Nesting Mechanism for d-symmetry Superconductors

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Abstract

A nested Fermi surface with nearly parallel orbit segments is found to yield a singlet d-wave superconducting state at high temperatures for a restricted range of the on-site Coulomb repulsion that avoids the competing spin density wave instability. The computed superconducting transition temperature drops dramatically as the nesting vector is decreased, in accord with recent photo-emission data on the Bi2212 and Bi2201 cuprates.

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Even though the BCS theory [1] provides a successful description of conventional superconductors, the concept of alternate electron pairing states of finite angular momentum has evolved [2] to encompass various physical systems. Spin fluctuations suppress [3,4] the BCS isotropic pair binding induced by phonon exchange, and hence materials with strong repulsive interactions are prospects for anisotropic pairing. Superfluid $^3\text{He}$ exhibits p-wave pairing [5], and heavy Fermion superconductors offer another unconventional case at very low temperatures.

Copper oxides with high superconducting transition temperatures $T_c$ exhibit abnormal electrical transport and optical properties. The observed linear temperature variation of the resistivity was attributed by Lee and Read [6] to electron-electron collisions on a perfectly nested Fermi surface in the form of a square, and the anomalous linear frequency variation of the damping has been derived for a partly nested Fermi liquid (NFL). [7,8] However, nesting models need to consider the competing spin density wave (SDW) instability.

The evident correlation of high $T_c$ values in cuprates with departures from the standard Fermi liquid behavior suggests that the physical origin of the anomalous damping is a key source of the superconductivity. This connection is found here by the present microscopic theory for a partially nested Fermi surface. The on-site Coulomb repulsion $U$ provides the primary interaction, while the nested orbit topology is the key determinant of the attraction. The pairing symmetry and binding via exchange of spin fluctuations are determined by the nesting vector $\vec{Q}$. The $d$ angular momentum state is found to be favored in the Bi2212 cuprate where our calculations reveal the existence of superconductivity for values of $U$ that avoid the SDW instability.

Our investigation was inspired by the discovery of Scalapino et al. [9] that $d$-wave pairing may be possible in a Hubbard model. Similar correlations were found in Monte Carlo simulations [11] on a small lattice. However, for the band fillings and Fermi surface topologies treated by Scalapino [9] and others [11,13], the lowest order estimates give very small $T_c$ values. Other anisotropic pairing proposals have been applied to organic compounds [14] and heavy Fermion superconductors [15].
We consider the Hubbard Hamiltonian

\[
H = \sum_{\vec{k},\sigma} E(\vec{k}) c_{\vec{k},\sigma}^{\dagger} c_{\vec{k},\sigma} + U \sum_{\vec{p},\vec{q},\vec{k}} c_{\vec{p}+\vec{q},\uparrow}^{\dagger} c_{\vec{p},\uparrow} c_{\vec{k}-\vec{q},\downarrow}^{\dagger} c_{\vec{k},\downarrow},
\]

(1)

where the electron (or hole) energy band \(E(k)\) is represented by the tight–binding expression

\[
E(\vec{k}) = -2t(\cos k_x + \cos k_y - B \cos k_x \cos k_y + \frac{\mu}{2}),
\]

(2)

\(U\) is the Coulomb repulsion between electrons at a given site, and \(c_{\vec{k},\sigma}^{\dagger}(c_{\vec{k},\sigma})\) represent creation (destruction) operators of momentum \(k\) and spin \(\sigma\). The Fermi surfaces for this model are shown in Figure 1 for a rounded orbit (Fermi liquid FL), and a nested surface that resembles photoemission experimental data by Dessau et al. \[16\] and Shen et al. \[17\] on Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_8\).

Electron scattering in the singlet spin channel involves a direct Coulomb term and the exchange of spin fluctuations \[4\] of the form shown in Figure 2. The phase space for the scattering and the susceptibility enhancement near the nesting vector are important for the d-wave pairing as well as for the SDW instability condition \(U\chi' = 1\).

We compute the real part of the susceptibility, \(\chi'(\vec{q},\omega)\), using the standard definition \[18\] and include self energy corrections of the NFL form \[4\]. The results for the \(E(k)\) model chosen to represent Bi2212 are shown as a function of momentum in Figure 3. The double peak structure at low frequencies is similar to the neutron spectra for the La\(_{2-x}\)Sr\(_x\)CuO\(_4\) superconductor \[19\]. Another consequence of nesting is the scaling of the spin susceptibility as a function of \(\omega/T\) which has been confirmed by neutron scattering on several cuprates \[20\]. The SDW constraint on the susceptibility requires \(U \leq 1.1\) eV in the case of Bi2212 where the bandwidth is estimated to be 1.5 eV from photoemission data.

Decomposition of the two-particle scattering into angular momentum channels yields an effective pairing coupling \[9\]

\[
\lambda_l = - \frac{\sum_{\vec{k}k'} g_l(\vec{k}) V(\vec{k},\vec{k}') g_l(\vec{k}') \delta[E(\vec{k})] \delta[E(\vec{k}')] \sum_{\vec{k}} g_l^2(\vec{k}) \delta[E(\vec{k})]}{\sum_{\vec{k}} g_l^2(\vec{k}) \delta[E(\vec{k})]}.
\]

(3)

The conventional symmetry classification of the basis set \(g_l\) \[3, 13\] is \(g_s = 1\) for the s-wave states, \(g_p = \sin k_x\) for p-waves and the d-wave states with \(g_{x^2-y^2} = \cos k_x - \cos k_y\) and \(g_{xy} = \sin k_x \sin k_y\).
The primary pairing interaction $V(\vec{k}, \vec{k}')$ (see Fig. 2) is given by the term with two spin fluctuation bubbles, $U^3\chi'^2(\vec{k} - \vec{k}')$, and the exchange term proportional to $U^2\chi'(\vec{k} + \vec{k}')$. If $\chi'(\vec{q}, 0)$ is approximately constant, an inspection of Eq. 3 reveals that superconductivity by this mechanism is not possible because $\lambda < 0$.

To calculate the coupling, we represent the susceptibility by a Gaussian form

$$\chi'(\vec{q}, 0) = A + B(\vec{Q}) \exp \left[ -\frac{(|q_x| - Q_x)^2 + (|q_y| - Q_y)^2}{2\alpha^2} \right]$$

where $\vec{q} = \vec{k} - \vec{k}'$, $\vec{Q} = (\pi, \pi)$, and the constants $A$ and $B(\vec{Q})$ determine the normalization for the Gaussian. This model yields a reasonable fit to the computed Bi2212 susceptibility shown in Figure 3. The actual nesting peaks for our Bi2212 model are at $\vec{Q}_1 = (\xi\pi, \pi)$, $\vec{Q}_2 = (\pi, \xi\pi)$, $\vec{Q}_3 = (2\pi - \xi\pi, \pi)$ and $\vec{Q}_4 = (\pi, 2\pi - \xi\pi)$, with $\xi = 0.91$, but this four-peak structure produces only small corrections to the $T_c$ determined by the simple Gaussian in Eq. 4.

Our previous analytic derivation [7] of the NFL susceptibility using the nesting approximation $E(\vec{k} + \vec{Q}) \approx -E(\vec{k})$ gave a logarithmic temperature variation of $\chi'_{NFL}(\vec{Q}, 0)$. However, the present calculation gives a smaller susceptibility (see Fig. 3), with a weaker temperature dependence. The susceptibility reduction is caused by the rounded corners in our Fermi surface model and the influence of the NFL self-energy $\Gamma = \text{Max}(T, |\omega|)$. Together, these features avoid the SDW formation at intermediate values of the interaction, such as $U \simeq 0.96$ eV (compared to the bandwidth $8t = 1.5$ eV) that is used here.

Numerical integration over momenta gives the coupling $\lambda_{x^2-y^2}$, and our computed susceptibility indicates an energy cut-off $\omega_c \simeq 0.3$ eV. The leading order evaluation of the superconducting temperature becomes

$$T_c = \omega_c \exp\left(\frac{-1}{\lambda_{x^2-y^2}}\right).$$

We first find that the Fermi Liquid topology (dashed curve in Figure 1) gives $\lambda_{x^2-y^2} = 0.016$ which corresponds to a vanishing $T_c$. This example is qualitatively similar to other cases studied by several groups [9–13]. The random phase approximation (RPA) contributions enhance this coupling near the SDW instability [9–11][13].
Nesting topologies increase the attraction in a d-wave channel as we demonstrate for the Bi2212 cuprate model. Using band parameters that yield the nested Fermi surface in Fig. 1, \( U = 1.0 \, \text{eV} \) and \( \chi'_{\text{max}} = 0.92 \, \text{eV}^{-1} \), we obtain a d-wave coupling in the lowest order \( \lambda_{x^2-y^2} = 0.27 \) that gives \( T_c = 90 \, \text{K} \).

If the Coulomb coupling is of intermediate strength, e.g. \( U\chi' = 0.9 \), the RPA enhancement of the nested case would elevate the coupling to \( \lambda_{x^2-y^2} = 2.7 \) and thereby predict an enormous \( T_c \). This situation should stimulate further research on vertex corrections and self energy effects that may offset the RPA series enhancement.

The sensitivity of the coupling to the magnitude of the nesting vector is illustrated in Figure 4. The Bi2201 cuprate exhibits a low \( T_c = 6 \, \text{K} \) despite having abnormal resistivities and optical properties in league with the high \( T_c \) cuprates. Shen et al. [21] have discovered by photoemission spectroscopy that this cuprate possesses a nesting vector close to \( 0.8\vec{Q} \), as compared to the ideal half filled case of \( \vec{Q} = (\pi, \pi) \) and the Bi2212 situation with a nesting vector of \( 0.9\vec{Q} \). This correlation is compatible with a sharp drop in the calculated \( T_c \) values as seen in Figure 4. Our model predicts that the spin susceptibility peaks seen in Figure 3 for the Bi2212 case should spread apart in Bi2201 and this feature may be tested by neutron scattering measurements.

We do not find superconductivity of \( xy \) symmetry for our Fermi surface geometry. The \( x^2-y^2 \) state for the present nesting model is consistent with photoemission measurements of the energy gap anisotropy in Bi2212 [17]. If the Fermi surface is rotated in other cuprates, as suggested by photoemission spectra of YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) by Liu et al. [22], then states of other symmetry should be examined in more detail. We find a vanishing \( T_c \) for p-wave symmetry pairing using \( g_x = \sin k_x \) in both the Fermi liquid model and the nested Fermi surface.

Our model for Bi2212 yields a Van Hove singularity in the density of states that is located 0.04 eV\( \approx \) 500 K above the Fermi energy. An arbitrary increase of the chemical potential towards the logarithmic singularity would result in a SDW phase as shown in Fig. 1.

Impurity scattering should be detrimental to anisotropic pairing as well as for the SDW formation. By analogy with the Abrikosov-Gorkov theory, [23] d-wave suppression by dis-
order constrains $T_c$ in the cuprates \cite{24}. Similarly, non-magnetic impurities also impede the competing SDW transition \cite{25}. The case of chromium reveals a further sensitivity of the SDW to impurity induced shifts of the band structure \cite{26}. Impurities at sites in the copper oxide planes should be more destructive for d–wave superconductivity than those at interplanar sites.

The origin of nesting features in cuprates is evident in band structure calculations \cite{27} because of the nearly half-filled d-bands in two dimensions. Logically, the relative persistence of parallel segments in a given band subjected to doping may be stabilized by a second band that acts as a charge reservoir.

Theoretical extensions of the present work may be relevant to higher order spin fluctuation graphs, including the “spin bag” variety \cite{28}, and the self-energy and vertex corrections. Nesting of a two-dimensional electronic structure produces \cite{7,8} a linear frequency variation of the quasiparticle damping that bears similarities to the Luttinger theory \cite{29} for a one dimensional electron gas, which also exhibits remarkable charge and spin dynamics \cite{30}, \cite{31}.

Nevertheless, nesting in two dimensions is distinguished by a crossover temperature $T^\ast$ below which the electronic response reverts to standard Fermi liquid behavior. Accordingly, the concept of a well-defined Fermi surface is valid in the NFL approach, despite the unusual damping features that arise above $T^\ast$ and a corresponding frequency crossover $\omega^\ast$ that are determined by the nesting geometry.

Our analysis may provide a guide to the design of new superconducting materials. The primary ingredients for the d-wave pairing are a Fermi surface topology with a nesting vector restricted to a narrow range, a Coulomb repulsion $U$ of intermediate strength, and a planar electronic structure that accepts intercalant atoms with weak impurity scattering of electrons (or holes) in the conducting layers.

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FIGURES

FIG. 1. A nested Fermi surface (NFL) shown by the solid curve was calculated to fit the photoemission data points of Dessau et al. [16] using the tight–binding model of Eq. 2 with $B = 0.165$ and $\mu = -0.56$. The nesting vector is $\vec{Q}^* \simeq 0.91(\pi, \pi)$ in this case. By contrast, the dashed curve for the same value of $B$ but a chemical potential $\mu = -1.6$ shows a rounded orbit reminiscent of a standard Fermi Liquid (FL).

FIG. 2. Diagrams for the electron-electron scattering in the singlet channel show the direct Coulomb repulsion by a dotted line and the spin fluctuation exchange processes with a bubble representing the susceptibility. In the d-wave channel for a nested Fermi surface, the leading order attractive contributions from the graphs involving the susceptibility are of the same order, whereas the direct bare Coulomb repulsion gives no contribution in the Hubbard model, because $U$ is assumed to be momentum–independent.

FIG. 3. The calculated real part of the susceptibility for the Bi2212 band parameters $B = 0.165$ and $\mu = -0.56$ is shown as a function of momentum $|\vec{q}|$ along the direction $q_x = q_y$ by the solid curve for the damping $\Gamma_{NFL} = \text{Max}(T, |\omega|)$, and by the dashed curve for a damping $\Gamma = 0$. The calculated maximum $\chi'(\vec{Q}^*) \simeq 0.97 \text{ eV}^{-1}$ constrains $U < 1 \text{ eV}$ which compares with the bandwidth $8t = 1.5 \text{ eV}$ that we estimated from the photoemission data of Ref. 16. The dot-dashed curve represents the Gaussian model of Eq. 4 with $\alpha = 1.2$.

FIG. 4. $T_c$ values as a function of the nesting vector $\vec{Q}^*$ calculated using the tight-binding model of Eq. 2 are shown by the solid curve. The Bi2212 parameters are $B = 0.165$ and $\mu = -0.56$. The points are the experimental values. A surface with a nesting vector $\vec{Q}^* \simeq 0.8(\pi, \pi)$ appropriate to the Bi2201 photoemission data [22] was simulated using $B = 0.33$ and $\mu = -1.36$ which lowers $T_c$. Intermediate $\vec{Q}^*$ cases were found by linear interpolation of the band structure. The shaded region designates the spin-density wave (SDW) regime.