Two-band model with an occupation-influenced hopping rate: Kondo enhancement and superconductivity

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A two-band hopping model is treated where one narrow band lies near the Fermi energy. As the size of an atomic orbit depends on the occupations of the atomic levels, an occupation-influenced hopping rate with a form factor is introduced. Correlations of a new type involving orbital and spin degrees of freedom build up. The possible phase transitions are studied by logarithmic approximation in one dimension. For a particular range of the position of the Fermi energy, attractive interaction and superconductivity are generated as a consequence of the form factor.

The highly correlated electron systems are the center of interest[1,2] because of their role in phenomena such as heavy fermions and high-temperature superconductivity. The challenge is to enhance the couplings and to obtain attractive electron-electron interactions for conduction electrons in the presence of large intra-atomic (on-site) repulsive interaction.[3] The possibility of triplet superconductivity also has attracted considerable interest.[4] The models which have been treated thus far are based on the Anderson and Hubbard models. The model to be presented has two bands, one heavy and one light. The influence of the light electron screening on the hopping motion of the heavy particle has been extensively studied and results in a reduced hopping rate but not in enhancement of the couplings.[5] The electron-assisted hopping first proposed by Kondo[6] in the case of a two-site model leads to logarithmic enhancement of the couplings.[7] Recently, a hopping model on a lattice has been studied with similar results,[8] but as a uniform conduction band has been treated its relevance for highly correlated systems is limited.

The present model is a tight-binding two-band hopping model where correlation can be easily incorporated. Instead of the conduction electron-assisted tunneling, an occupation-dependent hopping is introduced. As a change in the occupation of an atomic orbital results in a change of the size of the orbital, the hopping rate between neighboring sites is influenced. Such interaction is also contained by the two-particle interaction and it is known as the interaction between the charge of an atomic orbital and the bond charge.[9] Kivelson, Su, Schrieffer, and Heeger[10] have already considered such terms in treating the extended Hubbard model. In the present model that interaction is introduced for extra orbitals with heavy mass.

The goal of the present Brief Report is to demonstrate that the small new interaction leads to logarithmic corrections. The summation of the diagrams to infinite order with logarithmic accuracy leads to power-law enhancements in the couplings. To our knowledge it is shown for the first time that the off-diagonal interaction term results in the formation of correlation of a new type in which both the orbital and spin degree of freedom are involved. That correlation induces electron-electron interaction which can be attractive in the presence of on-site Coulomb repulsion. The generated interaction differs from the excitonic mechanism proposed by Varma, Schmitt-Rink, and Abrahams.[11] As in the present case, one of the particles in the two-particle intermediate state is heavy; thus, logarithmic corrections appear.

The role of such occupation-dependent hopping rate is studied by treating the possible phase transitions as charge-density wave (CDW) and spin-density wave (SCW), and singlet (SS) and triplet superconductivity (TS). A narrow f band near the Fermi level is introduced, and the position of the Fermi level relative to the broad d band is the relevant parameter, as it is contained by this anomalous form factor in the off-diagonal interaction. That form factor is actually responsible for the correlations of the new type.

In the proposed f-d model there is a d-electron orbit at each site and a f-electron orbit at each second site (see Fig. 1). The sites with two orbits are labeled by integer and the others by half-integer indices. The electrons with spin σ are created by the operators $d^{\dagger}_{j\sigma}$ and $f^{\dagger}_{i\sigma}$, respectively, where $j=0,\frac{1}{2},1$ and $i=1,2,\ldots$. Hopping occurs between nearest neighbors and the on-site f-d mixing is taken at zero because of symmetry. Thus, the unperturbed

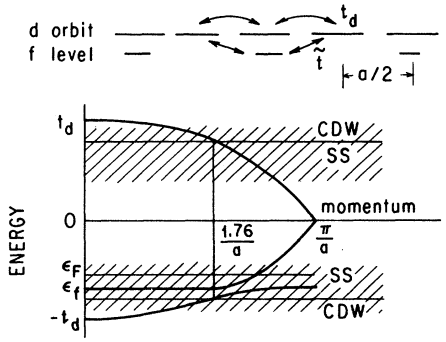

FIG. 1. The position of the d and f levels and the possible hopping indicated by arrows are shown . On the band dispersion curve the shadowed area indicates that region of the Fermi energy ε_F where the renormalization is the most effective. In the case of interactions $\tilde{t}$ and U the region of ε_F for singlet superconductivity (SS) and CDW are shown.

Hamiltonian H_0 is

$$H_0=\varepsilon_f\sum_{i,\sigma}f_{i\sigma}^{\dagger}f_{i\sigma}+\varepsilon_d\sum_{j,\sigma}d_{j\sigma}^{\dagger}d_{j\sigma}+\left(t_d\sum_{i,\delta,\sigma}d_{i\sigma}^{\dagger}d_{i+\delta\sigma}+t\sum_{i,\delta,\sigma}f_{i\sigma}^{\dagger}d_{i+\delta\sigma}\right)+\text{H.c.}, \quad (1)$$

where t_d and t are the hopping energies, $\delta=\pm\frac{1}{2}$, ε_f and ε_d are the energies of the localized levels, measured from the Fermi energy, and it is assumed that the f level is near the Fermi energy, thus $|\varepsilon_f|<t_d$. The energy bands are shown in Fig. 1. Consider the case, e.g., $\varepsilon_d>0$; only the lower d band is important. The states at site $R_j=ja$ can be expressed by Bloch states with momentum k as

$$d_{j\sigma}\sim\sum_k e^{ikR_j}d_{k\sigma},\quad f_{i\sigma}\sim\sum_k e^{ikR_i}f_{k\sigma}. \quad (2)$$

The d-f hopping rate $\tilde{t}_d$ influenced by the d-electron occupation with opposite spin and the on-site d-f Coulomb interaction U are described by the Hamiltonian $H'=H_{\tilde{t}}+H_U$, where

$$H_{\tilde{t}}=\tfrac{1}{2}\tilde{t}_d\sum_{i,\delta,\sigma}f_{i\sigma}^{\dagger}d_{i+\delta\sigma}n_{di+\delta-\sigma}+\text{H.c.} \quad (3)$$

and

$$H_U=U\sum_{i,\sigma,\sigma'}n_{fi\sigma}n_{di\sigma'}, \quad (4)$$

and $n_{dj\sigma}=d_{j\sigma}^{\dagger}d_{j\sigma'}$, $n_{fi\sigma}=f_{i\sigma}^{\dagger}f_{i\sigma}$. The direct Coulomb interaction contributes also to $H_{\tilde{t}}$.[9] The roles played by the possible other occupations ($n_{fi\sigma}$ and $n_{di\sigma}+n_{di-\sigma}$), influenced hopping terms, and by the further on-site Coulomb interactions such as U_d and U_f between d-d and f-f electrons will be discussed later.

In the Bloch representation defined by Eq. (2), the interaction Hamiltonian $H_{\tilde{t}}$ contains a form factor $e^{ik_f\delta a}$ where k_f is the momentum of the f electron. Summation over δ results in terms like

$$\cos(\tfrac{1}{2}k_fa)f_{k_f\sigma}^{\dagger}d_{k_3-\sigma}^{\dagger}d_{k_2-\sigma}d_{k_1\sigma}.$$

The form factor carries a memory of the scattering just like the spin matrix elements in the Kondo problem.[8] Without this form factor, e.g., the first two diagrams in group (a) depicted in Fig. 2 cancel.

The summation of the contributions of the diagrams will be performed in logarithmic approximation; thus, only the term with the highest power of $\ln|\varepsilon_f/D|$ and of $\ln|\omega/D|$ are kept, where ω is a small energy variable and D is an appropriate d-band-width cutoff ($D\sim t_d$). The logarithmic corrections arise from intermediate states with only one energy variable ε to integrate over the interval $D>|\varepsilon|>0$. There are two types of corrections.

(i) One d and one f electron in the intermediate state; thus, the correction is proportional to $\ln(\varepsilon_f/D)$.

(ii) Two d particles in the intermediate state, with only one energy integration due to momentum conservation, which contributes by $\ln|\omega/D|$. These diagrams have been treated in the theory of one-dimensional electron gas.[12]

The relevant skeleton diagrams are depicted in Fig. 2. The corrections to the vertex $\tilde{t}_d$ by the interaction U are shown by diagrams in Fig. 2(a) which are of type (i). The diagrams in Fig. 2(b) with renormalized $\tilde{t}$ contribute to the effective d-d interactions called g's in the "g-ology" theory of the one-dimensional (1D) electron gas and these corrections are also of type (i). The obtained d-d interactions are the starting values of the couplings in the g-ology theory which is based on skeleton diagrams in Fig. 2(c).[12]

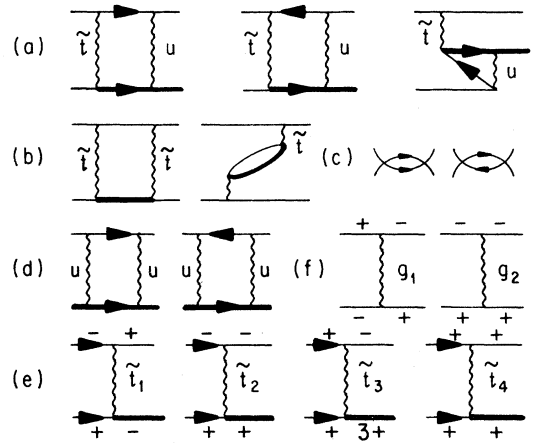

FIG. 2. (a)–(f) Time-ordered skeleton diagrams with light d-electron and heavy f-electron lines with the wavy lines indicating interactions; (a) corrections to vertex $\tilde{t}$, (b) effective interaction g, (c) basic diagrams in g-ology, (d) corrections to vertex U, (e) the four different momentum channels for vertex $\tilde{t}$, (f) the channel for the vertex in g-ology.

In the following $\varepsilon_f>0$ is taken, but the opposite case is obtained by electron-hole transformations. Furthermore, dimensionless coupling is introduced multiplying by $(2\pi v_f)^{-1}$ where v_F is the Fermi velocity for a linearized d-electron band. These are denoted by the corresponding small letters u, u_d, u_f, and g; furthermore, $\tilde{t}=(2\pi v_F)^{-1}\tilde{t}_d$. Taking $t_d=1$ eV, $U=1$ eV, $t=0.1$ eV, and $\tilde{t}_d=10^{-1}t$, the dimensionless parameters are $u\sim1$, $t\sim0.1$, $\tilde{t}\sim10^{-2}$. The d electrons near the Fermi energy contribute most. The right- and left-hand side of the Fermi region with momenta $\pm k_F$ will be denoted by $+$ and $-$. The relevant channels for the vertex $\tilde{t}$ and the electron-electron vertex g labeled according to the scheme used in "g-ology" (see Fig. 3).[12] In the channel $\tilde{t}_3$ all the

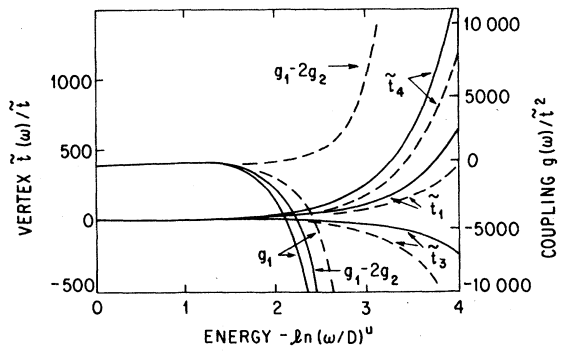

FIG. 3. Solution of vertex Eq. (1) for $\theta=0.7$ (solid line) and $\theta=0.9$ (dashed line) and the corresponding couplings g_1 and g_1-2g_2 are also indicated.

electrons are near the Fermi energy; thus the f electron has a momentum approximately $3k_F$ called 3+ (that is not an umklapp process). In contrast to g-ology[12] $\tilde{t}_4$ is relevant. Considering the form factor expressed by $\theta=\frac{1}{2}k_F a$, the unrenormalized vertexes are

$$\tilde{t}_1=\tilde{t}_2=\tilde{t}_4=\tilde{t}\cos\theta,\quad \tilde{t}_3=\tilde{t}\cos 3\theta. \tag{5}$$

Renormalization of the vertex $\tilde{t}$: The self-consistent "parquet" equation is based on the skeleton diagrams depicted in Fig. 2(a), which can be written in a schematic form as

$$\tilde{t}(\omega)=\tilde{t}-\cdots\int_{\max\{|\omega|,\varepsilon_f\}}^{D}\tilde{t}(\varepsilon)\frac{1}{\varepsilon}u(\varepsilon)d\varepsilon, \tag{6}$$

where $\tilde{t}(\omega)$ and $u(\omega)$ are the frequency-dependent renormalized vertexes. Here, ω represents the smallest energy variable of the d lines considering the intermediate states with one d and one f line. $u(\omega)$ renormalized according to the two diagrams in Fig. 2(d) which cancel each other; therefore, $u(\omega)=u$. Taking into account the different channels, Eq. (6) can be written in the form of a differential equation with a new variable, $x=(\omega/D)^u$, as

$$\frac{d}{d\ln x}\begin{pmatrix}\tilde{t}_1\\ \tilde{t}_2\\ \tilde{t}_3\\ \tilde{t}_4\end{pmatrix}_x=-\begin{pmatrix}1&-1&1&1\\ -1&1&1&1\\ 1&1&1&-1\\ 1&1&-1&1\end{pmatrix}\begin{pmatrix}\tilde{t}_1\\ \tilde{t}_2\\ \tilde{t}_3\\ \tilde{t}_4\end{pmatrix}_x, \tag{7}$$

where the components of the matrices are determined by the diagrams in Fig. 2(a). This equation can be solved after diagonalizing the matrix and the initial values are given by Eq. (5) and $\tilde{t}_1(\omega)=\tilde{t}_2(\omega)$. As a result of the cutoff $\tilde{t}(\omega)=\tilde{t}(\varepsilon_f)$ for $|\omega|<\varepsilon_f$. The solution strongly depends on θ. Typical solutions are shown in Fig. 3. If $u\sim 1$, then $\tilde{t}(x)$ varies by one or two orders of magnitude as x decreases by a factor 10.

The effective electron-electron interactions g_1 *and* g_2. The diagrams depicted in Fig. 2(b) provide the skeletons for the equation for the $g(\omega)$. Similar to Eq. (6),

$$g(\omega)=\int_{\omega}^{D}\tilde{t}(\varepsilon)\frac{1}{(-\varepsilon)}\tilde{t}(\varepsilon)d\varepsilon\sim-\frac{\tilde{t}^2(\omega)}{2u} \tag{8}$$

holds for $g(\omega)$. The actual calculation of diagrams in Fig. 2(b) provides the effective couplings g_1 and g_2,

$$g_1\sim 4(\tilde{t}_1^2-\tilde{t}_1\tilde{t}_4),\quad g_2\sim 2(\tilde{t}_1^2-\tilde{t}_3^2), \tag{9}$$

which disappear for $\theta=0$, $\pi/2$, as then $\tilde{t}_1=\tilde{t}_2=\tilde{t}_3=\tilde{t}_4$. Thus, the largest couplings are obtained for intermediate θ's. Furthermore, $g_1<0$ and g_1-2g_2 changes sign $(-\rightarrow+)$ as the increasing δ passes the value $\delta\approx 0.88$.

g-ology. An effective d-d interaction scales by bandwidth cutoff. As this scaling is much slower than the variation of $g(\omega)\sim\tilde{t}^2(\omega)(|\omega|>\varepsilon_f)$, thus the scaling can be started at $\omega=\varepsilon_f$ with values $g_1(\varepsilon_f)$ and $g_2(\varepsilon_f)$. The scaling of these quantities can be represented on the g_1-g_2 plane shown in Fig. 4.[12] The scaling lines are $g_1-2g_2=$const, g_1 always decreases and the $g_1=0$ is a singular line. The corresponding phase instabilities are also indicated. As for g_1 given by Eq. (9), $g_1<0$ holds; therefore, the possible phases are CDW and singlet superconductivity (SS). The latter occurs when $g_1-2g_2>0$ ($\delta>0.88$). This result is shown also in Fig. 1.

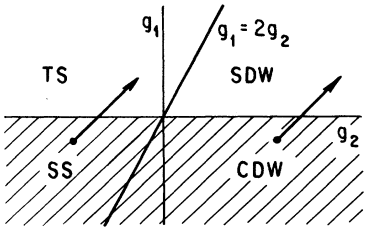

FIG. 4. The phase diagram in g-ology (Ref. 10). In the case of interactions $\tilde{t}$ and U the area of strongest renormalization is shadowed. The shift due to an additional on-site d-d interaction u_d is also indicated.

Finally, it is worth mentioning that the contributions of the diagrams with two f lines in the intermediate state are proportional to $\tilde{t}^2D/\varepsilon_f$ which can be ignored as far as the coupling $\tilde{t}$ is weak.

Roles of other couplings. For many physical systems $u_f>1$ can be expected. In the case of $u_f=\infty$ and $\varepsilon_f<0$, each site is occupied by a single electron with up or down spin. As there is only one dispersionless f line in each intermediate state (disregarding the vicinity of the d-f hybridization point) , only a probability factor $\frac{1}{2}$ therefore is associated with any creation of an f hole.

There may be further terms in a general Hamiltonian responsible for the d-f hopping influenced by the occupations of sites with two orbits. For d-occupation influenced hopping $\tilde{t}_d$, the form factors associated with d electrons are the same in each channel and, therefore, the vertices are given by a single function $\tilde{t}_d(\omega)$. Then the couplings must be replaced as $\tilde{t}_m(\omega)\rightarrow\tilde{t}_m(\omega)+\tilde{t}_d(\omega)$ $(m=1,2,3,4)$. In the case of $u_f=\infty$, f-occupation influenced hopping does not occur.

The direct d-d interacting $u_d>0$ contributes as $g_1\rightarrow g_1+u_d$ and $g_2\rightarrow g_2+u_d$ if the renormalization in the energy range $\varepsilon_f<\varepsilon<D$ is neglected. That replacement is very relevant as it can shift the coupling to the upper half of the g_1-g_2 plane (see Fig. 4) where the system exhibits either triplet superconductivity or SDW behavior.

It is worth mentioning that if there are f orbits at each site, but they do not overlap directly, that does not change the qualitative conclusions. Similarly, the signs of ε_d and ε_f are irrelevant.

The main features of the result can be summarized as follows:

(i) The combination of the occupation influenced hopping rate can lead to an essential enhancement of the effective d-d couplings, g_1 and g_2, if the Fermi level and the f level are close.

(ii) The enhancement is the largest when the Fermi level is in the middle region of the upper or lower d band.

(iii) Without on-site d-d interaction the SS or CDW phase occurs in the d band.

(iv) The on-site d-d interaction may play a crucial role in obtaining TS or SDW.

(v) *Attractive d-d interaction can be generated in spite*

of the on-site repulsion.

(vi) *The phase diagrams depend crucially on the occupation of the d level* (parameter θ) and are insensitive to the presence of a large on-site f-f repulsion *provided that the system is in one of the valence fluctuation regions* [$\varepsilon_f < 0$, $|\varepsilon_f|/D \ll 1$ or $\varepsilon_f + U > 0$, $(\varepsilon_f + U)/D \ll 1$].

The presence of the large logarithmic correction due to the occupation-influenced hopping is not limited to one dimension. A similar effect can be obtained for any hopping model where a flat band is close to the Fermi energy, at least, in part of the Brillouin zone, and the correlations are large and also for a single impurity orbital.[13] The application of the model to the heavy fermionic systems is rather straightforward and is challenging to the highly correlated superconductors.

Finally, it is worth mentioning that the correlation formed at low temperature shows analogy to the spin Kondo problem, but it is not identical because of its orbital origin (see also Refs. 7 and 8).

Note added. In the case of high-temperature superconductors the nonbonding $p\pi$ oxygen orbitals may play the role of the extra orbitals.

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