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Critical Values for Electron Pairing in t–U–J–V and t–J–V Models

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The critical values for pairing of s^*- and d-wave symmetry are calculated within the t–U–J–V and the t–J–V models in renormalized mean field theory. It is shown that the first model yields the proper critical values in the low density limit while the other does not. Renormalized mean field theory strongly decreases the absolute value of (negative) critical values for larger electron densities.

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1. Introduction

High-temperature superconductivity (HTSC) has been an object of intensive research for many years. It is a phenomenon appearing in narrow band systems, with short coherence length, small value of the Fermi energy and other features, placing their low-temperature physics somewhere between the BCS scenario and Bose–Einstein condensation (BEC) [1]. Thus the problem of crossover between these limits is a very interesting one.

The cuprate high-temperature superconductors are commonly described by the Hubbard model and its derivatives. In the strong coupling limit of these models we can take an advantage of exact solutions for two-electron bound pairs. The BCS equations for singlet pairing smoothly connect to these solutions in the limit of low electron density ($n \to 0$) [2, 3]. If HTSC were driven by (Bose) condensation of such bound pairs, then their existence would be directly connected to the existence of superconductivity. Actually, there is a theorem of Randeria et al. [4], claiming that the existence of such pairs is a necessary condition for appearing of superconductivity but only of s-wave type in two dimensions. We can calculate the critical value for appearance of such a two-body bound state, which should be retrieved in the low density limit of applied theories. It can be accomplished in the mean-field approach (MFA) to the Hubbard model, but, surprisingly, not in some more sophisticated treatments.

The t–J model, as a strong coupling limit of the Hubbard model, should be even more appropriate for comparison with low-density solutions. It turns out nevertheless that it does *not* yield proper critical values. For what seems, the restriction of no-doubly occupied sites is too strong; it is correct for an infinite on--site repulsion, while in reality the repulsion although big is finite, and small, finite on-site correlations should be allowed in the model. Thus our approach will be to start with the t–U–J model and take the $U \to \infty$ limit in the end. The on-site Hubbard term yields non-zero on-site gap even in this case [5], which results in correct critical values.

To improve results of the Hartree–Fock MFA the present paper applies renormalized mean-field theory (RMFT) [6] to the t–U–J–V model in the $U = \infty$ limit to obtain the proper low density properties on one hand and to compare the effects of RMFT renormalization on J and V terms on the other.

2. The method

We start with the effective t–U–J–V Hamiltonian [7]:

$$H = -t \sum_{\langle ij \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) - \mu \sum_i n_i + U \sum_i n_{i\uparrow} n_{i\downarrow}$$
$$+ J \sum_{\langle ij \rangle} \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \frac{1}{4} n_i n_j \right) + V \sum_{\langle ij \rangle} (n_{i\uparrow} n_{j\downarrow} + n_{i\downarrow} n_{j\uparrow}), \tag{1}$$

where $\langle ij \rangle$ means single summation over nearest neighbor (nn) sites and U, J, V are independent parameters [8]. As we are interested in singlet pairing the parallel--spin part of the V interactions is omitted. This way the Fock terms connected with V will not appear in the mean-field equations. For consistency we also omit the Fock terms connected with antiferromagnetic coupling. In the end the limit $U \to \infty$ will be taken, so the Hartree shifts in the chemical potential are also not explicitly included, and only the effective, self-consistent chemical potential μ will be calculated.

The $U \to \infty$ limit imposes the constraint of no doubly-occupied sites: $n_{i\uparrow} n_{i\downarrow} = 0$, implying $\langle c_{i\downarrow} c_{i\uparrow} \rangle = 0$. The on-site component of BCS superconducting gap (the full gap includes also terms connected with nn interactions, see Eq. (10)): $\Delta_0 = U \langle c_{i\downarrow} c_{i\uparrow} \rangle$ remains nevertheless constant [5]. This way the effect of on-site term is preserved, despite no-doubly-occupied sites condition enforced. Thus to examine the ground state we can use the Gutzwiller-projected BCS function and RMFT

$$|\psi\rangle = P_d |\psi_0\rangle, \qquad |\psi_0\rangle = \prod_{\boldsymbol{k}} (u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow}) |0\rangle, \tag{2}$$

where $P_d = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$ is the Gutzwiller projection operator, $|0\rangle$ is vacuum state and $u_{\boldsymbol{k}}$, $v_{\boldsymbol{k}}$ are variational parameters subject to constraint: $|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 = 1$. Our aim is to replace the averages in projected states $|\psi\rangle$ (henceforth denoted as $\langle . \rangle$) by unrestricted averages in the states $|\psi_0\rangle$ (denoted as $\langle . \rangle_0$). We assume RMFT relations

$$\langle c^\dagger_{i\sigma} c_{j\sigma} \rangle = g_t \langle c^\dagger_{i\sigma} c_{j\sigma} \rangle_0, \qquad \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle = g_S \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle_0. \tag{3}$$

The weigting factors g_t and g_S are given by the ratios of the corresponding physical processes in the states $|\psi\rangle$ and $|\psi\rangle_0$, as [6]:

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

The energy of the system can be evaluated now as

$$\langle H(t,U,J,V)\rangle = \langle H(\tilde{t},U,\tilde{J},V)\rangle_0, \tag{5}$$

where $\tilde{t} = g_t t$ and $\tilde{J} = g_S J$. Let us note that the diagonal interaction terms: U and V stay unrenormalized, both in projected and unprojected states. With $\widetilde{H} \equiv H(\tilde{t},U,\tilde{J},V)$ we perform standard BCS-like decoupling procedure to obtain the following ground-state equations in the reciprocal space in the singlet channel:

$$\Delta_{\boldsymbol{k}} = \frac{1}{N}\sum_{\boldsymbol{q}} V^s_{\boldsymbol{k},\boldsymbol{q}} \langle c_{-\boldsymbol{q}\downarrow} c_{\boldsymbol{q}\uparrow}\rangle = \frac{1}{N}\sum_{\boldsymbol{q}} V^s_{\boldsymbol{k},\boldsymbol{q}} \frac{\Delta_{\boldsymbol{q}}}{2E_{\boldsymbol{q}}}, \tag{6}$$

$$V^s_{\boldsymbol{k},\boldsymbol{q}} = U + (V-\tilde{J})\gamma_{\boldsymbol{k}-\boldsymbol{q}}, \tag{7}$$

$$E_{\boldsymbol{q}} = \sqrt{(\tilde{\epsilon}_{\boldsymbol{q}} - \mu)^2 + |\Delta_{\boldsymbol{q}}|^2}, \tag{8}$$

$$\tilde{\epsilon}_{\boldsymbol{q}} = -\tilde{t}\gamma_{\boldsymbol{q}} = -g_t t \gamma_{\boldsymbol{q}} = g_t \epsilon_{\boldsymbol{q}}. \tag{9}$$

The gap equation is solved by the ansatz

$$\Delta_{\boldsymbol{k}} = \Delta_0 + \Delta_\gamma \gamma_{\boldsymbol{k}} + \Delta_\eta \eta_{\boldsymbol{k}}, \tag{10}$$

where $\gamma_{\boldsymbol{k}} = 2(\cos k_x + \cos k_y)$ and $\eta_{\boldsymbol{k}} = 2(\cos k_x - \cos k_y)$, which leads us to the set of self-consistent equations for (extended) s^*-wave pairing in the $U \to \infty$ limit

$$\left[\begin{pmatrix} 0 & 0 \\ 0 & -\frac{4}{V-\tilde{J}} \end{pmatrix} - \begin{pmatrix} \Phi_0 & \Phi_\gamma \\ \Phi_\gamma & \Phi_{\gamma^2} \end{pmatrix}\right] \begin{pmatrix} \Delta_0 \\ \Delta_\gamma \end{pmatrix} = 0, \tag{11}$$

where

$$\Phi_0 = \frac{1}{N}\sum_{\boldsymbol{q}} \frac{1}{2E_{\boldsymbol{q}}}, \qquad \Phi_\gamma = \frac{1}{N}\sum_{\boldsymbol{q}} \frac{\gamma_{\boldsymbol{q}}}{2E_{\boldsymbol{q}}}, \qquad \Phi_{\gamma^2} = \frac{1}{N}\sum_{\boldsymbol{q}} \frac{\gamma^2_{\boldsymbol{q}}}{2E_{\boldsymbol{q}}}. \tag{12}$$

The $d_{x^2-y^2}$-wave gap equation together with the equation for chemical potential are shown below

$$-\frac{4}{V-\tilde{J}} = \frac{1}{N}\sum_{\boldsymbol{q}} \frac{\eta^2_{\boldsymbol{q}}}{2E_{\boldsymbol{q}}}, \qquad n-1 = -\frac{1}{N}\sum_{\boldsymbol{k}} \frac{\epsilon_{\boldsymbol{k}} - \mu}{E_{\boldsymbol{k}}}. \tag{13}$$

Let us note that in RMFT $\Delta_{\boldsymbol{k}}$ and μ are just variational parameters. The order parameter Δ^{sc} is given by: $\Delta^{\text{sc}}_{\boldsymbol{k}} = g_t \Delta_{\boldsymbol{k}}$, while the true chemical potential μ^{sc}:

$$\mu^{\text{sc}} = \mu + \left\langle \frac{\partial}{\partial n}(\widetilde{H} + \mu n) \right\rangle_0. \tag{14}$$

3. Results

The calculations were done for square lattice. The results are shown in Fig. 1 and describe critical values for s^*- and d-wave pairings. Infinitesimally small attraction leads to pairing of d-wave symmetry, so there is no critical value for this kind of pairing except the trivial one: as the potential has the form $\sim (V - J)$ we can have pairing for any $V < J$, e.g., for $V < 0$ in t–V model ($J = 0$) or for $V < 1/3$ in the t–J–V model with $J = 1/3$ (a common choice). In RMFT the critical value $V_{\rm cr} = J$ only for $n = 0$; it increases with electron density to reach $V_{\rm cr} = 4J$ at half-filling. It is depicted by the uppermost, dotted line in the figure. Let us note that in the standard approach to the t–J model the above mentioned values are also critical values for the existence of s^*-wave superconductivity. As we know from the exact two-electron solution, the proper value for s^*-wave is $V_{\rm cr} = -2t$ (or $V - J = -2t$ for $J \neq 0$). In the figure the two full lines describe the Hartree–Fock (HF) solutions for the existence of s^*-wave superconductivity in the hard-core limit, obtained by setting $\Delta_{\boldsymbol{k}} = 0$ in self-consistent equations [9]. The lower one is for $J = 0$, the upper one is for $J = 1/3$. As we can see, the solutions attain the proper low density limit. For larger densities the critical values increase in absolute value in HF, reflecting the increased screening of charges. The situation is definitely changed in RMFT theory; the critical values decrease in absolute value (for $V < 0$) as shown by dashed lines. For half-filling they reach the values obtained within standard approach to the t–J–V model.

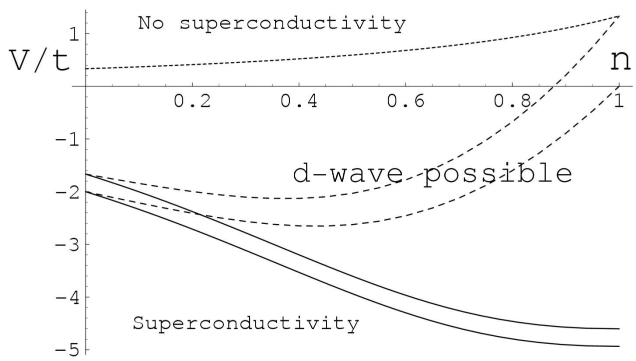

Fig. 1. The critical values for the existence of superconductivity in the t–U–J–V model in the $U = \infty$ limit. Dotted line — RMFT (also for s^*-wave in the t–J–V model) for $J/t = 1/3$. Upper dashed line — RMFT, $J/t = 1/3$, lower dashed line — RMFT, $J = 0$, upper full line — HF, $J/t = 1/3$, lower full line — HF, $J = 0$.

In general, the corrections of RMFT are the largest close to $n = 1$, where the model starts to behave like the t–J–V model and our trick with introducing t–U–J–V, so important close to $n = 0$, loses its significance.

Let us note that close to the half filling band there is competition with antiferromagnetism and for large, negative V the phase separation is probable.

For $V > 0$ the CDW-phase should be also considered. All those problems are not addressed by the present paper.

In conclusion, the present paper shows that taking $U \to \infty$ limit of t–U–J–V model yields proper critical values for $n = 0$ unlike standard approach to the t–J or t–J–V models. The RMFT strongly influences the critical values for larger densities, especially close to the Mott–Hubbard limit ($n = 1$). The results are also applicable to the t–J and t–U–J models as the t–J–V model is equivalent to anisotropic t–J one.

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