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Mixed State in $t-U-J-V$ Model

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The $t-U-J-V$ model in the $U \to \infty$ limit is treated by renormalized mean-field theory for arbitrary electron density. Superconductivity of $s + \mathrm{i}d$ symmetry is found in the large parts of the phase diagram. Calculations also show a possibility of phase separation.

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1. Introduction

The mean-field approximation (MFA) is one of the most widespread methods in the theory of the condensed matter. It is relatively simple but quite crude, so the need for more refined treatments emerges. One of them is renormalized mean-field approximation (RMFA) [1, 2], similar in use to MFA but in spirit reminding the Gutzwiller method or its slave-boson variations [3]. Applied to Hubbard- or $t-J$-like models amounts to adding a doping-dependent weighting factors both to the hopping and to the interaction parts of the Hamiltonian, followed by the MFA scheme. The hopping-term weighting factor is precisely the band-narrowing factor of the slave-boson theory [4].

In the present paper the RMFA method is applied to the $t-U-J-V$ model in the $U \to \infty$ limit. The results are applicable also to $t-J$-like models in general. Keeping finite on-site repulsion U during intermediate stages of calculations, to take $U \to \infty$ limit in the end enables us to obtain proper low density limit (i.e., two-electron bound state with finite critical value), incorrectly given in standard $t-J$ model treatment [5]. Considering the V-term is equivalent to using anisotropic $t-J$ model.

2. The method

We start with the extended Hubbard Hamiltonian $t-U-J-V$:

$$H = -t\sum_{\langle ij\rangle\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma} + \text{h.c.}) - \mu\sum_i n_i + U\sum_i n_{i\uparrow}n_{i\downarrow}$$
$$+J\sum_{\langle ij\rangle}(S_i\cdot S_j - \tfrac{1}{4}n_in_j) + V\sum_{\langle ij\rangle\sigma} n_{i\sigma}n_{j-\sigma}. \qquad (1)$$

We calculate operator averages in the BCS states $|BCS\rangle = \prod_k(u_k + v_k c^{\dagger}_{k\uparrow}c^{\dagger}_{-k\downarrow})|0\rangle$ with the double occupancies projected out by the Gutzwiller projector $P_G = \prod_i(1 - n_{i\uparrow}n_{i\downarrow})$. Then we use the Gutzwiller approximation, which introduces the doping dependent factors g_t and g_S (multiplying hopping integral and interaction J, respectively), while taking the averages back in the BCS states. In the end the MFA is done and $U = \infty$ limit is taken. To be exact, the projection removes the double occupancy term and all correlations induced by it, but such a procedure seems too stringent. Even in the $U = \infty$ limit, where there is no doubly occupied states, some U-induced correlations remain, e.g., a superconducting gap, defined as $\Delta_0 = U\langle c_{i\downarrow}c_{i\uparrow}\rangle$ [6]. Therefore, we retain the U-term during MFA, keeping the on-site term in the mean-field superconducting gap, and take $U = \infty$ limit in the end of calculations, omitting U-terms in the free energy and chemical potential. In MFA we calculate the charge density $\langle n\rangle$ and superconducting averages of the type $\langle c_{i\downarrow}c_{j\uparrow}\rangle$ and $\langle c_{i\downarrow}c_{i\uparrow}\rangle$, omitting Fock-type averages $\langle c^{\dagger}_{i\sigma}c_{j\sigma}\rangle$ to simplify calculations. Thus, we retain only the antiparallel spin terms in the nearest-neighbor Coulomb interaction in Eq. (1).

The Hamiltonian which is subject to MFA decomposition is given by Eq. (1), with integrals t and J replaced by $g_t t$ and Jg_S respectively, where

$$g_t = 2\frac{1-n}{2-n}, \qquad g_S = \frac{4}{(2-n)^2}. \qquad (2)$$

After introducing standard order parameters and after the procedure of minimization (see, e.g. [7]) the free energy takes the form

$$F/N = \overline{\mu}(n-1) + (\tfrac{1}{2}Jg_S + V)n^2$$
$$+\frac{1}{N}\sum_k\frac{|\Delta_k|^2}{2E_k} - \frac{2}{\beta N}\sum_k \ln 2\cosh\frac{\beta E_k}{2}, \qquad (3)$$

where $E_k = \sqrt{(-tg_t\gamma_k - \overline{\mu})^2 + |\Delta_k|^2}$. The self-consistent equation for superconducting gap: $\Delta_k = \sum_q V^s_{kq}\langle c_{-q\downarrow}c_{q\uparrow}\rangle$ is given by

$$\Delta_k = \sum_q V^s_{kq}\frac{|\Delta_q|^2}{2E_q}, \qquad (4)$$

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where $V^s_{kq} = U - (V - Jg_S)\gamma_{k-q}$ is singlet pairing potential, $\gamma_k = 2(\cos k_x + \cos k_y)$, $\eta_k = 2(\cos k_x - \cos k_y)$. The gap equation can be further simplified using an ansatz: $\Delta_k = \Delta_0 + \Delta_\gamma\gamma_k$, $\Delta_k = \Delta_\eta\eta_k$, $\Delta_k = \Delta_0 + \Delta_\gamma\gamma_k + \Delta_\eta\eta_k$, $\Delta_k = \Delta_0 + \Delta_\gamma\gamma_k + \mathrm{i}\Delta_\eta\eta_k$ for s^*-wave, d-wave, $s+d$-wave and $s+\mathrm{i}d$-wave pairing, respectively. Inserting the ansatz in Eq. (4) we can obtain equations for variational parameters Δ_0, Δ_γ, Δ_η; e.g., in case of pure on-site pairing the equation for Δ_0 is $1/U = (1/N)\sum_k \Delta_0/2E_k$. Limit $U \to \infty$ simplifies this equation to $0 = (1/N)\sum_k \Delta_0/2E_k$. In the most complicated case of $s + d$ pairing, we have to solve three equations in the form

$$0 = \Delta_0\Phi_1 + \Delta_\gamma\Phi_\gamma + \Delta_\eta\Phi_\eta, \tag{5}$$

$$-\frac{z}{V - Jg_S}\Delta_\gamma = \Delta_0\Phi_\gamma + \Delta_\gamma\Phi_{\gamma^2} + \Delta_\eta\Phi_{\eta\gamma}, \tag{6}$$

$$-\frac{z}{V - Jg_S}\Delta_\eta = \Delta_0\Phi_\eta + \Delta_\gamma\Phi_{\eta\gamma} + \Delta_\eta\Phi_{\eta^2}, \tag{7}$$

where z is number of nearest neighbors. In the ground state, for $T = 0$, $\Phi_1 = \frac{1}{N}\sum_k \frac{1}{2E_k}$, $\Phi_\eta = \frac{1}{N}\sum_k \frac{\eta_k}{2E_k}$, etc. Equations for d-wave and extended s-wave can be obtained by omitting respective deltas in Eqs. (5)–(7). In case of $s + \mathrm{i}d$-pairing, equations for s and d formally decouple (yet they stay still connected by E_k). All these equations have to be solved together with the equation for electron density n:

$$n - 1 = -\frac{1}{N}\sum_k \frac{-tg_t\gamma_k - \overline{\mu}}{E_k}. \tag{8}$$

Let us note that, unlike the standard BCS-MFA, Δ's are only variational parameters. The true superconducting gap is $g_t\Delta$ [1]. Also $\overline{\mu}$ is variational parameter; the true chemical potential is given by $\partial(F/N)/\partial n$; in the ground state

$$\begin{aligned}\mu = \overline{\mu} &+ \frac{\partial}{\partial n}((\tfrac{1}{2}Jg_S + V)n^2) \\ &+ \frac{\partial}{\partial g_t}\left(-\frac{1}{N}\sum_k E_k - \frac{1}{N}\sum_k \frac{|\Delta_k|^2}{2E_k}\right)\frac{\partial g_t}{\partial n} \\ &+ \frac{\partial}{\partial g_S}\left(-\frac{1}{N}\sum_k E_k - \frac{1}{N}\sum_k \frac{|\Delta_k|^2}{2E_k}\right)\frac{\partial g_S}{\partial n}.\end{aligned} \tag{9}$$

To perform these calculations we need the derivative of Δ_k with respect to electron density. The way to do it is shown below, on an example of s^*-wave pairing

$$\frac{\partial\Delta_k}{\partial\, g_S} = -J\sum_q \frac{1}{z}\gamma_q\langle c_{-q\downarrow}c_{q\uparrow}\rangle\gamma_k = -J\frac{\Delta_\gamma}{V - Jg_S}\gamma_k. \tag{10}$$

Chemical potential calculated this way is more complicated than simple $\overline{\mu}$ and shows nonmonotonic behavior, as will be shown in the next section.

3. Results

Calculations have been performed on a two-dimensional square lattice with nearest neighbor hopping in the ground state. The Hartree-Fock (HF) results show stabilization of superconductivity for attractive intersite interaction V [8]. For V larger than threshold value for binding of two-electron pair, s-wave superconductivity appears for small electron densities [9]. d-wave is possible for the whole range of densities, yet for small $|V|$ its energy gain over normal state is exponentially small. The phase diagram for the pure phases is shown in Ref. [10]. Present calculations show that most of the phase diagram is occupied by the mixed phase of the symmetry $s + \mathrm{i}d$ (see also [11]). The phase diagram obtained within HF MFA for $J = 0$ and $U = \infty$ is shown in Fig. 1 by a thin full line.

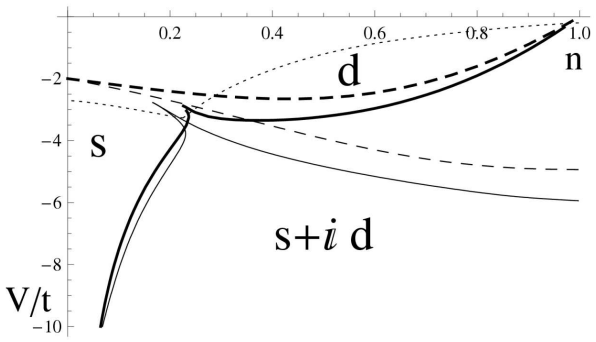

Fig. 1. Phase diagram of the t–U–J–V model for $J = 0$ in the $U = \infty$ limit within the HF MFA (thin full line) and RMFT (thick full line) method. Dotted lines show where the condensation energy of the d- and s-wave pairing, calculated within HF MFA, is the order of 10^{-6}. The dashed lines are boundaries, below which solutions of pure s-wave pairing exist: upper, thick one calculated in RMFT, lower one in HF.

Within the area surrounded by this line (i.e., for larger $|V|$ and larger fillings) the mixed, $s + \mathrm{i}d$-wave pairing is stabilized. Above the quasi-horizontal thin full line only the d-wave pairing can exist. Virtually for the whole range of attractive interaction V, but in practice at the dotted line the condensation energy reaches 10^{-6}. Above this line the condensation energy is even smaller, so we call this area a quasi-normal phase. To the left of the quasi-vertical thin, full line only s-wave pairing exists. At the dotted line the condensation energy again reaches 10^{-6}. The lower dashed line is line of possible second order transition: $\Delta \to 0$. This mean-field boundary line for the existence of s-wave type superconductivity smoothly goes over into an exact threshold for the existence of a bound 2-electron pair in the $n \to 0$ limit. It is also a threshold for s-wave superconductivity for low densities [9]. The upper dashed line is the same boundary line calculated within RMFT. It is strongly renormalized for larger electron densities relative to HF values and reaches $V = 0$ at half-filled band, meaning that there is no threshold for existence of mean-field s-wave solutions at $n = 1$. Therefore the use of RMFT enhances $s + \mathrm{i}d$-wave pairing for larger electron densities on the expense of pure d-wave. Nevertheless, at half-filling and close to it the superconductivity is not realized due to settling of antiferromagnetic (AF) phase. In present paper AF phase is not calculated, yet the existence of non-superconducting state close to half-filling

shows by appearing of the phase-separation close to the $n = 1$. The phase-separation appears both in calculations of free energy, using the Maxwell construction as well as in negative compressibility $\mathrm{d}\mu/\mathrm{d}n$, in calculations of true chemical potential using Eq. (9).

The thick full lines show the boundary of $s + \mathrm{i}d$ phase calculated within RMFT. The s-wave, quasi-vertical boundary is relatively close to the HF one, the renormalizations are small for small n. The boundary with pure d-wave is shifted much in the direction of smaller $|V|$ and reaches $V = 0$ for the half-filled band. This boundary also lies close to the RMFT pure-s border, just as in HF case.

In conclusion, the HF MFA and RMFT methods were used to analyze superconductivity in the $t-U-J-V$ model in the $U = \infty$ limit. Both pure phases and $s + \mathrm{i}d$ phase were examined, showing the domination of the latter over the pure ones. Almost always in the areas where both components $\Delta_s^{s+\mathrm{i}d}$ and $\Delta_d^{s+\mathrm{i}d}$ are non-zero the mixed phase $s + \mathrm{i}d$ dominates over pure ones. The $\Delta_s^{s+\mathrm{i}d}$ disappears close to the boundary of existence of pure s-wave mean field solutions. These conclusions are obtained by both the HF and RMFT methods, with the difference that in RMFT for larger fillings the region of d-wave pairing is suppressed in favor of $s + \mathrm{i}d$-wave.

The present calculations did not take into account the fugacity factors [12]. The Gutzwiller projection without those factors change the average number of electrons in the system, which can have influence on the chemical potential and other density-dependent functions. This problem is under investigation.

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References

[1] F.C. Zhang, C. Gros, T.M. Rice, H. Shiba, *Supercond. Sci. Technol.* **1**, 36 (1988).

[2] B. Edegger, V.N. Muthukumar, C. Gros, *Adv. Phys.* **56**, 927 (2007).

[3] M.C. Gutzwiller, *Phys. Rev. Lett.* **10**, 159 (1963).

[4] M. Bak, R. Micnas, *J. Phys., Condens. Matter* **10**, 9029 (1998).

[5] M. Bak, *Acta Phys. Pol. A* **114**, 275 (2008).

[6] R. Micnas, J. Ranninger, S. Robaszkiewicz, *J. Phys. C, Solid State Phys.* **21**, L145 (1988).

[7] R. Micnas, J. Ranninger, S. Robaszkiewicz, *Phys. Rev. B* **39**, 11653 (1989).

[8] C. Bastide, C. Lacroix, A. da Rosa Simoes, *Physica C* **159**, 347 (1989).

[9] M. Randeria, J. M. Duan, L.-Y. Shieh, *Phys. Rev. B* **41**, 327 (1990).

[10] F. Pistolesi, Ph. Nozieres, *Phys. Rev. B* **66**, 054501 (2002).

[11] B. Tobijaszewska, R. Micnas, *Phys. Status Solidi B* **243**, 159 (2006).

[12] B. Edegger, N. Fukushima, C. Gros, V.N. Muthukumar, *Phys. Rev. B* **72**, 134504 (2005).