Hybridized mechanism of pairing and the heavy fermion state: Exactly solvable two-band model with strong hybridized interactions

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The two-band model describing strongly hybridized degenerated electron states in a chain is proposed and solved exactly by means of the Bethe ansatz. The fermions of the subbands interact with each other via one-particle and one-particle correlated on-site hybridized interactions. The chain of electrons is reduced to the model with two noninteracting subbands with a given total number of electrons, in which fermions interact via different effective constants of interactions. In the case of strong hybridized interaction the on-site repulsive interaction is compensated by hybridized interaction, which leads to an effective attractive interaction between particles and the formation of spinless bound states of Cooper type. This electron liquid component determines both heavy fermion- and superconducting-type behavior of electron properties.

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The discovery of high-T_c superconductivity has greatly stimulated the investigation of new mechanisms of superconductivity and formulation of adequate models of strongly correlated electron systems. Among the relevant models the t-J model[1] should be noted, where the motion of electrons is strongly influenced by spin fluctuations through antiferromagnetic coupling. Another approach to high-temperature superconductivity has been proposed by Hirsch.[2] According to Ref. 2 the charge carriers of high-T_c superconductors are holes, the kinetic energy of hole hopping between nearest-neighbor sites depends on the occupation of these sites, and the correlated hopping energy is compensated by the repulsive interaction for holes. Although the main interest lies in the physics of 2D systems, it is also extremely useful to investigate 1D variants of such models related to high-T_c superconductivity. Exact solutions of simplified versions of these models on a chain, that keep the main ideas of approach to superconductivity,[1,2] enable us to realize the mechanisms of effective attractive interaction between particles.[3] The models of strongly correlated electrons with a bond-charge interaction, which conserves a number of double occupied sites, are simple examples of strongly correlated electron systems which exhibit superconductivity.[4] The merit of these models is their complete integrability.

In this report a two-band degenerate model of fermions with strongly hybridized electron states is proposed. The model is exactly solvable and has a tendency to superconductivity in strong hybridized interaction; the "superconducting" component of an electron liquid has a heavy fermion transport mass also. We assume that this mechanism of an effective attractive interaction between electrons is realized in real superconductors and can describe the behavior of heavy fermion systems. The model Hamiltonian includes two terms $\mathcal{H}=\mathcal{H}_0+\mathcal{H}_{int}$:

$$\mathcal{H}_0 = -\sum_{j=1}^{L}\sum_{\sigma}(c_{j\sigma}^{\dagger}c_{j+1\sigma}+a_{j\sigma}^{\dagger}a_{j+1\sigma}-Vc_{j\sigma}^{\dagger}a_{j\sigma}+\text{H.c.}), \quad (1)$$

$$\mathcal{H}_{int} = U\sum_{j=1}^{L}(n_{j\uparrow}n_{j\downarrow}-\eta_j^{\dagger}\eta_j-\sigma_j^{\dagger}\sigma_j) + W\sum_{j=1}^{L}\sum_{\sigma}(c_{j\sigma}^{\dagger}a_{j\sigma}+a_{j\sigma}^{\dagger}c_{j\sigma})n_{j-\sigma}, \quad (2)$$

where $c_{j\sigma}$ ($c_{j\sigma}^{\dagger}$) and $a_{j\sigma}$ ($a_{j\sigma}^{\dagger}$) are operators of fermions with spin $\sigma=\uparrow,\downarrow$ at lattice site j, $\eta_j=c_{j\downarrow}c_{j\uparrow}-a_{j\downarrow}a_{j\uparrow}$, $\sigma_j=c_{j\downarrow}^{\dagger}c_{j\uparrow}+a_{j\downarrow}^{\dagger}a_{j\uparrow}$, the particle number operator for electrons is defined by $n_{j\sigma}=c_{j\sigma}^{\dagger}c_{j\sigma}+a_{j\sigma}^{\dagger}a_{j\sigma}$, L denotes the length of the chain, and we assume periodic closure. The hopping integral in (1) is equal to unity, V and W are the parameters of one-particle and one-particle correlated on-site hybridized interactions, U is the on-site Coulomb repulsion (it defines the exchange and two-particle on-site hybridized interaction also). The model Hamiltonians conserve the total number of particles $\mathrm{N}=N_c+N_a$, and the total spin $\mathrm{M}=M_c+M_a$; here N_c,M_c and N_a,M_a are the total numbers and total spin of fermions of each subband, $0\leqslant N_c,N_a,M_c,M_a\leqslant \mathrm{N}$. Under the combined electron-hole symmetry $c_j\rightarrow(-1)^j c_{j\sigma}^{\dagger}, a_{j\sigma}\rightarrow(-1)^j a_{j\sigma}^{\dagger}$ the Hamiltonian transforms to the similar form $\mathcal{H}(1,V,U,W)\rightarrow\mathcal{H}(1,-V-2W,U,W)+3U(2L-N)$.

The model may be viewed as a two-chain ladder model ("c" and "a" denote the chains of spinless fermions) with the hopping between nearest-neighbor sites along the chains and the inner chain on-site Coulomb interaction (U). The interaction between chains is defined by the interchain on-site Coulomb repulsion (U), one-particle (V), one-particle correlated (W), and two-particle tunneling (U) between chains.

The advantage of this model (1) and (2) is its integrability. Below we present the exact solution of the model obtained by the Bethe ansatz. The eigenvector $|\psi\rangle$ with N particles is defined as

$$|\psi\rangle = \sum_{N_c=0}^{N}\delta_{N_a,N-N_c}\sum_{\{(x_j,y_j,\sigma_j,\alpha_j)\}}\psi_{\sigma_1\ldots\alpha_1\ldots}^{c\ldots a\ldots}(x_1,\ldots,y_1,\ldots)\times|x_1\sigma_1,\ldots,y_1\alpha_1,\ldots\rangle,$$

where the Bethe function takes a traditional form:

$$\psi^{c\ldots a\ldots}_{\sigma_1\ldots\alpha_1\ldots}(x_{Q1},\ldots,y_{Q1},\ldots,x_{QN_c},\ldots,y_{QN_a}) = \sum_P (-1)^P A^{c\ldots a\ldots}_{\sigma_1\ldots\alpha_1\ldots}(x_{Q1},\ldots,y_{Q1},\ldots,x_{QN_c},\ldots,y_{QN_a}) \times \exp\left(i\sum_{j=1}^{N_c} k_{Pj}x_{Qj} + i\sum_{j=1}^{N_a} k_{Pj}y_{Qj} \right), \quad (3)$$

where the P summation extends over all permutations of the momenta $\{k_j\}$, $Q=\{Q_1,\ldots,Q_N\}$ is the permutation of the N particles such that the coordinates satisfy $1\leqslant x_{Q1}\leqslant\cdots\leqslant y_{Q1}\leqslant\cdots\leqslant x_{QN_c}\leqslant\cdots\leqslant y_{QN_a}\leqslant L$, and δ_{ij} denotes the Kronecker delta. The coefficients $A(P/Q)$ arising from different permutation Q are connected via the scattering matrices as follows: $A^{\cdots\gamma_j\gamma_i\cdots}_{\cdots\beta_j\beta_i\cdots}(\ldots,z_j,z_i,\ldots) = S_{ij}(k_i\chi_i,k_j\chi_j)A^{\cdots\gamma_j\gamma_i\cdots}_{\cdots\beta_j\beta_i\cdots}(\ldots,z_i,z_j,\ldots)$, here $z_j=x_j$ or $z_j=y_j$, $\beta_j=\sigma_j$ or $\beta_j=\alpha_j$, and $\gamma_j=c$ or $\gamma_j=a$. The index $\chi_j=\pm1$ defines the electron subbands with the dispersion $\epsilon(k,\chi) = -2\cos k+\chi V$ (the value of V shifts the energy of subbands, later we shall hold $V\leqslant 0$ and $W>0$ for convenience). The two-particle scattering matrix is given by

$$S_{ij}(k_i\chi_i,k_j\chi_j) = \frac{\sin k_i - \sin k_j + i\delta_{\chi_i,\chi_j}c(\chi_j)\mathcal{P}_{ij}}{\sin k_i - \sin k_j + i\delta_{\chi_i,\chi_j}c(\chi_j)},$$

where the operator $\mathcal{P}_{ij}$ interchanges the spins of the electrons and $c(\chi)=U+\chi W$ is the constant of an effective electron-electron interaction.

The S matrix is defined by the mutual scattering of electrons of each subband. The particles of different subbands are not scattered, and S_{ij} is equal to unity for different values of χ_i and χ_j; the particles with the same wave vectors are not scattered: $S_{ij}(k_i\chi_i,k_i\chi_j)=1$. The amplitudes of the Bethe function (3) satisfy the Pauli principle $\psi^{\cdots\gamma_i\cdots\gamma_j\cdots}_{\cdots\sigma_i\cdots\sigma_j\cdots}(\ldots,z_i,\ldots,z_j\ldots)=0$ for $x_i=x_j$, $\sigma_i=\sigma_j$ (or $y_i=y_j$, $\sigma_i=\sigma_j$), and the Bethe function is the solution of the Schrödinger equation for an arbitrary number of the particles. Due to the form of the solution for the S matrix, the Yang-Baxter equations are satisfied for an arbitrary number of electrons on the site; since, according to (4), the electrons of different subbands are not scattered, an alternative proof of integrability of the model is given in Ref. 5.

Using periodic boundary conditions for the Bethe function (3) $\psi^{\cdots\gamma_j\cdots}_{\cdots\sigma_j\cdots}(\ldots,z_j,\ldots)=\psi^{\cdots\gamma_j\cdots}_{\cdots\sigma_j\cdots}(\ldots,z_j+L,\ldots)$ we define the T_j matrix $\exp(ik_jL)\psi=T_j\psi$ that depends on the momenta and the band index of j particle $T_j=T(k_j\chi_j)$:

$$T_j = S_{jj+1}(k_j\chi_j,k_{j+1}\chi_{j+1})\cdots S_{jN}(k_j\chi_j,k_N\chi_N) \times S_{j1}(k_j\chi_j,k_1\chi_1)\cdots S_{jj-1}(k_j\chi_j,k_{j-1}\chi_{j-1}). \quad (4)$$

The coefficients $A(P/Q)$ are defined by the single S matrix (4), which is the same for two kinds of electrons (c and a), so that we obtain the same T_j matrix for the set of the partial [with different N_c (or N_a) number] function in (3).

The energy eigenstates are characterized by sets of wave numbers k_j $[j=1,\ldots,N(\chi_j)]$ for the particles and additional spin rapidities λ_α $[\alpha=1,\ldots,M(\chi_j)]$, that satisfy the Bethe equations

$$\exp(ik_jL) = \prod_{\alpha=1}^{M(\chi_j)} \frac{\sin k_j - \lambda_\alpha + \frac{i}{2}c(\chi_j)}{\sin k_j - \lambda_\alpha - \frac{i}{2}c(\chi_j)},$$

$$\prod_{j=1}^{N(\chi_j)} \frac{\lambda_\alpha - \sin k_j + \frac{i}{2}c(\chi_j)}{\lambda_\alpha - \sin k_j - \frac{i}{2}c(\chi_j)} = \prod_{\beta=1}^{M(\chi_j)} \frac{\lambda_\alpha - \lambda_\beta + ic(\chi_j)}{\lambda_\alpha - \lambda_\beta - ic(\chi_j)}, \quad (5)$$

where $N(\chi_j)$ and $M(\chi_j)$ are the total number of electrons and number of down spin electrons of the subbands, $N(1)=N_1$, $N(-1)=N_2$ and $M(1)=M_1$, $M(-1)=M_2$.

The model (1) and (2) is reduced to two noninteracting subbands of electrons with different values of the effective interaction between particles. The electron subbands are connected via the constraint according to which the total number of the particles is conserved, $N=N_1+N_2$. The value of N_1 (or N_2) corresponds to the minimum of the ground-state energy $E=\sum_{j=1}^{N_1}\epsilon(k_j,1)+\sum_{j=1}^{N_2}\epsilon(k_j,-1)$ at given N.

The first subband with dispersion $\epsilon(k,1)=-2\cos k+V$ is a Hubbard subband with a repulsive interaction $c_1=U+W$ and the second subband with dispersion $\epsilon(k,-1)=-2\cos k-V$ is the subband with the constant of an effective interaction $c_2=U-W$; here $c_2>0$ for $W<U$ and $c_2<0$ for $W>U$. As a result, in the first subband the particles form one-particle states and in the second they are coupled in pairs in the case of a strong hybridized interaction $W>U$. In other words, one subband is a metallic band and the other has the properties of a superconducting band in the case of an attractive effective interaction. We cannot really say that the constant of the correlated hybridized interaction is larger than the corresponding constant of the on-site interaction in cuprates. In the absence of direct calculations of the correlated hybridized parameter W we shall extract the value of W using LDA calculations for La_2CuO_4: the parameters of the on-site interactions of different d and p orbitals $U_{dd'}=6.58$ eV and $U_{pp'}=2.54$ eV, for the same orbitals $U_{dd}=8.96$ eV and $U_{pp}=4.19$ eV.[8] On the one hand, the parameters of the on-site interactions of different orbitals take into account the Coulomb interaction of electron orbitals, on the other hand the overlap of the wavefunction of these orbitals. If we associate the value of W with $U_{dd'}$ or $U_{pp'}$ we can see that W and U_{dd} or W and U_{pp} have the same order, thus the value of W can be really large U in some superconductors.

Let us consider the two-electron liquid state in detail. The densities of electrons $n=N/L$ and ground-state energy $\varepsilon=E/L$ are defined as the sum of the partial densities $n=n_1+n_2=\int_{-\Lambda_1}^{\Lambda_1}\rho_1(k)dk+\int_{-\Lambda_2}^{\Lambda_2}\rho_2(k)dk$ and $\varepsilon=\int_{-\Lambda_1}^{\Lambda_1}\epsilon(k,1)\,\rho_1(k)dk+\int_{-\Lambda_2}^{\Lambda_2}\epsilon(k,-1)\,\rho_2(k)dk$, where $\rho_1(k)$ and $\rho_2(k)$ are the distribution functions of the charge rapidities. The filling of the subbands is defined by the chemical potential of the system, which is the same for different subbands under their partial filling. This condition corresponds to the minimum of the ground-state energy under given total number of particles. The model in which the phase states depend on the density of

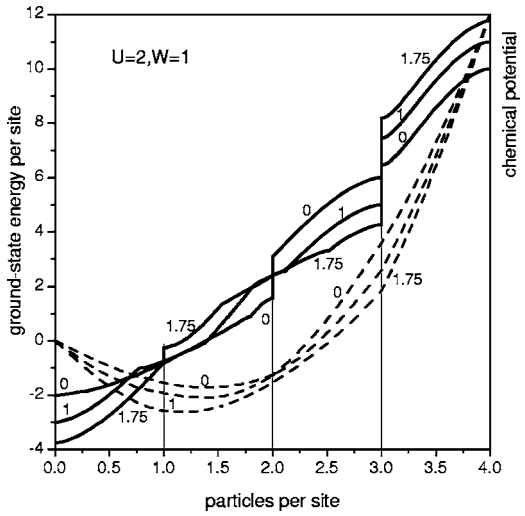

FIG. 1. The chemical potential (solid lines) and the density of the ground-state energy (dashed lines) as a function of the total density in the case of a weak hybridized interaction at $U=2$, $W=1$. Individual curves are labeled by value of $V=0,1,1.75$.

particles and values of the coupling constants has a rich phase diagram. In the case of a weak hybridized interaction $W<U$ the constants of the effective interactions in the subbands are positive, thus the phase diagram includes the metallic phases separated by the Mott-Hubbard transitions. In contrast to the traditional Hubbard model, where the model at half-filling is an insulator for an arbitrary repulsive interaction,[6,7] the proposed model has a set of the Mott-Hubbard transitions for quarter- ($n=1$), half- ($n=2$), and three-quarter- ($n=3$) band filling ($n=4$ satisfies to full-filled subbands). The calculations of the chemical potential and the ground-state energy as a function of the density of the particles for $U=2$, $W=1$, and several values of V ($V=0,1,1.75$) are represented in Fig. 1, where the jumps of the chemical potential describe the Mott-Hubbard transitions. The paradigm of the realization of the Mott-Hubbard transitions is shown in Fig. 1: at $V=0$ and $V=1.75$ there are two Mott transitions at $n=2$, $n=3$ and $n=1$, $n=3$, respectively; at $V=1$ we have one transition at $n=3$ only. At a weak splitting of the subbands the bands overlap and therefore the Mott-Hubbard transitions at the filling $n=1$, or 2, or 3 are not realized. The gap of the charge excitations is either closed or opened at a critical value V_c depending on the constants of the effective interactions c_1, c_2 and the band filling, thus $V_c=V_n$ for $n=1,2,3$ is equal to $V_1=1.456$, $V_2=0.766$, $V_3=-0.223$. According to Fig. 1 the gap is opened at V_1 and closed at V_2 and V_3. Note that *the gapless insulator state is realized at a critical value* V_c. At strong splitting of the subbands, when their energies are not overlapped, the properties of the system are defined by a partially filled subband and the charge excitations are gapped at a full-filled subband, as a result of the Mott-Hubbard transition. Depending on the interaction parameters the system is a metal for an arbitrary band filling and can undergo the Mott transitions at $n=1,2,3$. For positive constants of effective interaction the metal phase is characterized by dominating density-density fluctuations.

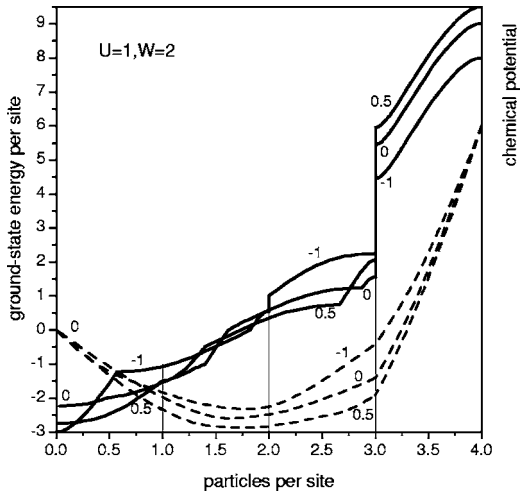

FIG. 2. The chemical potential and the density of the ground-state energy in the case of a strong hybridized interaction at $U=1$, $W=2$, similar to Fig. 1.

In a strong coupling $W>U$ an attractive effective interaction is realized in one of the subbands, thus spinless bound states of Cooper-type form the ground state of the subband. We show numerical results of the chemical potential and the density of the ground-state energy as a function of the band filling at $U=1, W=2$, and $V=-1,0,0.5$ (see Fig. 2). According to the calculations obtained the gaps are opened at values $V_1=0.5$ and $V_2=-0.777$ and closed at $V_3=-2.105$, where in contrast to Fig. 1, we have an electron liquid state with "normal" and "abnormal" components. The normal component is defined by a repulsive effective electron-electron interaction, abnormal an attractive interaction. In Fig. 3 the effective transport mass of particles in each subband is shown as a function of the band filling, $m/m_e=D_e/D$, where $D=(1/4\pi)v_F\alpha$ is the charge stiffness, v_F is the Fermi velocity, $\alpha=2[\xi(\Lambda_{1,2})]^2$, $\xi(\Lambda_{1,2})$ is the dressed charge, D_e

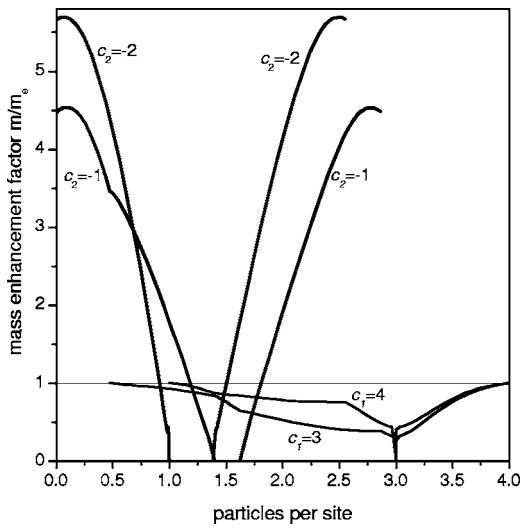

FIG. 3. The mass enhancement factor as a function of the total density in the case of a strong hybridized interaction $U=1$, $W=2$, $V=0$ and $U=1$, $W=3$, $V=0$. Individual curves are labeled by value of effective coupling constant c_1, c_2.

$=(1/\pi)\sin(\pi n_{1,2})$ is the charge stiffness of the spinless fermions. The calculations are obtained at $U=1$, $W=2$, $V=0$ and $U=1$, $W=3$, $V=0$, lower curves correspond to a normal electron component with $c_1=1,4$; an abnormal component is calculated at $c_2=-1,-2$; and the zero value of the mass enhancement factor is reached at the full-filled subband. The effective mass of current carries of a normal component becomes less than the mass of spinless fermions, while at the same time an abnormal electron component has a large effective mass (with the exception of a small density region near the full-filling of the subband). In the U-infinity limit ($U>0$) we have two subbands of spinless fermions, since the on-site Coulomb interaction forbids the realization of two electrons with different spins on the same lattice site. The mass enhancement factor of an abnormal electron component is proportional to the constant of effective interaction and reaches 4.54 and 5.68 for $c_2=-1$ and $c_2=-2$, respectively, thus the Cooper pairs form a heavy fermion electron liquid also. The critical exponent α is defined as the asymptotic of the singlet-pair correlator; in the marginal Luttinger liquid the superconducting correlations are dominant in the case of $\alpha>1$. The condition $\alpha>1$ is realized for an arbitrary density of Cooper pairs, thus the abnormal electron component corresponds to both a heavy fermion and a superconducting type phase. In Fig. 4 we see a clear realization of the behavior of the effective transport mass due to the realization of Cooper-type pairs in one of the subbands. The curves are calculated in the case of weak $U=2$, $W=1$ and strong $U=1$, $W=2$ hybridized interaction. In the case of a large shift of the subbands "pure" electron states are realized in the system and the model is reduced to two noninteracting Hubbard subbands with a given number of electron subbands or one-component electron liquid.

In summary, we have presented a soluble model of two degenerated strongly correlated electron subbands, having the nontrivial Luttinger liquid behavior. An exact solution has been obtained by means of the nested Bethe ansatz. The proposed model is reduced to two noninteracting Hubbard chains with different constants of effective electron-electron interaction. In the case of strong hybridized interaction the constant of effective electron-electron interaction of one of the subbands is negative; as result, the electron state of the system is defined by the Cooper-type pairs also. This electron component leads to both superconducting and heavy fermion behavior of electron properties.

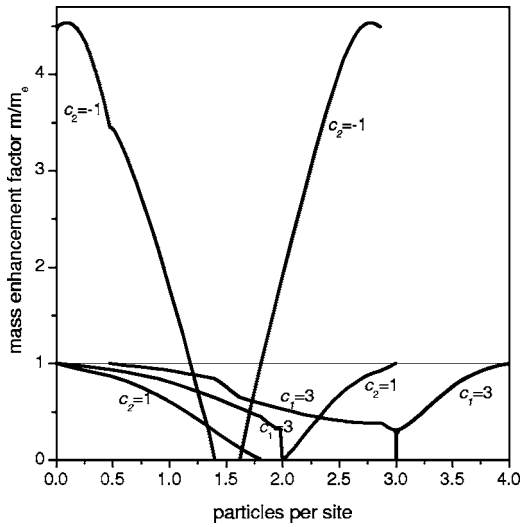

FIG. 4. The mass enhancement factor as a function of the total density in the case of weak $U=2$, $W=1$ and strong hybridized interaction $U=1$, $W=2$, similar to Fig. 3.

The results of the calculations of 1D models do not allow direct application to real 2D and 3D systems. Nevertheless, one can expect that the mechanism of pairing via the correlated hybridization is realized in real high-T_c superconductors and leads to formation of heavy fermion states in real compounds.

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