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SUPERCONDUCTIVITY IN HUBBARD MODEL WITH CORRELATED HOPPING

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Using the slave-boson method in its spin- and charge-rotational invariant representation we determine stability of the superconducting state in the Hubbard model with correlated hopping. In general the term with correlated hopping violates electron–hole symmetry, however, in the special case when the correlated hopping integral X is equal to the uncorrelated hopping integral t the electron–hole symmetry remains. We investigate this case and show that correlations induced by onsite Coulomb interactions U yield to the normal state with exactly single occupied sites (corresponding to $|U=\infty\rangle$). The phase diagram of the superconducting state is determined for the different electron concentration n. At the half-filled band ($n=1$) a direct transition from the Mott insulator to the superconducting state occurs.

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1. Introduction

High-T_c superconductors have many properties, which classify them as a strongly correlated electron system, and therefore, a great interest in the Hubbard model and its extensions since the discovery of new superconductors has been fully justified. The model is the simplest one, which describes Coulombic interactions of electron on the lattice. An important question which arises is a mechanism of formation of Cooper pairs in the presence of strong Coulomb repulsion. In some circumstances even not strong intersite interactions may overwhelm onsite repulsion and lead to superconductivity [1, 2]. It was shown that such a case may be in the Hubbard model with correlated hopping ($t-X$ Hubbard model) described by the following Hamiltonian:

$$H=\sum_{\langle i,j\rangle,\sigma}(c_{i\sigma}^{+}c_{j\sigma}+c_{j\sigma}^{+}c_{i\sigma})[-t+X(n_{i-\sigma}+n_{j-\sigma})]+U\sum_{i}n_{i+}n_{i-}. \quad (1)$$

The parameter t, X and U are the hopping integral, the correlated hopping integral of electrons between nearest neighbor sites and the onsite Coulomb integral, respectively. In cuprates, fullerides, barium bismuthates one can estimates the parameters as $t\approx X\approx 0.2$ eV and $U\approx 1$ eV. The model (1) has been investigated extensively in the mean-field approximation (MFA) [1]. This approach neglects, however, electron correlations, crucial for the normal metallic state and in consequence for stability of superconductivity. Recent studies [2] of the model performed by an exact method for the 1D chain in the case $t = X$ have shown that the normal state is a strongly correlated metallic state with singly occupied sites.

We want to study the model (1) for $t = X$ by means of the slave-boson (SB) method in its spin- and charge-rotational invariant representation [3]. The method takes into account electron correlations and is very effective in studies of superconductivity (as well as other phases) in the extended Hubbard model. We will determine the stability conditions for the superconducting phase and its ground state characteristics. We want to study the phase transition from the Mott insulating phase to the superconducting phase, which occurs in the system at $n = 1$ electron/site.

2. Slave-boson approach

In the spin- and charge-rotational invariant SB representation [3] the doublet of states corresponding to a single occupied site $|\sigma\rangle_i$ and the doublet $|\rho\rangle_i$ corresponding to a doubly occupied site ($\rho = 2$) and an empty site ($\rho = 0$), are expressed by the Bose operators $p_{i,\sigma\sigma'}$, $b_{i,\rho\rho'}$ and the Fermi operators $f_{i,\sigma}$. In order to express the Hamiltonian (1) by these operators we use the Hubbard operators

$$X_i^{\sigma 0} \equiv |\sigma\rangle_i\,{}_i\langle 0| \equiv (1-n_{i\bar{\sigma}})c_{i\sigma}^{+} = \sum_{\sigma'} p_{i,\sigma\sigma'}^{+}(b_{i,00}f_{i,\sigma'}^{+} - \sigma' f_{i,\bar{\sigma}'}b_{i,20}), \tag{2}$$

$$X_i^{\sigma 2} \equiv |\sigma\rangle_i\,{}_i\langle 2| \equiv -\sigma n_{i\sigma}c_{i\bar{\sigma}} = \sum_{\sigma'} p_{i,\sigma\sigma'}^{+}(b_{i,02}f_{i,\sigma'}^{+} - \sigma' f_{i,\bar{\sigma}'}b_{i,22}) \tag{3}$$

and

$$X_i^{22} \equiv |2\rangle_i\,{}_i\langle 2| \equiv n_{i+}n_{i-} = 2\sum_{\rho} b_{i,2\rho}^{+}b_{i,\rho 2}. \tag{4}$$

The superconducting order parameter is defined by

$$\Delta_i \equiv \langle c_{i-}c_{i+}\rangle = 2\sum_{\rho}\langle b_{i\rho 2}^{+}b_{i0\rho}\rangle. \tag{5}$$

The SB mean-field solution gives results in agreement with the Gutzwiller approximation if one properly normalizes the slave-boson operators [4]. We used the normalization procedure described in Ref. [3]. In order to find stable solutions the boson operators are treated as c-numbers and used as variational parameters in the free energy

$$F = F_{\mathrm{f}} + F_{\mathrm{b}} = -\frac{1}{\beta}\sum_{k}\{\ln[1+\exp(\beta E_k)] + \ln[1+\exp(-\beta E_k)]\}$$

$$+\frac{UN}{2}(b^2+2\delta) - \lambda_0 N(1+2\delta) - 2\lambda_S N\Delta. \tag{6}$$

Here, N is the number of the lattice sites, $E_k = [(2\tilde{t}\eta_k+\lambda_0)^2+(2r\eta_k+\lambda_S)^2]^{1/2}$, for the hypercubic lattice $\eta_k = \sum_{\delta_\alpha}\cos(k\delta_\alpha)$, λ_0 and λ_S are the Lagrange multipliers for the constraints corresponding to the condition for the number of electrons and the order parameter (5). The parameter $\tilde{t} = -4t\delta\alpha^2 b_0^2$ and $r = -4t\Delta\alpha^2 b_0^2$, where δ

is connected with the electron concentration $n = 1+2\delta = 1+2(\langle b_{22}\rangle - \langle b_{00}\rangle)$, $\alpha^2 = p^2/[b_0^2(1-4\delta^2-4\Delta^2)]$, $b_0 = 2\langle b_{22}\rangle + 2\langle b_{00}\rangle$, $b^2 = 2\langle b_{22}^+ b_{22}\rangle + 2\langle b_{00}^+ b_{00}\rangle + 2\langle b_{20}^+ b_{02}\rangle + 2\langle b_{02}^+ b_{20}\rangle$, and for paramagnetic state $p = \langle p_{++}\rangle = \langle p_{--}\rangle$, $\langle p_{+-}\rangle = \langle p_{-+}\rangle = 0$. The stable solution is determined from a set of equations for the minimum of the free energy F (Eq. (6)). At $t = X$, the spectrum of Cooper pairs is gapless for any n and U. In this case it is easy to find the energy of the superconducting state at $T = 0$

$$F^{\mathrm{S}}/N = -\frac{W}{8}\left(1-\frac{U}{W}\right)^2 + U\delta \qquad \text{for} \quad -W < U < U_{\mathrm{c}}, \tag{7}$$

$$F^{\mathrm{S}}/N = \frac{U}{2}n \qquad \text{for} \quad U < -W, \tag{8}$$

where the order parameter and the critical value of U are

$$|\bar{\delta}| = \sqrt{\delta^2 + \Delta^2} = \frac{1}{4}\left(1 - \frac{U}{W}\right), \tag{9}$$

$$U_{\mathrm{c}} = W(1 - 4|\delta|). \tag{10}$$

For large $U > -2|\delta|W$ the normal metallic state is with singly occupied sites only, and for $n = 1$ it is the Mott insulator. The state brought about only by doubly occupied sites is more stable for $U < -2|\delta|W$. The free energy corresponding to these cases is

$$F_1{}^{\mathrm{N}}/N = -W|\delta|(1-2|\delta|) + U(|\delta| + \delta) \quad \text{and} \quad F_2{}^{\mathrm{N}}/N = Un/2, \tag{11}$$

respectively. The above results are obtained for the rectangular density of states ($\rho(E) = 1/W$ for $|E| < W/2$) in the system of noninteracting electrons. For comparison in the 1D chain our approach gives the critical value U_{c}

$$\frac{U_{\mathrm{c}}}{4t} = \frac{4}{\pi}\frac{\sin[\frac{\pi}{2}(1-2|\delta|)]}{(1+2|\delta|)^2} - 4|\delta|\frac{\cos[\frac{\pi}{2}(1-2|\delta|)]}{1+2|\delta|} \tag{12}$$

and the exact result is [2]

$$\frac{U_{\mathrm{c}}}{4t} = -\cos[\pi(1-2|\delta|)]. \tag{13}$$

The results obtained in the MFA with the rectangular DOS are qualitatively different. The critical value of U is

$$U_{\mathrm{c}}^{\mathrm{MFA}} = \frac{W}{4}\frac{1-12|\delta|^2}{|\delta|}. \tag{14}$$

The free energies of the normal and the superconducting state are

$$F_{\mathrm{MFA}}^{\mathrm{N}}/N = \frac{U}{4}n^2 - \frac{W}{2}|\delta|(1-4\delta^2), \tag{15}$$

$$F_{\mathrm{MFA}}^{\mathrm{S}}/N = \frac{U}{4}n^2 - U\delta^2 + \frac{U^2}{54W^2}(U - \sqrt{U^2+3W^2})$$

$$+\frac{1}{36}(3U - 2\sqrt{U^2+3W^2}) \qquad \text{for} \quad -W < U < U_{\mathrm{c}}, \tag{16}$$

$$F_{\mathrm{MFA}}^{\mathrm{S}}/N = \frac{U}{4}n^2 + \frac{U}{4}(1-4\delta^2) \qquad \text{for} \quad U < -W. \tag{17}$$

3. Conclusions

We showed that the slave-boson study of the Hubbard model with correlated hopping gives qualitatively similar results to those obtained by the exact method in a 1D system at $t = X$ and in contrast to the mean-field results. The reason is that the SB method takes into account correlations, which are neglected in the MFA. It is clearly seen in the n dependences of U_c (Eqs. (10) and (14)). In the limit $n \to 0$ ($n \to 2$), where correlations become irrelevant, both results converge to each other. It is important to point that at $t = X$ for any n there is no gap in the excitation spectrum of Cooper pairs. Electric current in such a system is carried by electrons as well as Cooper pairs and any dissipation leads to a finite resistance, there is no superconductivity. We expect unusual electromagnetic properties as the subsystem with Cooper pairs may respond in a different way to the electromagnetic field. The SB method also shows that the normal metallic state is the state either only with singly occupied sites (for $U > -2|\delta|W$) or only with doubly occupied sites (for $U < -2|\delta|W$). At $n = 1$ the normal state is the Mott insulator state and there is a direct insulator-to-superconductor transition.

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