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ORIGINAL PAPER

Superconductivity, Charge Orderings, Magnetism, and Their Phase Separations in the Ground State of Lattice Models of Superconductor with Very Short Coherence Length

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Abstract We present the ground state results for lattice models of superconductor (SC) with extremely short coherence length, which also involve the interplay with charge (CO) and (anti-)ferromagnetic orderings. Our preliminary results at zero temperature (derived by means of the variational approach which treats the on-site interaction term exactly and the intersite interactions within the mean field approximation, exact in $d \to +\infty$), yields that the SC phase can coexist with the CO or magnetic (M) phases in states with electron phase separation (PS:SC/CO and PS:SC/M, respectively).

Keywords Extended Hubbard model · Phase separation · Superconductivity · Magnetism · Charge ordering · Pair hopping · Phase diagrams

1 Introduction

The interplay and competition between superconductivity (SC) and other electron orderings, such as charge orderings (CO) or various magnetic (M) orderings is currently under intense investigations in broad range of materials including cuprates, bismutates, iron-pnictides, organic conductors and heavy-fermion systems (for review, see e.g. refs. [1–14] and references therein). Moreover, the phase separation (PS) has been evidenced (by various microscopy techniques such as STM, MFM, etc.) in some of the materials from the groups mentioned previously, especially in iron-pnictides (PS with M), bismutates (PS with CO) and cuprates.

In this paper, we study a simplified model which can pertain to that problem. The effective model considered has a form of single-band extended Hubbard model with pair hopping at the atomic limit ($t = 0$) [4–17]:

$$\begin{aligned}\hat{H} = {} & U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu\sum_i \hat{n}_i \\ & -I\sum_{\langle i,j\rangle}\left(\hat{\rho}_i^+\hat{\rho}_j^- + \hat{\rho}_j^+\hat{\rho}_i^-\right) + \frac{W}{2}\sum_{\langle i,j\rangle}\hat{n}_i\hat{n}_j \\ & -2J^z\sum_{\langle i,j\rangle}\hat{s}_i^z\hat{s}_j^z - J^{xy}\sum_{\langle i,j\rangle}\left(\hat{s}_i^+\hat{s}_j^- + \hat{s}_j^+\hat{s}_i^-\right),\end{aligned} \tag{1}$$

where $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^+\hat{c}_{i\sigma}$, $\hat{n}_i = \sum_\sigma \hat{n}_{i\sigma}$, $\hat{\rho}_i^+ = (\hat{\rho}_i^-)^\dagger = \hat{c}_{i\uparrow}^+\hat{c}_{i\downarrow}^+$, $\hat{s}_i^z = (1/2)(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$ and $\hat{s}_i^+ = (\hat{s}_i^-)^\dagger = \hat{c}_{i\uparrow}^+\hat{c}_{i\downarrow}$. $\hat{c}_{i\sigma}^+$ and $\hat{c}_{i\sigma}$ denote the creation and annihilation operators, respectively, of an electron with spin σ ($\sigma = \uparrow, \downarrow$) at site i, which fulfil standard anticommutation relations for fermionic operators. μ is the chemical potential. The nearest-neighbors interactions U, I, W, J^z and J^{xy} are effective model parameters and are assumed to include all the possible renormalizations and contributions like those coming from the strong electron-phonon coupling or from the coupling between electrons and other electronic subsystems in solid or chemical complexes.

The analysis of the ground state of model (1) has been performed by means of a variational approach (VA) in the grand canonical ensemble [6–14], which treats on-site U term exactly and the intersite interactions within the mean-field approximation (MFA). The MFA is a rigorous treatment of the intersite terms in the limit of infinite dimensions $d \to +\infty$ (or large coordination number z); thus, the result obtained in this paper for model (1) are also exact in the limit $d \to +\infty$. This approach allows us to calculate the

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grand canonical potential per site $\omega = \langle \hat{H} \rangle / L$ and the (free) energy per site $E = \langle \hat{H} + \mu \sum_i \hat{n} \rangle / L = \omega + \mu n$ (at $T = 0$, L is a number of lattice sites). $\langle \hat{A} \rangle$ is an average value of operator $\hat{A}$.

Let us introduce the following mean-field order parameters:

$$n_{\vec{q}} = \frac{1}{N} \sum_i \exp(i\vec{q} \cdot \vec{r}_i) \langle \hat{n}_i \rangle, \tag{2}$$

$$\Delta_{\vec{q}} = \frac{1}{N} \sum_i \exp(i\vec{q} \cdot \vec{r}_i) \langle \hat{\rho}_i^- \rangle, \tag{3}$$

$$m_{\vec{q}}^{\alpha} = \frac{1}{N} \sum_i \exp(i\vec{q} \cdot \vec{r}_i) \langle \hat{s}_i^{\alpha} \rangle, \tag{4}$$

where $\vec{r}_i$ determines the location of i-site and $\alpha = z, \pm$ ($m_{\vec{q}}^{+} = (m_{\vec{q}}^{-})^*$). We restrict ourselves only to a case of two sublattice orderings on the alternate lattices, i.e. $\vec{q} = \vec{0}, \vec{Q}$, where $\vec{Q}$ is a half of the smallest reciprocal lattice vector. $n \equiv n_{\vec{0}}$ is an electron concentration in the system. In the charge-ordered (CO) phase $n_{\vec{Q}} \neq 0$. Model (1) exhibits a symmetry between $I > 0$ (SC with s-pairing, $\Delta_{\vec{0}} \neq 0$) and $I < 0$ (SC with η-pairing, $\Delta_{\vec{Q}} \neq 0$) cases. Similar symmetry occurs for spin orderings in both direction ($\alpha = z, \pm$) between ferro- (with $m_{\vec{0}}^{\alpha} \neq 0$) and antiferro- (with $m_{\vec{Q}}^{\alpha} \neq 0$) magnetic (M) phases. Notice that for general case of both J^{xy} and J^z nonzero that symmetry is valid only for VA results. The boundary between M phases with orderings in z-direction and xy-direction is for $|J^{xy}/J^z| = 1$ (in VA). Thus, we define $|J| = \max\{|J^z|, |J^{xy}|\}$. Both symmetries in the above-mentioned discussion are for model (1) on the alternate lattices (i.e. lattices, which consist of two interpenetrating lattices). In the presence of finite single electron hopping $t \neq 0$, both of the above-mentioned symmetries are broken in the general case [18–30], but the detailed discussion of effects of $t \neq 0$ is beyond the scope of this publication. Moreover, because of the particle-hole symmetry of model (1) the phase diagrams obtained are symmetric with respect to $\bar{\mu} = 0$ ($\bar{\mu} = \mu - U/2 - W_0$, $W_0 = zW$) as well as $n = 1$. The equations for energies of phases and states for $n \geq 1$ can be obtained using the relation $\bar{E}(2 - n) = E(n) + (U + 2W_0)(1 - n)$, where $E(n)$ is the energy for $n \leq 1$ ((10)–(15) and (17)) and $\bar{E}(n)$ is the energy for $n \geq 1$. For order parameters, the relation $\bar{\psi}(2 - n) = -\psi^*(n)$ is fulfilled ($n \neq 1$), where $\psi = \Delta_{\vec{q}}, m_{\vec{q}}^{\alpha}, n_{\vec{Q}}$ ($n_{\vec{Q}} = n_{\vec{Q}}^*$, $(m_{\vec{q}}^z)^* = m_{\vec{q}}^z$).

The PS state (macroscopic separation) is a state in which two domains with different electron concentrations (n_+ and n_-) exist in the system (coexistence of two homogeneous phases). The energies of the PS states are calculated from minimization of the expression

$$E_{\mathrm{PS}}(n_+, n_-) = mE_+(n_+) + (1 - m)E_-(n_-), \tag{5}$$

where $E_{\pm}(n_{\pm})$ are values of the energy of two separating phases at $n_{\pm}$ corresponding to the lowest homogeneous solution for a given phase, m is the fraction of the system with charge density n_+, and $mn_+ + (1 - m)n_- = n$ [8, 31–34].

In this paper, we focus on the ground state of model (1) in two cases: (i) $J = 0$ and $U \leq 0$ – Section 2.1; as well as (ii) $W = 0$ – Section 2.2. Names of transition orders used are consistent with our earlier works [7–14, 33–36]. In particular, a transition between a homogeneous phase and the PS state is symbolically named as a "third-order" transition.

2 The ground state results ($T = 0$)

2.1 Superconductivity and charge orderings ($J = 0$ and $U \leq 0$)

For any $U \leq 0$ and J^z, $J^{xy} = 0$ the ground state phase diagrams of model (1) are shown in Fig. 1. Figure 1a is a result of comparison of the grand canonical potentials of particular phases, which are as following:

$$\omega_{\mathrm{NO}}^{a} = 0, \qquad (n = 0) \tag{6}$$

$$\omega_{\mathrm{NO}}^{b} = -2\bar{\mu}, \qquad (n = 2) \tag{7}$$

$$\omega_{\mathrm{CO}} = -\bar{\mu} - W_0, \qquad (n = 1,\ n_{\vec{Q}} = 1) \tag{8}$$

$$\omega_{\mathrm{SC}} = -\frac{(\bar{\mu} + |I_0| + W_0)^2}{2(|I_0| + W_0)}, \left(n = 1 + \frac{\bar{\mu}}{|I_0| + W_0}\right) \tag{9}$$

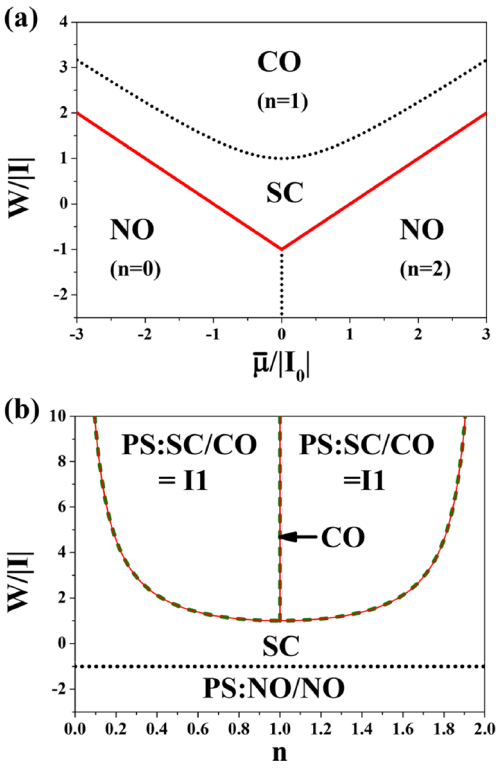

Fig. 1 Ground state diagram for $U \leq 0$ and $J = 0$ as a function of μ (**a**) and as a function of n (**b**). *Dotted, solid* and *dashed lines* denote first-order, second-order and "third-order" transitions, respectively. Details in text

where $I_0 = zI$ and $W_0 = zW$. The second-order NO–SC phase boundary is determined by $W_0/I_0 = |\bar{\mu}/I_0| - 1$ (n and $\Delta_{\vec{q}}$ are continuous). The first-order SC–CO transition occurs for $(W_0/I_0)^2 = (\bar{\mu}/I_0)^2 + 1$, at which $\Delta_{\vec{q}}$ and $n_{\vec{Q}}$ are discontinuous. n changes (discontinuously, except $\bar{\mu} = 0$) from $n_{\mathrm{SC}} = 1 \mp \sqrt{(W_0 - |I_0|)/(W_0 + |I_0|)}$ in the SC phase (for $n \lessgtr 1$, respectively) to $n_{\mathrm{CO}} = 1$ in the CO phase. A first-order NO–NO transition occurs for $\bar{\mu} = 0$ and $W/|I| < -1$.

As a function of n, the energies of the particular homogeneous phases are as follows (for $n \leq 1$):

$$E_{\mathrm{NO}} = \tfrac{1}{2}(U + W_0 n)\, n, \tag{10}$$

$$E_{\mathrm{SC}} = \tfrac{1}{2}\left[(U + 2W_0)n - (|I_0| + W_0)n(2-n)\right], \tag{11}$$

$$E_{\mathrm{CO}} = \tfrac{1}{2}Un, \ (n_{\vec{Q}} = n) \tag{12}$$

$$E_{\mathrm{I1}} = E_{\mathrm{SC}} + \\ -\tfrac{1}{2}\left[\sqrt{W_0 + |I_0|}(1-n) - \sqrt{W_0 - |I_0|}\right]^2, \tag{13}$$

where we also consider the mixed phase (I1) in which three order parameters: $n_{\vec{Q}}$, $\Delta_{\vec{0}}$ and $\Delta_{\vec{Q}}$ are non-zero (microscopic coexistence of SC and CO). In the SC phase, $|\Delta|^2_{\vec{0}/\vec{Q}} = \frac{1}{4}n(2-n)$, $|\Delta|^2_{\vec{Q}/\vec{0}} = 0$ (for $I \gtrless 0$, respectively), and $n_{\vec{Q}} = 0$. For the I1 phase (in the range of its definiteness and $n \leq 1$) one obtains: $|\Delta|^2_{\vec{0}/\vec{Q}} = \frac{1}{4}\left\{n(2-n) - \left[1 + (n-1)\sqrt{\frac{W_0+|I_0|}{W_0-|I_0|}}\right]\right\}$, $|\Delta|^2_{\vec{Q}/\vec{0}} = \frac{1}{4}(n-1)\left[1 - n - \sqrt{\frac{W_0-|I_0|}{W_0+|I_0|}}\right]$ (for $I \gtrless 0$, respectively), and $n^2_{\vec{Q}} = 1 + (n-1)^2 + (n-1)\frac{2W_0}{\sqrt{W_0^2 - I_0^2}}$. In this phase $\bar{\mu}_{\mathrm{I1}} = \mp\sqrt{W_0^2 - I_0^2}$ (for $n \lessgtr 1$, respectively), what implies that the I1 phase can occur only at the SC–CO boundary in Fig. 1a. Notice that in the I1 phase the $\bar{\mu}$-dependences of n, $n_{\vec{Q}}$, $\Delta_{\vec{0}}$ and $\Delta_{\vec{Q}}$ are indefinite, whereas in the SC phase, it can be easily obtained by using (9) (i.e. $n = n(\bar{\mu})$).

The first-order boundaries (for fixed $\bar{\mu}$) can be associated with the existence of the PS states in defined ranges of n (for fixed n). In our model, two such states can occur: (i) PS:SC/CO with concentrations in domains: $n_{\mathrm{SC}} = 1 \mp \sqrt{(W_0 - |I_0|)/(W_0 + |I_0|)}$ ($n \lessgtr 1$, respectively) and $n_{\mathrm{CO}} = 1$ as well as (ii) PS:NO/NO with concentrations in domains: $n^a_{\mathrm{NO}} = 0$ and $n^b_{\mathrm{NO}} = 2$. Using (5) and (10)–(12) one obtains (for $n \leq 1$):

$$E_{\mathrm{PS:SC/CO}} = \tfrac{1}{2}Un + (1-n)\left[\sqrt{W_0^2 - I_0^2} - W_0\right], \tag{14}$$

$$E_{\mathrm{PS:NO/NO}} = \left(\tfrac{1}{2}U + W_0\right)n. \tag{15}$$

Comparing energies (10)–(15), we obtain the diagram shown in Fig. 1b. The I1 phase and the PS:SC/CO state are degenerated in the whole ranges of their occurrences, but at $T > 0$, this degeneration is removed and only the PS:SC/CO state exists [13]. The SC–I1 and I1–CO transitions are second-order, whereas the SC–PS:SC/CO and PS:SC/CO–CO transitions are "third-order". At the PS:NO/NO–SC transition, the sizes of domains change discontinuously as well as the occurring orderings change; thus, we classified this transition as first-order rather than "third-order" (cf. the definitions of phase boundaries in [33–36]). Notice that in all above-mentioned phases and states, there are no single occupied sites ($\sum_i \langle|\hat{s}^z_i|\rangle/L = 0$ and $m^{\alpha}_{\vec{q}} = 0$) and all electrons are locally paired. The results obtained are in agreement with those for $U \to -\infty$ (VA, fixed n) [32, 37]. In that limit, the results derived by RPA approach for $d = 1, 2, 3$ lattices [4, 38, 39] are consistent with Fig. 1b; but for these dimensions, the critical concentration $n_c \neq 0$ exist that for $0 < n < n_c$ only the SC phase exists (for any $W/|I| > 0$, here: $n, n_c < 1$). The PS:SC/CO state for $W > 0$ has not been considered in [4, 37–39].

2.2 Superconductivity and magnetism ($W = 0$)

For $W = 0$ and $T = 0$, the phase diagrams of model (1) are shown in Fig. 2. On the diagram, as a function of $\bar{\mu}$ (shown in Fig. 2a) the NO (with $n = 0$ or $n = 2$), SC, and M phases

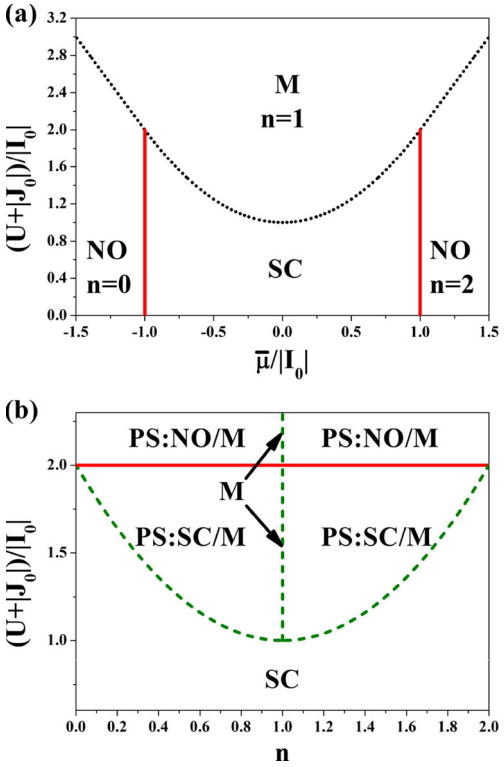

Fig. 2 Ground state diagram for $W = 0$ and $J \neq 0$ as a function of μ (**a**) and as a function of n (**b**). Denotations are the same as in Fig. 1. Details in text

occur, whose grand potentials are given by (6), (7), (9) (for $W_0 = 0$), and

$$\omega_{\mathrm{M}} = -\bar{\mu} - U/2 - |J_0|/2 \qquad (n = 1,\ m_{\vec{q}}^{\alpha} = 1/2), \quad (16)$$

respectively, ($|J_0| = z|J|$). The first-order SC–M boundary is located at $(U + |J_0|)/|I_0| = (\bar{\mu}/I_0)^2 + 1$. The SC–NO transitions at $|\bar{\mu}/I_0| = 1$ are second order.

Similarly, as in the previous section, we derived the energies of particular phases and possible PS states for fixed n. For the M phase, we obtain ($n \leq 1$):

$$E_{\mathrm{M}} = -\tfrac{1}{2}|J_0|n^2, \qquad \left(m_{\vec{q}}^{\alpha} = n/2\right) \quad (17)$$

whereas the energies: (i) $E_{\mathrm{PS:SC/M}}$ of the PS:SC/M state with concentrations in domains: $n_{\mathrm{SC}} = 1 \mp \sqrt{(U + |J_0|)/|I_0| - 1}$ (for $n \lesseqgtr 1$) and $n_{\mathrm{M}} = 1$; (ii) $E_{\mathrm{PS:NO/M}}$ of the PS:NO/M state with concentrations in domains: $n_{\mathrm{NO}}^{a} = 0$ ($n < 1$) or $n_{\mathrm{NO}}^{b} = 2$ ($n < 1$) and $n_{\mathrm{M}} = 1$ as well as E_{SC} for the SC phase can be derived from (5) and (10), (11) (with $W_0 = 0$) and (17).

The resulting diagram as a function of n is shown in Fig. 2b. Notice that in the M phase, $\mu_{\mathrm{M}} = -|J_0|n$ and $\frac{\partial \mu}{\partial n} < 0$ for $n < 1$. Thus, the M phase occurs only for $n = 1$ and $(U + |J_0|)/|I_0| > 1$ (cf. refs. [12, 40–42]). The mixed phase (I2) in which order parameters $\Delta_{\vec{q}}$ and $m_{\vec{q}}^{\alpha}$ are non-zero (microscopic coexistence of SC and M) does not exist in any range of $\bar{\mu}$ and n. The PS:SC/M–PS:NO/M is second-order transition between two PS states, because in the SC domain, $\Delta_{\vec{q}}$ goes continuously to zero, whereas in the other domain (M), $m_{\vec{q}}^{\alpha} \neq 0$ and it changes continuously [33–36]. The PS:SC/M–M and PS:NO/M–M transitions are "third-order" ones.

For $J = 0$ the M phase reduces into the NO′ phase with $\omega_{\mathrm{NO}'} = -\bar{\mu} - U/2$ ($n = 1$) and $E_{\mathrm{NO}'}(n) = 0$ (for $n < 1$) [8–11], and the PS states on Fig. 2b change into PS′:SC/NO′ and PS′:NO/NO′ states, whose energies can be derived from (5) analogously. The energies of this NO′ phase and the PS′:NO/NO′ state are equal at $T = 0$, but at $T > 0$ the PS′ does not occur. In such a case, the PS′:SC/NO′-PS′:NO/NO′ is a second-order transition between two PS states [33–36], whereas the PS′:SC/NO′–NO′ transition is "third-order".

3 Summary and final comments

The analysis of the model considered shows that the superconductivity can coexists with magnetism only in the state with phase separation (PS:SC/M for $1 < (U + |J_0|)/|I_0| < 2$, $W = 0$), whereas superconductivity and charge orderings—in the state with phase separation (PS:SC/CO) as well as in homogeneous mixed I1 phase (for $U < 0$, $W/|I_0| > 1$ and J^z, $J^{xy} = 0$). These last mentioned two states are degenerated at $T = 0$. This degeneration can be removed in the presence of long range (at least between next-nearest neighbors) interactions [32]. The mixed homogeneous phases I2 (coexistence of SC and M orderings) does not appear on the phase diagrams.

Let us discuss how the properties of the system in the PS states evolve with n. If the SC fraction of the system is rather large (as it occurs near the boundary with the homogeneous SC phase, i.e. for $n \gtrsim n_{\mathrm{SC}}$), for example, the measured penetration depth will remain constant with increasing n (since $n_{-} = n_{\mathrm{SC}}$ is independent of n) [8, 31, 32]. On the other hand, near half-filling ($n \approx 1$) the SC fraction is strongly reduced and there will be only diluted SC domains (with $n_{\mathrm{SC}} < 1$) in a insulating or semiconducting CO/M background (with $n_{\mathrm{CO/F}} = 1$). When the SC domains do not percolate, one should observe a partial Meissner effect but without zero resistance. On the contrary, in the homogeneous mixed phases (I1, I2) behaviour of the SC characteristics would be totally different, because the whole system exhibits superconductivity and all of its SC properties (in particular, a penetration depth) would change with n, but with a full Meissner effect and zero resistance [37–39].

Notice that the results of Section 2.1 together with results of [13, 32, 37, 43–46] give the full picture of behavior of model (1) for $U \leq 0$, $W \neq 0$, and J^z, $J^{xy} = 0$ within VA approach. Cases of $U > 0$ as well as J^z, $J^{xy} \neq 0$ are left to future works. Some analyses concerning the interplay between W and J^z, J^{xy} interactions for $I = 0$ have been performed in [5, 47–49].

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