Saddle-Point Pairing: An Electronic Mechanism for Superconductivity

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It is shown that the interactions in a strongly correlated quasi-two-dimensional electron gas with the Fermi level lying at a saddle point (Van Hove singularity) in ε_k can give rise to superconductivity by exchange of excitations with a characteristic low electronic energy scale E^*. Application to cuprate superconductors shows that this mechanism along with a conventional electron-phonon interaction can explain the high T_c's and the anomalous behavior of the isotope shift as a function of doping.

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Electronic pairing mechanisms, proposed in the context of potential high-temperature *s*-wave superconductors, remain subject to the long-standing problem of identifying an electronic energy scale low enough relative to the Fermi energy so as to satisfy [1] the Migdal theorem and to renormalize the Coulomb repulsion. So far no electronically paired *s*-wave superconductors have ever been convincingly identified.

In this paper we present a new electronic pairing mechanism which does have a low-energy scale and which under the right conditions can lead to high-temperature superconductivity. This pairing mechanism arises in strongly interacting quasi-2D electron systems having the Fermi level close to a logarithmic Van Hove singularity in the density of states (DOS), at which point the energy surfaces form a saddle point (Fermi surface nesting is *not* desirable). This type of Fermi system has unusual low-frequency electron-hole excitations, which provide a decay channel for an excited quasiparticle, leading to an anomalously large quasiparticle lifetime broadening [2–4] $1/\tau$, scaling linearly with quasiparticle energy ω from the Fermi level [2,3] instead of the usual ω^2 dependence. Here we shall show that the exchange of the same low-frequency excitations gives rise to a strongly **q**- and ω-dependent interquasiparticle interaction which leads to pairing. Although the electron-hole excitations themselves (unlike phonons) do not have any characteristic low-energy scale, they manifest the new scale in their *coupling* to quasiparticles.

The cuprate superconductors supply all the conditions for the new pairing mechanism to occur. They are nearly 2D strongly interacting electron systems, band structure [4] and angle-resolved photoemission data [4] support the presence of the Van Hove singularity (VHS) near ε_F, and evidence for the linear dependence of $1/\tau$ on quasiparticle energy [2–5] exists. Discussion of other phenomena associated with the VHS may be found in available reviews [6]. However, it has not been possible to achieve adequate T_c's and the extremely low observed isotope shifts for the cuprates within a convincingly parametrized strong-coupling framework [7] based on phonons alone, even when the VHS is taken into account. In this paper we show as an application of the electronic pairing mechanism that it does lead to high T_c's and very low isotope shifts, while correctly describing the trend of isotope shift [8–10] as the Fermi level is displaced away from the VHS.

The basic model, from which the quasiparticle interactions can be derived, is the strongly interacting one, which is widely accepted for the cuprates, in which the local short-range Coulomb interaction U between electrons is taken to be much larger than the kinetic energy terms. An initial Fermi-liquid solution to this strong-interaction problem, derived for example from the extensively studied slave-boson mean-field approach, can be assumed to be very close to reality, based on its consistency with photoemission data on both the band dispersion [11] and the shape of the Luttinger Fermi surface [11,12]. This formulation, involving a $1/N$ expansion, gives a convenient expression for the quasiparticle-quasiparticle interaction at the $1/N$ level, which has been used in several earlier treatments of superconductivity in strongly correlated systems [13]. These treatments, however, did not take into account the possibility of the Fermi level lying near a VHS.

The interquasiparticle interaction $V_{\rm eff}(\mathbf{q},\omega)$ to order $1/N$ in the slave-boson theory comes from single slave-boson exchange [Fig. 1(a)] and is given by the slave-boson propagator $D(\mathbf{q},\omega)$. A useful low-frequency approximation to $D(\mathbf{q},\omega)$ (which is in general a 2×2 matrix) is given by [14]

$$V_{\rm eff}(\mathbf{q},\omega)\simeq 1/\Pi(\mathbf{q},\omega)\,, \tag{1}$$

where Π is the **q**- and ω-dependent polarizability [Fig. 1(b)]. The approximation (1) is rigorously valid in the

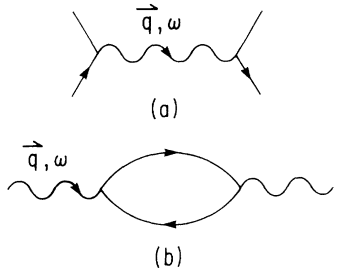

FIG. 1. (a) Interquasiparticle interaction $V_{\rm eff}(\mathbf{q},\omega)$. (b) Polarizability $\Pi(\mathbf{q},\omega)$.

Kondo limit, but earlier numerical studies [15] have also shown it to be reasonable in the practical parameter region for high-temperature superconductors, which are relatively strongly correlated systems. In the limit $\omega=0$, $\mathbf{q}\rightarrow 0$, we retrieve from (1) the widely used approximation $V_{\rm eff}\simeq[2\rho(\varepsilon_F)]^{-1}$, where $\rho(\varepsilon_F)$ is the DOS at the Fermi level.

Suppose that we model the band structure for the CuO_2 plane, $\varepsilon_{\mathbf{k}}$, within a region $|k_x|<k_c$, $|k_y|<k_c$ around the VHS, with the rectangular hyperbolic form

$$\varepsilon_{\mathbf{k}}=k_xk_y/m\,, \tag{2}$$

where m is the effective mass. Here the simplification of rectangular asymptotes is irrelevant and can be removed by rescaling the axes. Then the polarizability $\Pi(\mathbf{q},iv)$ at $T=0$ for imaginary frequency iv is given by $\Pi=(f/2D)\{P(Z,q_x/k_c)+P(Z,q_y/k_c)\}$, where

$$P(Z,x)=g(1)-g(-1)-g(1/x)+g(-1/x)$$
$$-g(1-1/x)+g(-1+1/x)\,, \tag{3}$$

and $g(u)=(Z+u)\ln|Z+u|$. In (3), $D=k_c^2/m$ and $Z=iv/\varepsilon_{\mathbf{q}}$. Equation (3) is based on the assumption of one VHS occupying a fraction f of the area of the Brillouin zone, and a spin degeneracy of 2.

The interaction $V_{\rm eff}$ from (1) and (3) is illustrated in Fig. 2. When the Fermi level lies right at the VHS this function has extremely unusual behavior, in having a cusplike $\mathbf{q}$-dependent minimum as a function of imaginary frequency. At small $\mathbf{q}$ the function changes by order 1 eV in tens of millivolts, abrupt behavior reminiscent of the attraction induced by phonons. Of course the potential in the cusp region is not intrinsically attractive (Fig. 2), but it becomes so when the pseudopotential effect, arising from a node in the gap at higher energy, is included: Such pairing by purely repulsive interactions has long been known to be possible [16], but nonphononic examples have been lacking. When a displacement E of the Fermi level away from the VHS is introduced the cusp region, and hence the pairing tendency, tends to disappear (Fig. 2).

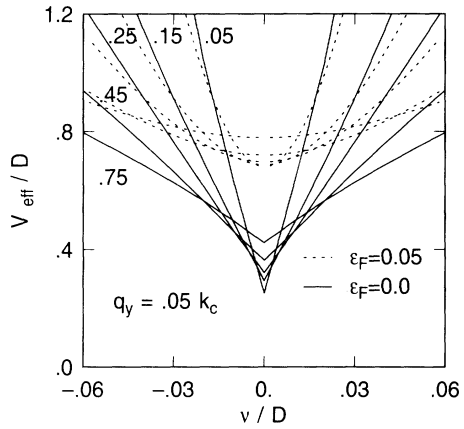

FIG. 2. Interquasiparticle interaction $V_{\rm eff}(\mathbf{q},iv)$ as a function of imaginary frequency v, for various values of q_x in units of k_c (labels on curves), at fixed $q_y=0.05k_c$. $f=0.5$. Solid curves, $\varepsilon_F=0$ [Eq. (3)]; dashed curves, $\varepsilon_F=0.05D$ (obtained by carrying out the zero-T $\mathbf{k}$ sum numerically).

For low frequencies the $T=0$ potential $V_{\rm eff}$ can be modeled to considerable accuracy, for small $\varepsilon_{\mathbf{q}}$, by the form $V_{\rm eff}(\mathbf{q},iv)\simeq V_0+\zeta|v|(D/|\varepsilon_{\mathbf{q}}|)^{1/2}$. Our conclusions are not sensitive to the detailed behavior of $V_{\rm eff}$ at large v, and since $V_{\rm eff}$ tends to saturate, we define a saturation value V_c in the high-frequency region. Hence, including the electronic Z factor Z_e (see below), a model for $V_{\rm eff}$ over an extended frequency range is then

$$V_{\rm eff}(\mathbf{q},iv)\simeq\frac{Z_e}{f}\left\{V_0+\frac{\zeta|v|D^{1/2}}{|\varepsilon_{\mathbf{q}}|^{1/2}}\right\},\quad |v|<(E^*|\varepsilon_{\mathbf{q}}|)^{1/2}\,,$$
$$V_{\rm eff}(\mathbf{q},iv)=V_c,\quad |v|>(E^*|\varepsilon_{\mathbf{q}}|)^{1/2}\,, \tag{4}$$

where the characteristic electronic energy scale E^* is given by

$$E^*\equiv\frac{[fV_e/\zeta Z_e]^2}{D}\,. \tag{5}$$

At $T=0$, $V_e=V_c-Z_eV_0/f$, and from Fig. 2 the constants ζ and V_0 are $\zeta=0.86$ and $V_0=0.16D$. The behavior (4) can also be obtained in the limit of weak interaction ($U\ll D$), using the RPA, with U now entering instead of V_c.

Physically, the energy scale E^* arises as the condition when the dispersion relation of the interaction V_e, $v=fV_e\varepsilon_{\mathbf{q}}^{1/2}/\zeta Z_e\sqrt{D}$, intersects the dispersion relation $v=\varepsilon_{\mathbf{q}}$ for the quasiparticles—a kind of velocity matching condition. At this scale the quasiparticle can be thought of as in resonance with the retarded interaction between them.

To model the reduction in well depth V_e due to Fermi-level displacement E (Fig. 2) and also finite temperature T, we adopt the interpolative form

$$V_e=V_C-(V_e/f)\{V_0^\gamma+V_E^\gamma+V_T^\gamma\}^{1/\gamma}$$

which exactly describes the separate E- and T-well depth reductions if $V_E=D/\ln(D/|E|)$ and $V_T=D/\ln(D/0.88T)$.

We now shall demonstrate how the interaction (4) gives rise to pairing in which E^* plays a role, analogous to the phonon frequency in conventional superconductivity, as the characteristic energy scale for electronic pairing. In the limit where E^* is small, a Migdal-type phase-space argument [1] will rigorously justify the treatment of electronic and phononic pairing on the same footing. The essential principle may be manifested by approximating the $\mathbf{k}$-dependent part of (4) by a square-well interaction. To take account of phonons, we shall consider the Einstein model, also modeling the kernel by the square-well approximation [1], giving the linearized strong-coupling gap equation

$$\bar{\Delta}(\mathbf{k},\nu_n)=T\sum_{n'}\sum_{\mathbf{k}'}K(\mathbf{k}-\mathbf{k}',\nu_n-\nu_{n'})\frac{\bar{\Delta}(\mathbf{k}',\nu_{n'})}{\varepsilon_{\mathbf{k}'}^2+\bar{\nu}_{n'}(\mathbf{k}')^2}\,, \tag{6}$$

where the kernel takes the form

$$K(\mathbf{q},\nu_n)=-V_c+V_e\theta((E^*|\varepsilon_{\mathbf{q}}|)^{1/2}-|\nu_n|) +V_p\theta(\omega_E-|\nu_n|)\,; \tag{7}$$

barred quantities involve implicit multiplication by the Z factor $Z(\mathbf{k},\nu_n)$. In (7) $\nu_n=(2n+1)\pi T$ is the fermionic Matsubara frequency, ω_E is the Einstein frequency, and V_p is the electron-phonon coupling. If there were only the Coulomb and phonon terms in (7), it would be possible to momentum average and retrieve the Eliashberg equation [1,7]. But, as we shall see, the **q**-dependent term coming from the interaction of Fig. 2 leads to very different physics.

Preliminary numerical studies of (6) and (7) suggest two simplifying approximations—(a) ignoring the **k** dependence of Z, and (b) using a separable model for the kernel. The model is then

$$Z\sim 1+\sigma_e\theta(E^*-|\nu_n|)+\sigma_p\theta(\omega_E-|\nu|)\,,$$

$$K\sim -V_c+V_e\theta((E^*|\varepsilon_{\mathbf{k}}|)^{1/2}-|\nu_n|)\theta((E^*|\varepsilon_{\mathbf{k}'}|)^{1/2}-|\nu_{n'}|) +V_p\theta(\omega_E-|\nu_n|)\theta(\omega_E-|\nu_{n'}|)\,.$$

The σ_α are estimated from $Z=-d\Sigma(\mathbf{k},\omega)/d\omega|_{\omega=0}$ at $T=0$. Assuming $E^*\gg\omega_E$, the electronic Z factor is first calculated by solving

$$Z_e=1+V_e f\{\ln[D/(E+Z_e^2E^*)]+\ln[D/(\sqrt{E}+Z_e(E^*)^{1/2})^2]\}/2D,\quad \mathbf{k}\to 0\,, \tag{8a}$$

and then Z is calculated from

$$Z=Z_e+V_p f\ln[D/(\omega_E^2Z^2+E^2)^{1/2}]/2D\,. \tag{8b}$$

Note the somewhat analogous appearance of E^* in (8a) in the role of energy scale played by ω_E in (8b).

Now the transition temperature is given by the solution to

$$\det\begin{bmatrix}F_c+\gamma_c & F_e & F_p\\ F_e & F_e-\gamma_e & F_{ep}\\ F_p & F_{ep} & F_p-\gamma_p\end{bmatrix}=0\,, \tag{9}$$

where $\gamma_\alpha=1/V_\alpha$ and the functions F_α are

$$F_\alpha=T\sum_{\mathbf{k}}\sum_n\frac{f_\alpha}{\varepsilon_{\mathbf{k}}^2+\bar{\nu}_n^2}\,, \tag{10}$$

with $f_c=1$, $f_e=\theta((E^*|\varepsilon_{\mathbf{k}}|)^{1/2}-|\nu_n|)$, $f_p=\theta(\omega_E-|\nu_n|)$, and $f_{ep}=f_ef_p$.

Let us consider the qualitative physics in the absence of electron-phonon coupling. Putting then $V_p=0$, we need only consider the top left 2×2 submatrix in (9). A rough weak-coupling evaluation of F_e gives

$$F_e\simeq\int d\varepsilon\rho(\varepsilon)\{\tanh(\varepsilon/2T)-(2/\pi)\tan^{-1}[(\varepsilon/E^*)^{1/2}]\}/2\varepsilon\,,$$

whence putting $f=1$ we obtain intuitive (but not accurate) forms for T_c and the effective coupling constant,

$$T_c=1.36D\exp\{-[2/\lambda_{\text{eff}}+\ln^2(D/E^*)-1]^{1/2}\}\,, \tag{11}$$

$$\lambda_{\text{eff}}=D^{-1}\left[V_e-\frac{V_c}{1+V_c\ln^2(E^*/D)/4D}\right].$$

Equations (11) are identical with the standard results [17–21] for pairing at a VHS in the BCS approximation except that V_e replaces the electron-phonon coupling and E^* plays the role of the phonon cutoff.

For a more accurate evaluation we first replace the artificial step-function cutoffs by more tractable smooth ones, $\theta(\omega_E-|\nu|)\to\omega_E^2/(\nu^2+\omega_E^2)$ and $\theta((E^*|\varepsilon|)^{1/2}-|\nu|)\to\varepsilon^2/[\varepsilon^2+(\nu^2/E^*)^2]$, then carry out the $\varepsilon_{\mathbf{k}}$ integration first, giving expressions for the F's in terms of adequately convergent frequency sums, which are readily carried out numerically.

The results are illustrated in Fig. 3, where we have adjusted V_c to give a T_c of order 90 K. The electronic T_c is seen to have a pronounced maximum at $E=0$, both due to the higher DOS in the neighborhood of the VHS and due to the maximization of the electronic binding strength at this point (Fig. 2). We then add a phonon coupling V_p, corresponding to dimensionless coupling strength at the Fermi level of $\lambda\sim 0.2$, a value consistent with the mean free path [22]. With phononic pairing included, a somewhat broader T_c maximum is obtained; the width is similar to that found in a recent quantitative

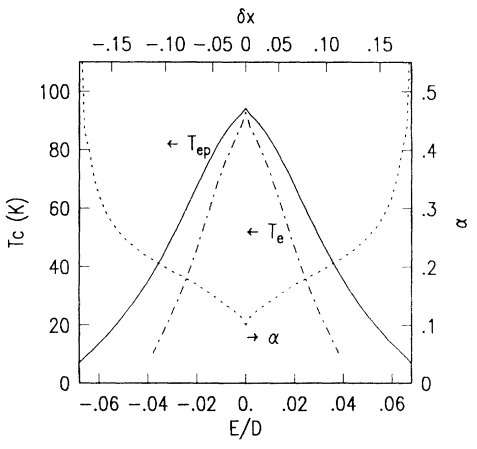

FIG. 3. T_c for electronic interaction only (T_e), and for electronic plus phononic interaction (T_{ep}), and isotope shift α plotted vs shift E of Fermi level from center of VHS. Top scale indicates doping change δx relative to ε_F at VHS. In the absence of electronic pairing T_c peaks at 20 K with an isotope shift of 0.31 rising to 0.5 at large E. Parameters: $D=1.6$ eV, $f=0.7$, $\gamma=3$, $V_c=1.3D$, $V_p=0.2D$, $\omega_E=0.04$ eV ($E^*=0.44D$ at $E=0$).

study of the specific heat jump in the 1:2:3 material [23]. The isotope shift undergoes a strong variation from 0.1 to 0.6 as E displaces the Fermi level away from the VHS, in agreement with isotope-shift data on the 1:2:3 material [9,10]. This contrasts with the much shallower dip in α found in strong coupling from purely phononic pairing, whether treated in the Eliashberg approach [7] or in the present separable approximation (however, the BCS approach gave a strong variation in the isotope shift even for phononic pairing [21]).

The value of $E^*=0.44D$ is deceptively large; E^* is merely an upper cutoff on a pairing spectrum. As a result of peaking of the logarithmic DOS at low frequency, the important pairing frequency is much below E^*. This is seen quantitatively by examining the behavior of the F integrals, and indeed in the existence of pairing itself.

In the future we plan to examine the behavior of other quantities, such as the gap and spin-lattice relaxation time, for more specific experimental comparison with cuprate superconductors.

In summary, a strongly interacting 2D electron gas with the Fermi level lying close to a VHS is found to have an electronic contribution to pairing which can explain the high T_c's found in the cuprate superconductors and the trend of the isotope shift. The pairing mechanism is associated with a characteristic low electronic energy scale.

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