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**d-wave superconductivity from electron-phonon interactions**

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I examine electron-phonon mediated superconductivity in the intermediate coupling and phonon frequency regime of the quasi-two-dimensional Holstein model. I use an extended Migdal-Eliashberg theory that includes vertex corrections and spatial fluctuations. I find a d-wave superconducting state that is unique close to half filling. The order parameter undergoes a transition to s-wave superconductivity on increasing filling. I explain how the inclusion of both vertex corrections and spatial fluctuations is essential for the prediction of a d-wave order parameter. I then discuss the effects of a large Coulomb pseudopotential on the superconductivity (such as is found in contemporary superconducting materials like the cuprates), which results in the destruction of the s-wave states, while leaving the d-wave states unmodified.

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The discovery of high transition temperatures and a d-wave order parameter in the cuprate superconductors are remarkable results and have serious implications for the theory of superconductivity. The presence of large Coulomb interactions in the cuprates that have the potential to destroy conventional s-wave BCS states has prompted the search for new mechanisms that can give rise to superconductivity. However, electron-phonon mediated superconductivity is still not well understood, especially in lower dimensional systems. In particular, the electron-phonon problem is particularly difficult at intermediate couplings with large phonon frequency (such as found in the cuprates) and the electron-phonon mechanism cannot be fully ruled out. It is therefore of paramount importance to develop new theories to understand electron-phonon mediated superconductivity away from the BCS limit.

The assumption that electron-phonon interactions cannot lead to high transition temperatures and unusual order parameters was made on the basis of calculations from BCS theory, which is a very weak coupling mean-field theory (although, of course, highly successful for pre-1980s superconductors). In the presence of strong Coulomb interaction, the BCS s-wave transition temperature is vastly reduced. However, the recent measurement of large couplings between electrons and the lattice in the cuprate superconductors means that extensions to the conventional theories of superconductivity are required. In particular, low dimensionality, intermediate dimensionless coupling constants of ~1, and large and active phonon frequencies of ~75 meV mean that BCS or the more advanced Migdal-Eliashberg (ME) theory cannot be applied. In fact, the large coupling constant and a propensity for strong renormalization in two-dimensional (2D) systems, indicate that the bare unrenormalized phonon frequency could be several times greater than the measured 75 meV.

Here I apply the dynamical cluster approximation (DCA) to introduce a fully self-consistent momentum-dependent self-energy to the electron-phonon problem. Short-ranged spatial fluctuations and lowest-order vertex corrections are included, allowing the sequence of phonon absorption and emission to be reordered once. In particular, the theory used here is second order in the effective electron-electron coupling $U=\frac{g^2}{M\omega_n}$, which provides the correct weak coupling limit from small to large phonon frequencies. In this paper, I include symmetry broken states via the anomalous self-energy to investigate unconventional order parameters such as the d wave. No assumptions are made in advance about the form of the order parameter.

DCA (Refs. 6, 8, and 9) is an extension to the dynamical mean-field theory for the study of low-dimensional systems. To apply the DCA, the Brillouin zone is divided into $N_c$ subzones within which the self-energy is assumed to be momentum independent, and cluster Green functions are determined by averaging over the momentum states in each subzone. This leads to spatial fluctuations with characteristic range, $N_c^{1D}$. In this paper, $N_c=4$ is used throughout. This puts an upper bound on the strength of the superconductivity, which is expected to be reduced in larger cluster sizes. To examine superconducting states, DCA is extended within the Nambu formalism. Green functions and self-energies are described by $2\times2$ matrices, with off-diagonal terms relating to the superconducting states. The self-consistent condition is

$$G(K,i\omega_n) = \int_{-\infty}^{\infty} d\epsilon \frac{D_1(\epsilon)}{[\zeta(K,i\omega_n) - \epsilon]^2 + \phi(K,i\omega_n)^2},$$

$$F(K,i\omega_n) = -\int_{-\infty}^{\infty} d\epsilon \frac{D_1(\epsilon)\phi(K,i\omega_n)}{[\zeta(K,i\omega_n) - \epsilon]^2 + \phi(K,i\omega_n)^2},$$

where $\zeta(K,i\omega_n)=i\omega_n + \mu - \Sigma(K,i\omega_n)$, $\mu$ is the chemical potential, $\omega_n$ are the Fermionic Matsubara frequencies, $\phi(K,i\omega)$ is the anomalous self-energy, and $\Sigma(K,i\omega)$ is the normal self-energy. $G(K,i\omega_n)$ must obey the lattice symmetry. In contrast, it is only $|F(K,i\omega_n)|$ that is constrained by this condition, since $\phi$ is squared in the denominator of Eq. (1). Therefore the sign of $\phi$ can change. For instance, if the anomalous self-energy has the rotational symmetry $\phi(\pi,0)=-\phi(0,\pi)$, the on-diagonal Green function, which represents the electron propagation, retains the correct lattice symmetry.
The phonons couple to the local electron density via a momentum-independent coupling constant \( G_{\text{VC}} \). The electron self-energies are labeled with \( \Pi \), and \( \Sigma \) denotes the electron self-energies. Lines represent the full electron Green function and wavy lines the full phonon Green function.

\[
G(\pi,0) = G(0, \pi). \text{ Therefore, only inversion symmetry is required of the anomalous Green function representing superconducting pairs and the anomalous self-energy.}
\]

Here I examine the Holstein model\(^{11}\) of electron-phonon interactions. It treats phonons as nuclei vibrating in a time-averaged harmonic potential (representing the interactions between all nuclei), i.e., only one frequency \( \omega_0 \) is considered. The phonons couple to the local electron density via a momentum-independent coupling constant \( g_{\text{ME}} \).

\[
H = -\sum_{\langle ij \rangle} t c_i^\dagger c_j + \sum_{\nu} n_{\nu} (g r_i - \mu) + \sum_i \left( \frac{M \omega_0^2 r_i^2}{2} + \frac{p_i^2}{2M} \right).
\]

The first term in this Hamiltonian represents hopping of electrons between neighboring sites and has a dispersion \( \epsilon_k = -2\sum_{i=1}^{D} \cos(k_i) \). The second term couples the local ion displacement, \( r_i \) to the local electron density. The last term is the bare phonon Hamiltonian, i.e., a simple harmonic oscillator. The creation and annihilation of electrons is represented by \( c_i^\dagger \), \( p_i \) is the ion momentum, and \( M \) the ion mass. The effective electron-electron interaction is

\[
U(i\omega_n) = \frac{U \omega_n^2}{\omega_n^2 + \omega_0^2},
\]

where \( \omega_n = 2\pi n \omega \), \( s \) is an integer, and \( U = -g^2/M \omega_0^2 \) represents the magnitude of the effective electron-electron coupling. \( D=2 \) with \( t=0.25 \), resulting in a noninteracting bandwidth \( W=2 \). A small interplanar hopping \( t_{\perp} = 0.01 \) is included. This is necessary to stabilize superconductivity, which is not permitted in a pure 2D system.\(^{12}\)

Perturbation theory in the effective electron-electron interaction (Fig. 1) is applied to second order in \( U \), using a skeleton expansion. The electron self-energy has two terms, \( \Sigma_{\text{ME}}(\omega, \mathbf{K}) \) neglects vertex corrections [Fig. 1(a)], and \( \Sigma_{\text{VC}}(\omega, \mathbf{K}) \) corresponds to the vertex corrected case [Fig. 1(b)]. \( \Pi_{\text{ME}}(\omega, \mathbf{K}) \) and \( \Pi_{\text{VC}}(\omega, \mathbf{K}) \) correspond to the equivalent phonon self-energies. At large phonon frequencies, all second-order diagrams including \( \Sigma_{\text{VC}} \) are essential for the correct description of the weak coupling limit.

The phonon propagator \( D(z, \mathbf{K}) \) is calculated from

\[
D(i\omega_n, \mathbf{K}) = \frac{\omega_n}{\omega_n^2 + \omega_0^2 - \Pi(i\omega_n, \mathbf{K})},
\]

and the Green function from Eqs. (1) and (2). \( \Sigma = \Sigma_{\text{ME}} + \Sigma_{\text{VC}} \) and \( \Pi = \Pi_{\text{ME}} + \Pi_{\text{VC}} \). Details of the translation of the diagrams in Fig. 1 and the iteration procedure can be found in Ref. 7. Calculations are carried out along the Matsubara axis, with sufficient Matsubara points for an accurate calculation. The equations were iterated until the normal and anomalous self-energies converged to an accuracy of approximately 1 part in \( 10^5 \).

Since the anomalous Green function is proportional to the anomalous self-energy, initializing the problem with the noninteracting Green function leads to a nonsuperconducting (normal) state. A constant superconducting field with \( d \)-wave symmetry was applied to the system to induce superconductivity. The external field was then completely removed. Iteration continued without the field until convergence. This solution was then used to initialize self-consistency for other similar values of the parameters. The symmetry conditions used in Refs. 5 and 7 have been relaxed to reflect the additional breaking of the anomalous lattice symmetry in the \( d \)-wave state. This does not affect the normal-state Green function, but does affect the anomalous-state Green function.

In Fig. 2, the anomalous self-energy is examined for half filling. The striking feature is that stable \( d \)-wave superconductivity is found. This is manifested through a change in sign of the anomalous self-energy, which is negative at the \((\pi, 0)\) point and positive at the \((0, \pi)\) point. The electron Green function [Eq. (1)] depends on \( \phi^2 \), so causality and lattice symmetry are maintained. Since the gap function \( \phi(i\omega_n)/Z(i\omega_n) \) is directly proportional to \( \phi(i\omega_n) \), and \( Z(i\omega_n, \mathbf{K}_{(\pi,0)}) = Z(i\omega_n, \mathbf{K}_{(0,\pi)}) \), then the sign of the order parameter, i.e., the sign of the superconducting gap changes under \( 90^\circ \) rotation. \( Z(i\omega_n) = 1 - \Sigma(i\omega_n)/i\omega_n \).
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coupling, the off-diagonal Eliashberg self-energy has the form $-UT\Sigma_{Q,\omega}F(i\omega_n, Q)D_0(i\omega_n - i\omega)$, so it is clear (for the same reasons as the Coulomb pseudopotential) that this diagram has no contribution in the $d$-wave phase (the weak coupling phonon propagator is momentum independent for the Holstein model). Therefore, vertex corrections are the leading term in the weak coupling limit. Further, I have discussed the inclusion of Coulomb states to lowest order, which act to destabilize the $s$-wave states, while leaving the $d$-wave states unchanged. Since the Coulomb pseudopotential has no effect, then it is possible that electron-phonon interactions could explain the mechanism works for real materials such as the cuprates. The Coulomb filtering interactions are the mechanism inducing electron-phonon interactions and high phonon frequencies are seen in the electron and phonon band structures of the 2D Holstein model in the normal phase. It is clearly of interest to determine whether other features and effects in the cuprate superconductors could be explained with electron-phonon interactions alone.

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18. I also note the extensions to Eliashberg theory carried out by Grimaldi et al. (Ref. 14).
19. On the basis of a screened electron-phonon interaction, Abrikosov claims to have found stable $d$-wave states in a BCS-like theory (Refs. 15 and 16). However, with an unscreened Holstein potential, the transition temperature, the $d$-wave channel given by the standard theory is zero. Also, it is not completely clear that the assumed order parameter in his work has $d$-wave symmetry.