an axial $\mathbf{z}$ motion of a *buckled* O(2) atom:

$$V_3=\sum_i g[z_i^x(n_i+n_{i+x})+z_i^y(n_i+n_{i+y})]. \quad (7)$$

Here z_i^x is for an O(2) between the $\hat{i}$ and $\hat{i}+\hat{\mathbf{x}}$ sites and z_i^y is for an O(2) between the $\hat{i}$ and $\hat{i}+\hat{\mathbf{y}}$ sites. Linear coupling of this type is possible for buckled Cu-O-Cu bonds. The electron-phonon interactions considered here are diagonal in the electron number representation. We note that it would also be interesting to study the effects of phonon modes where the electron-phonon coupling is not diagonal in the electron number representation.

Assuming for the discussion that the lattice coordinate can be described as a local harmonic oscillator with frequency ω_0 (which just as g is of course different for the different modes), the effective electron-electron interaction mediated by the exchange of these phonons is

$$V_{\rm ph}=\frac{-2|g(\mathbf{q})|^2\omega_0}{\omega_m^2+\omega_0^2}, \quad (8)$$

where ω_m is the Matsubara frequency $2m\pi T$. Here for the local interaction, Eq. (5),

$$|g(\mathbf{q})|^2=\frac{|g|^2}{2M\omega_0}, \quad (9)$$

while for the breathing mode, Eq. (6),

$$|g(\mathbf{q})|^2=\frac{2|g|^2}{2M\omega_0}(\sin^2 q_x/2+\sin^2 q_y/2) \quad (10)$$

and for the axial mode, Eq. (7),

$$|g(\mathbf{q})|^2=\frac{2|g|^2}{2M\omega_0}(\cos^2 q_x/2+\cos^2 q_y/2), \quad (11)$$

with M the O ion mass.

In order to see how these interactions affect the pairing we examine the leading eigenvalue λ and eigenfunction $\phi(p)$ of the Bethe-Salpeter equation, neglecting self-energy contributions,[7]

$$\lambda\phi(p)=-\frac{T}{N}\sum_{p'}[V_{\rm SF}(p-p')+V_{\rm ph}(p-p')] \times G(p')G(-p')\phi(p'), \quad (12)$$

where $G(p)$ is the single-particle Green's function given by

$$G(p)=\frac{1}{i\omega_n-\varepsilon_p}. \quad (13)$$

Here and in the following we will measure energies in units of t. The chemical potential has been chosen so that the site occupation $\langle n_{i\uparrow}+n_{i\downarrow}\rangle=0.875$ and an effective Coulomb interaction $U=2$ has been taken. We will also take $\omega_0=0.25$ and $|g|^2/M\omega_0=1$ corresponding to an electron-phonon coupling strength $|g|^2N(0)/M\omega_0^2\simeq 0.8$, where $N(0)$ is the electron density of states at μ_F.

We find that the leading eigenvalue in the even frequency singlet channel has $d_{x^2-y^2}$ symmetry and the temperature dependence of the eigenvalue $\lambda_{x^2-y^2}(T)$ is shown in Figs. 1 and 2 for the electron-phonon interactions given by Eqs. (6) and (7), respectively. The solid line in each figure shows the eigenvalue in the absence of the phonon-mediated interaction ($g=0$), while the dashed curve shows the effect of including the phonon-mediated term. It is clear that the breathing mode interaction, Eqs. (6) and (10), suppresses $d_{x^2-y^2}$ pairing[6] while the axial O(2) mode of Eqs. (7) and (11) enhances the $d_{x^2-y^2}$ pairing, raising T_c. The local interaction, Eqs. (5) and (9), is orthogonal to the $d_{x^2-y^2}$ gap and hence does not affect the $d_{x^2-y^2}$ eigenvalue when self-energy effects are neglected. Including it in the self-energy will act to suppress T_c due to the wave function renormalization.[7] To understand the behavior shown in Figs. 1 and 2 we note that the strength of the coupling to the axial mode, Eq. (11), decreases as $\mathbf{q}$ approaches (π,π). Because the phonon-mediated interaction, Eq. (8), is negative, decreasing the magnitude of the coupling $|g(\mathbf{q})|^2$ acts to make the interaction *more positive* as the momentum transfer increases. As discussed above, this is the criteria for a $d_{x^2-y^2}$ gap to form when the system is near half-filling. Clearly it will be interesting to examine the isotope effect within models in which the strength of the electron-phonon coupling decreases at large momentum transfers.

Thus we conclude that a $d_{x^2-y^2}$ gap implies that the pairing interaction becomes more positive for large momentum

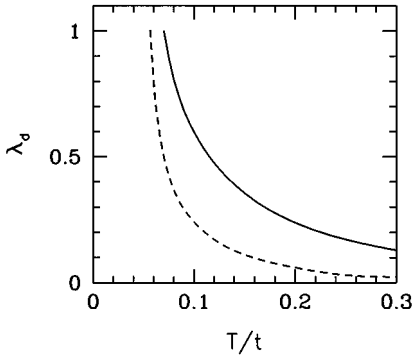

FIG. 1. The $d_{x^2-y^2}$ eigenvalue of Eq. (12) vs the temperature T in units of the hopping t. The solid curve gives the eigenvalue for just the spin-fluctuation interaction $V_{\rm SF}$ and the dashed curve shows the effect when the electron-phonon interaction V_2 associated with the breathing mode, Eqs. (6) and (10), is added to $V_{\rm SF}$. The coupling constants are given in the text.

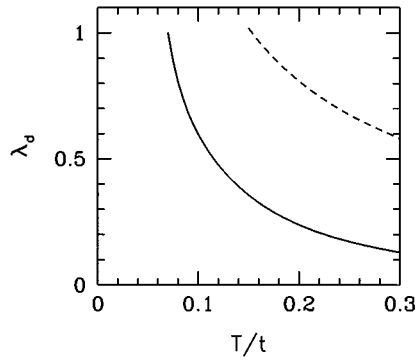

FIG. 2. Same as Fig. 1 except for the axial O electron-phonon interaction V_3, Eqs. (7) and (11).

transfers. This is clearly the case for the spin-fluctuation interaction, Eq. (3), but as shown it can also occur for the attractive phonon-mediated interaction if $|g(\mathbf{q})|^2$ *decreases* at large momentum transfers. This form of coupling would also give rise to an electron-phonon coupling constant λ which could be large compared to the effective coupling constant λ_{tr} entering transport processes since the transport coupling constant λ_{tr} weights large momenta transfers more heavily.[8,9] For small momentum transfers $\mathbf{q}$, a scattering of $(\mathbf{p}\uparrow,-\mathbf{p}\downarrow)$ to $(\mathbf{p}+\mathbf{q}\uparrow,-\mathbf{p}-\mathbf{q}\downarrow)$ with $\mathbf{p}$ near a corner of the Fermi surface connects regions which have the same sign of the $d_{x^2-y^2}$ gap so that according to Eq. (1) an attractive electron-phonon interaction [negative $V(q)$] enhances $\Delta_{\mathbf{p}}$. Another way to see that this latter case is similar to the spin-fluctuation interaction is to add U onto the phonon interaction, giving $U+V_{ph}$. For the $d_{x^2-y^2}$ channel, a constant has no effect, but if it is larger than the magnitude of the phonon-mediated interaction, Eq. (8), then as $|g(\mathbf{q})|^2$ decreases, the total interaction $U+V_{ph}$ is positive and increases as $\mathbf{q}$ becomes large, just as V_{SF}. In order to obtain more quantitative information on the role of the electron-phonon interaction, it would be useful to have band structure calculations[11] of the $d_{x^2-y^2}$ electron-phonon coupling constant for the ν mode:

$$\lambda^{\nu}_{d_{x^2-y^2}}=\frac{2\Sigma_{k,k'}g(k)g(k')(|M^{\nu}_{kk'}|^2/\omega_{k-k'})\delta(\varepsilon_k)\delta(\varepsilon_{k'})}{\Sigma_{\mathbf{k}}g^2(k)\delta(\varepsilon_k)}. \tag{14}$$

Here $g(k)\sim(\cos k_x-\cos k_y)$, ε_k is the band energy with k including the band index, and $M^{\nu}_{kk'}$ is the electron-phonon matrix element for the νth phonon mode.[12]

Note added in proof. We have recently been made aware of two other papers that are relevant to this work.[13,14]

The authors gratefully acknowledge support from the National Science Foundation under Grant No. DMR92-25027. The numerical computations reported in this paper were performed at the San Diego Supercomputer Center.

[1] B.G. Levi, Phys. Today **46** (5), 17 (1993), and references therein.

[2] J.R. Schrieffer, Solid State Commun. **92**, 129 (1994), and references therein.

[3] D.J. Scalapino, Phys. Rep. **250**, 329 (1995), and references therein.

[4] S.R. White *et al.*, Phys. Rev. B **39**, 839 (1989); N. Bulut, D.J. Scalapino, and S.R. White, *ibid.* **47**, 6157 (1993).

[5] We have previously found that this form provides a reasonable fit to the Monte Carlo results for the irreducible interaction: N. Bulut, D.J. Scalapino, and S.R. White, Phys. Rev. B **50**, 9623 (1994).

[6] H.-B. Schüttler and C.-H. Pao [Phys. Rev. Lett. **75**, 4504 (1995)] have also discussed this.

[7] The effect of the self-energy is to reduce the effective strength of the interactions due to wave function renormalization. Here we are interested in obtaining a qualitative understanding of the effect of the different electron-phonon interactions on the $d_{x^2-y^2}$ pairing channel and have neglected the self-energy and treated the coupling strength g as a parameter.

[8] V.H. Crespi and M.L. Cohen, Solid State Commun. **81**, 187 (1992).

[9] R. Zeyher, J. Supercond. **7**, 537 (1994).

[10] J. Song and J.F. Annett, Phys. Rev. B **51**, 3840 (1995) have discussed the electron-phonon coupling associated with in-plane breathing modes as well as out-of-plane tilting modes for an effective single-band Hubbard Hamiltonian.

[11] Such calculations for the s-wave $[g(\mathbf{k})=1]$ coupling λ of the cuprates have been carried out by O.K. Andersen, A.I. Liechtenstein, O. Rodriguez, I.I. Mazin, O. Jepsen, V.P. Antropov, O. Gunnarsson, and S. Gopalan, Physica C **185–189**, 147 (1991); H. Krakauer, W.E. Pickett, and R.E. Cohen, Phys. Rev. B **47**, 1002 (1993).

[12] For the cuprates it will also be important to take into account the strong electron-electron correlations in computing $M^{\nu}_{kk'}$.

[13] A. Nazarenko and E. Dagotto, Phys. Rev. B **53**, R2987 (1996).

[14] T. Dahm, D. Manske, D. Fay, and L. Tewordt, Phys. Rev. B **54**, 12 006 (1996).