Superconductivity Fluctuations in a One-dimensional Two Band Electron-Phonon Model with Strong Repulsive Interactions.

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We study a one-dimensional, two band model with short range electron-electron repulsions (onsite \(U\) and nearest-neighbour \(V\) terms) and electron-phonon coupling. We show that there is a region of \(U,V\) and band filling in which singlet superconductivity fluctuations are dominant. This region is absent without electron-phonon interactions and includes large values of \(U,V\).

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The physics of low dimensional strongly correlated fermion systems with repulsive interactions is a topic of active interest, largely due to the absence of a clear understanding of the origin of high-\(T_c\) superconductivity in cuprate oxides and the role of phonons in these correlated systems. In the framework of a simple one-dimensional (1-d) Cu-O chain model [1], we investigate the effects of both short range electron-electron (e-e) repulsive interactions (onsite \(U\) and nearest neighbour Cu-O repulsion \(V\)) and electron-phonon (e-p) coupling on the ground state of the system. We show that superconducting (SC) correlations are absent in the model if we take into account e-e interactions only. The inclusion of e-p interactions leads to the appearance of a region of \((U,V,\rho)\) (\(\rho\), the band filling) in which superconducting fluctuations are dominant. On the other hand the ground state of the system in the absence of e-e repulsion is a charge-density-wave (or spin-density-wave) state without a divergent SC response. Thus, the origin of the region with dominant SC response is the combined effect of e-e and e-p interactions for this model.

We use a renormalization group (RG) two cut-off approach, developed in earlier works [2,3]. With some assumptions on the model parameters our analysis is valid in the large \(U,V\) limit. The possibility of superconducting fluctuations in quasi-1-d systems with strong repulsive e-e interactions and e-p coupling was first raised in work of Zimanyi et.al. [3], where results are obtained for a massive Thirring model. The two-band model without e-p interactions was considered in [2], where numerical results are presented, pointing out the existence of SC fluctuations in a strong coupling limit.

We consider a chain consisting of two types of atoms: Cu on odd sites with d-orbitals and O on even lattice sites with p-orbitals. The Hamiltonian of the system is

\[
H = H_0 + H_{ee} + H_{ep}
\]

\[
H_0 = -t \sum_{<i,j>} c_{p,i}^+ c_{d,j} + h.c. + \sum_i \Delta (c_{p,i}^+ c_{p,i} - c_{d,i}^+ c_{d,i})
\]

(1)

\[
H_{ee} = \sum_{a=d,p} \sum_i U_a c_{a,i}^+ c_{a,i} + V \sum_{<i,j>} c_{d,i}^+ c_{d,j} c_{p,j}^+ c_{p,j}
\]

(2)

where \(t\) is the hopping integral, \(<i,j>\) are nearest-neighbour sites, \(\Delta = (E_p - E_d)/2\), \(E_p\) and \(E_d\) are site energies, \(U_d, U_p\) are Hubbard onsite repulsive energies, and \(V\) is the repulsion amplitude between nearest-neighbor sites. Direct antiferromagnetic coupling between Cu sites is omitted. Also

\[
H_{ep} = H_{ep,1} + H_{ep,2},
\]

(3)

and we consider two models of electron-phonon coupling: the molecular crystal (MC) model with the Hamiltonian \(H_{ep,1}\) in which optical phonons couple to the electron site energy; and the Su-Schrieffer-Heeger (SSH) model with the Hamiltonian \(H_{ep,2}\) in which the lattice distortions modulate the electron-hopping matrix element \(t\). The Hamiltonian \(H_{ep,1}\) consists of two parts \(H_{ep,1} = H_{ep,d} + H_{ep,p}\), where the each part has the form

\[
H_{ep} = \sum \frac{P_i^2}{2M} + \frac{1}{2} \kappa_i^2 + \lambda q_i \rho_i = \sum \omega_0 (d_i^+ d_i + 1) + \frac{g}{M \omega (d_i^+ d_i + 1)^2} \rho_i
\]

(4)

with \(\omega_0 = \kappa/M\), \(g = \lambda/(2M \omega_0)^{1/2}\), \(\rho_i = \sum c_{k+q}^+ c_{q}\) (\(M\) ion mass, \(\omega_0\) optic phonon frequency, \(\kappa\) elasticity constant, \(\lambda\) e-p coupling constant.) All terms in (4) have indices \(d\) or \(p\) and the sum is over odd or even sites for \(H_{ep,d}\), \(H_{ep,p}\) respectively. The Hamiltonian \(H_{ep,2}\) takes into account intermolecular phonon modes

\[
H_{ep,2} = \sum \frac{P_i^2}{2M} + \frac{1}{2} \kappa (q_i + q_{i+1})^2 - \sum_{<i,j>} \delta t_{i,j} c_{d,i}^+ c_{p,j}
\]

(5)

\[
\sum \omega_k (f_k^+ f_k + \frac{1}{2}) + \frac{1}{N \omega_q} \sum g(k,q) (f_q + f_{-q}^+ c_{d,k}^+ c_{p,k})
\]

where \(\delta t_{i,j} = \lambda (q_i - q_j)\), \(\omega_q = 2(\kappa/M)^{1/2} \sin(\alpha q/2)\) is the acoustic phonon frequency,
where $g_1$ is the back scattering amplitude, and $g_2, g_4$ are forward scattering. The "Umklapp" part $g_3$ exists only for the half filled case $\rho = 1$: for the sake of simplicity we will not consider this case. Since we use a RG approach below, we consider $g_1/\pi v_F \leq 1$, that is $Ua, V a \leq \pi v_F$ or $\sin \theta \ll 1$ for large $U, V$. We have spin - rotation invariance, i.e., $g_{\pm} = g_0$. Therefore, if it is not essential we are omitting spin indices. The effect of the $g_4$ term is taken into account separately: it simply produces a shift in the velocity of the spin and charge degrees of freedom: $v_s = v_F(1 + g_4), v_p = v_F(1 - g_4)$.

The usual RG equations defining the scaling behaviour of the system are

\begin{equation}
 g'_1 = \frac{1}{\pi v_\sigma} g_1^2 \tag{14}
\end{equation}

\begin{equation}
 g_c = g_1 - 2g_2 = \text{const.} \tag{15}
\end{equation}

For $g_1 \geq 0$ the excitation spectrum is gapless $g_1 \rightarrow g_1^* = 0$, and there is a gap if $g_1 < 0$. The charge excitation spectrum is gapless if $g_c \geq 0$ and has a gap $\Delta_g$ if $g_c < 0$. The ground state has a most divergent singlet (triplet) superconductivity (SC) response when $g_c \geq 0, g_1 < 0$ ($g_c \geq 0, g_1 \geq 0$). In our case

\begin{equation}
 g_c = -\frac{Ua}{2} \sin^4 \theta_F + 2Va \sin^2 \theta_F \cos^2 \theta_F (\cos(2kFa) - 2) < 0. \tag{16}
\end{equation}

Therefore there is no region $(U, V)$ with divergent SC fluctuations. Possible ground states are charge- or spin-density wave, depending on the sign $g_1$. (This sign can vary due to the cos $kFa$ term). We see that in order to obtain SC correlations it is necessary to have large positive $g_1^*$ or negative $g_2^*$ terms. As we will see below this condition can be achieved by taking into account e-p interactions.

Second order perturbation theory in e-p interaction produces a retarded e-e interaction \[\] for $\omega$ less than a Debye frequency $\omega < \omega_D \sim (\kappa/M)^{1/2}$. (We consider the case $\omega D < E_F$). The effective e-e interaction can be described in "g-ology" terminology: $g_{1,ph} = -2g^2(kF, 2kF)/\omega_{2kF}, g_{2,ph} = -2g^2(kF, 0)/\omega_0, g_{3,ph} = g_{1,ph}$ (half-filled band only). In the case of the MC model \[\]

\begin{equation}
 g_{1,ph} = g_{2,ph} = g_{3,ph} = -\frac{\lambda^2}{4\kappa}. \tag{17}
\end{equation}

whereas the SSH model \[\] gives

\begin{equation}
 g_{1,ph} = g_{3,ph} = -\frac{\lambda^2}{\kappa} (\sin^2 \theta_F \cos^2 \theta_F). \tag{18}
\end{equation}

The parameters $\kappa, \lambda$ in (17), (18) are, of course, different, as well as other similar parameters in Hamiltonians.
Note that all terms are negative, and \( g_{2ph} \) is due solely to onsite e-p coupling and does not contain renormalization terms \( \sin \theta_F, \cos \theta_F \). In the case \( \theta \ll 1 \) the onsite e-p interaction is dominant. We now have two types of e-e interactions with cutoffs \( E_F \) and \( \omega_D \). We thus use the RG procedure \([2],[3]\) for a two cut-off model. The one-loop scaling equations \([4],[5]\) for the \( g_i \) are unaffected by the presence of retarded interactions. The equations for the \( g_{i,ph} \), taking into account cross terms \( g_1 g_{j,ph} \), were derived in \([3]\):

\[
g_{1,ph} = \frac{1}{\pi v_p} \left( \frac{3}{2} g_1 + \frac{2}{2} g_{1,ph} \right) g_{1,ph} \quad (19)
\]

\[
g_{2,ph} = 0. \quad (20)
\]

We will consider the case \( g_{3,ph} = 0 \). The integration in \([18],[19]\) is taken from \( E_F \) to \( \omega_0 \sim \omega_D(\omega_0) \), where \( \omega_D(\omega_0) \) is the renormalized value of \( \omega_D \). As a result the combined action of different scattering processes is described by

\[
g_i^T = g_i^* + g_{i,ph}^*. \quad (21)
\]

The properties of the system at energies small compared to \( \omega_0 \) are derived from a model with single interactions \( g_i^T \) and bandwith \( \omega_0 \).

We now examine the solutions of equations \([4],[5],[19],[20]\). The initial conditions for \([4],[5]\) are defined by \([3]\). The initial conditions for \([19],[20]\) are defined by \([17],[18]\). We denote \( g_{1,ph}^{(0)} = -\gamma, g_{2,ph}^{(0)} = -\tilde{\gamma} \). If \( g_{1,ph}^{(0)} \geq 0 \) (we will see that this is the situation in the interesting region), from \([2]\) we obtain that \( g_1 \) scales toward small positive values \( g_1^* \leq g_1^{(0)} \). Note that in the case \( \theta \ll 1 \) we have \( g_{1,ph}^{(0)} \approx g_{2,ph}^{(0)}, \) that is \( \tilde{\gamma} \approx \gamma \). From \([3]\) it follows that \( g_1^* - 2g_2^* = g_1^{(0)} - 2g_2^{(0)} \). A positive derivative in \([19]\) implies that \( g_{1,ph} \) scales toward large negative values. We consider the opposite case \( g_{1,ph} < 0 \). Then, at least initially, \( g_{1,ph} \) will scale toward a small negative value. Therefore we demand that

\[
\frac{3}{2} g_1^{(0)} + \frac{1}{2} g_{e}^{(0)} + g_{1,ph}^{(0)} > 0, \quad (22)
\]

since \( g_{1,ph} < 0 \). The inequality \( (22) \) cannot be valid throughout the scaling process, since \( g_1 \) scales to small values. Therefore the value \( g_{1,ph}^* \) may not be very small. We do not require \( |g_{1,ph}^*| \ll \gamma \); for our purposes it is sufficient that \( g_{1,ph}^* > \gamma - 2\tilde{\gamma} \), as we show below. The value \( g_{2,ph} \) is not scaled as follows from \([20]\), i.e., \( g_{2,ph}^* = -\tilde{\gamma} \). This value does not contain the renormalization coefficient \( \sin \theta_F \). As a result of scaling we have the state with \( g_i^T = g_i^* \approx g_{1,ph}^* \). The ground state of the system with the new scaling amplitudes has dominant divergent SC susceptibility if

\[
g_c = g_1^* - 2g_2^* = g_1^{(0)} - 2g_2^{(0)} + g_{1,ph}^* + 2\tilde{\gamma} > 0. \quad (23)
\]

Since we suppose that \( g_{1,ph}^* \approx g_{2,ph}^* < 0 \), we have a state with spin gap \( \Delta_{\sigma} \). Therefore the dominant singularity is the singlet SC response with SC correlation function

\[
R(x) \sim x^{-\pi} \rho, \quad K_\rho = \sqrt{\frac{1 + g_c^2/2\pi v_p}{1 - g_c^2/2\pi v_p}} > 1. \quad (24)
\]

In this case the CDW response can be divergent with correlation function \( \propto x^{-\pi K_\rho} \). The inequalities \( (22),(23) \) define the region in which singlet SC correlations are dominant. In terms of \( u = Ua/\pi \sin \theta, \, v = V a \sin^2 \theta \cos^2 \theta \) we rewrite \( (22),(23) \) as

\[
\gamma + 2v(1 + 2\cos(\pi \rho/2)) < u < 2\gamma^* - 2v(2 + \cos(\pi \rho/2)), \quad (25)
\]

where \( 2\gamma^* = 2\tilde{\gamma} + g_{1,ph}^* \). It is easy to obtain the solution of \( (25) \). This is the region \( ABCD \) in Fig.1 delineated by lines: \( u = 0, \, v = 0, \, u = \gamma - 2v, \, u = 2\tilde{\gamma} + g_{1,ph}^* - 2v. \)

![FIG. 1. Phase diagram obtained by two cut-off RG scaling. Divergent SC response regions are I and II.](image)

Recall that in the case \( \theta \ll 1 \), Eq.\( (22) \), the bare repulsive energies \( U \sim u/\theta^2, \, V \sim v/\theta^2 \gg \gamma \). Thus our model includes the case of strong electron repulsion. For any point \( (u,v) \) in the region \( ABCD \) \( (23) \) is valid for

\[
\rho > 2\pi \cos^{-1}(\max\{u - \gamma - 2v/4v, \, 2\gamma^* - 4v - u/2v\}). \quad (26)
\]
In the case $t/\Delta \ll 1$ we can obtain the phase diagram in terms of the bare values $U, V$. Then the coordinates of points $A,B,C,D$ are $A = \{0,(4\gamma)/(\Delta/t)^4\}$, $B = \{0,2\gamma/(\Delta/t)^2\}$, $C = \{(\gamma/2)/(\Delta/t)^2,0\}$, $D = \{(\gamma^*/2)/(\Delta/t)^2,0\}$. The SC region is deformed to include region II due to the $\sin(\pi\rho/4)$ term. The equation of the curve $EF$ is

$$V = \frac{\Delta^2}{t^2} \left( (2\gamma^*-\gamma)k + 4\gamma + 16\gamma^* \right)^2 / 72(k+2)(\gamma + 2\gamma^*), \quad U = 2kV\Delta^2/t^2. \quad (27)$$

In the limit $k \to \infty$ we have $U \propto V^2$, but in this region $\rho \sim 1/U^{1/4} \to 0$. The inequality $\rho \sim v_0/(\Delta/t)$ with $t/\Delta \ll 1$ becomes

$$(U_1 + 8V_1)y^2 - 6V_1y - \gamma > 0,$$

$$(4V_1 - U)y^2 - 6V_1y + 2\gamma^* > 0, \quad (28)$$

where $V_1 = V(\Delta/t)^2$, $U_1 = \frac{2}{72}(\Delta/t)^4$, $y = \sin^2(\pi\rho/4)$. In region I the solution of (28) is $\rho_0 < \rho < 2$, where $\sin^2(\pi\rho/4) = y_0$ is the largest root of eqn. (28). In the region II we have $\rho_1(U,V) < \rho < \rho_2(U,V)$, where $\rho_1, \rho_2$ are easy obtained from (28). If $V = 0$ the solution is

$$\frac{4}{\pi} \sin^{-1} \left( \frac{\gamma}{U_1} \right)^{1/4} < \rho < \frac{4}{\pi} \sin^{-1} \left( \frac{2\gamma^*}{U_1} \right)^{1/4}. \quad (29)$$

for $U_1 > \gamma$; if $U = 0$, then in the region $\gamma/2 < V_1 < \gamma^*$ the solution is $\sin^2(\pi\rho/4) = y_0$, where $y_0$ is the largest root of eqn. (28) for $U = 0$.

In using the RG approach, we supposed as usual that $g_{i}/\pi v_{F} < 1$. For small $t/\Delta$ we have the initial value $v_{p}^{(0)} \sim (t/\Delta) \sin(\pi\rho/2)$. Recalling that $g_{i} \sim (t \sin(\pi\rho/4)/\Delta)^{2}$ or $(t \sin(\pi\rho/4)/\Delta)^{4}$, $g_{2,ph} = \text{const}$, we suppose that our results are reasonable if we are not too close to band edges, that is $\epsilon_{1} < \rho < 2 - \epsilon_{2}$, and $\rho \neq 1$ ($g_{1} = 0$). It follows from our analysis that in region III we have large spin and charge gaps, so that there is only a charge-density-wave divergent response. In the region IV we have $g_{c}^{T} < 0$, small $g_{T}^{T} < 0$ and thus divergent charge- and spin-density-wave (if $g_{1}^{T} \to 0$) responses.

In our consideration above we have not taken into account effects of $U_p$ repulsion. This is easily achieved by substituting $u$ into (24) in the form $u = (U a \sin^{4} \theta_{F} + U_{p} \cos^{2} \theta_{F})/2$. For small values of $U_p$, the RG approach remains valid, and all results in terms of the new $u, v$ are retained. For $t/\Delta \ll 1$ we have $\cos \theta_{F} \sim 1$, so that we can not consider the large $U_p$ limit in our approach.

In conclusion, using a two cutoff RG approach we have studied a two band, 1-d tight-binding model with e-e and e-p interactions. We included onsite $U$ and nearest neighbour $V$ electron repulsions, as well as intra- and inter-molecular e-p coupling. We have shown that there is no $U, V, \rho, t, \Delta$ parameter region with dominant divergent SC response in the absence of e-p interactions. In the lowest order RG approach we found that such a region does occur if we include e-p coupling with optical intra-molecular modes. Only this form of e-p interaction produces an effective renormalized $g_{2,ph}$ term. We have found that the singlet SC region includes large values of the $U, V$ repulsive interactions if $t \sin(\pi\rho/4)/\Delta \ll 1$. Note that this behavior is impossible in the framework of a one-band model, for which $\Delta = 0$. Then, instead of (28) we have

$$\gamma + 2V(1 - 2 \cos(\pi\rho)) < U < 2\gamma + g_{1,ph}^{(0)} - 2V(2 - \cos(\pi\rho)), \quad (30)$$

where $\gamma = g_{1,ph}^{(0)}$, $\gamma = g_{2,ph}^{(0)}$, $0 < \rho < 2$. The solution of (30) is the same region ABCD in Fig.1, provided $2\gamma + g_{1,ph}^{(0)} > \gamma$. However the bare values $U, V$ must be very small, of the order of phonon scattering strengths. Moreover, in this case the requirement $2\gamma + g_{1,ph}^{(0)} > \gamma$ can not be realized. (Recall that in the two band case we have $\gamma \sim \gamma$ in the limit $t/\Delta \ll 1$, since effective intersite phonon coupling terms are small due to the factor $(t/\Delta)^2$). Note also that we have used a RG approach. Therefore we did not consider the strong coupling limit where a phase separation instability could take place [2]: our results are valid in some vicinity of the SC fluctuation phase.

We have proposed one possible scenario for the origin of dominant SC fluctuations in quasi-one-dimensional systems as a result of the combined effect of repulsive e-e and attractive e-p interactions in a 2-band situation. We suggest that features of this picture will survive in analogous two-dimensional models of high-$T_c$ superconductors [3] in particular in 3-band Peierls-Hubbard models. However the orbital structure of the order parameter in this case (s-wave vs d-wave) is unclear without detailed calculations.

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