Electron phase separations involving superconductivity in the extended Hubbard models with pair hopping interaction

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In this work the extended Hubbard models with pair hopping interaction (at the atomic limit) are investigated within the variational approach, which treats the on-site interaction term exactly and the intersite interactions within the mean-field approximation (exact in $d \to +\infty$). We analyze mutual stability of the superconducting (SC) phase and charge (CO) or (ferro/antiferro-)magnetic (M) orderings as well as homogeneous mixed phases. Our preliminary results for $U = 0$ show that the SC phase can coexist with the CO or M phases only in states with electron phase separation.

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I. INTRODUCTION

The phase separation (PS) phenomenon involving superconductivity (SC) is under intense investigation and has been evidenced in broad range of currently investigated materials including iron pnictides, cuprates, bismutates, organic conductors and heavy-fermion systems (for review see e.g. Refs. [1–20] and references therein).

The effective model considered has a form of extended Hubbard model at the atomic limit ($t = 0$):

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

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. Interactions U, I, W, J^z, J^{xy} between the nearest neighbors (NN) are effective model parameters (assumed to include all the possible contributions and renormalizations) and μ is the chemical potential.

The analysis has been performed within a variational approach (VA) [2–7], which treats the U term exactly and the intersite interactions within the mean-field approximation (MFA), which is a rigorous treatment of the intersite terms in the limit of infinite dimensions $d \to +\infty$ or large coordination number (number of NN) z.

We introduce order parameters defined as: $\Delta_{\vec{q}} = \frac{1}{N} \sum_i \exp(i\vec{q} \cdot \vec{r}_i) \langle \hat{\rho}_i^- \rangle$, $n_{\vec{q}} = \frac{1}{N} \sum_i \exp(i\vec{q} \cdot \vec{r}_i) \langle \hat{n}_i \rangle$, $m_{\vec{q}}^\alpha = \frac{1}{N} \sum_i \exp(i\vec{q} \cdot \vec{r}_i) \langle \hat{s}_i^\alpha \rangle$ for two sublattice orderings on the alternate lattices, where N is the total number of lattice sites. The model exhibits a symmetry between $I > 0$ (SC with s-pairing, $\Delta_{\vec{0}} \neq 0$) and $I < 0$ (SC with η-pairing, $\Delta_{\vec{Q}} \neq 0$, $\vec{Q}$ is a half of the smallest reciprocal lattice vector) cases [3, 4]. Analogical 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 (for general case of both J^{xy} and J^z nonzero that symmetry is only for VA results). The boundary between M phases with ordering in z-direction and xy-direction is for $|J^{xy}/J^z| = 1$ (within VA). Thus we define $|J| = \mathrm{Max}\{|J^z|, |J^{xy}|\}$ and $|J_0| = z|J|$. In the presence of finite single electron hopping $t \neq 0$ the symmetries are broken in the general case and the effects of $t \neq 0$ have been also discussed in Refs. [11–20]. In the charge-ordered (CO) phase $n_{\vec{Q}} \neq 0$. $n \equiv n_0$ is electron concentration in the system. Notice that phase diagrams obtained are symmetric with respect to $n = 1$ ($\bar{\mu} = 0$, $\bar{\mu} = \mu - U/2 - W_0$, $W_0 = zW$) because of the particle-hole symmetry of the model.

In this paper we particulary focus on the interplay and competition between pair hopping (I) interaction and intersite magnetic (J) or density-density (W) interactions. The impact of on-site term U will not be analyzed, thus we restrict ourselves to $U = 0$ case. Names of transition orders used are consistent with our earlier works [3–8].

II. RESULTS AND DISCUSSION FOR $U = 0$

Let us consider the $U = 0$ case of the model analyzed. In such a case, for $|W|, |J| < |I|$ only the second-order transition SC–NO occurs with increasing temperature T and only the SC phase can be stable in low

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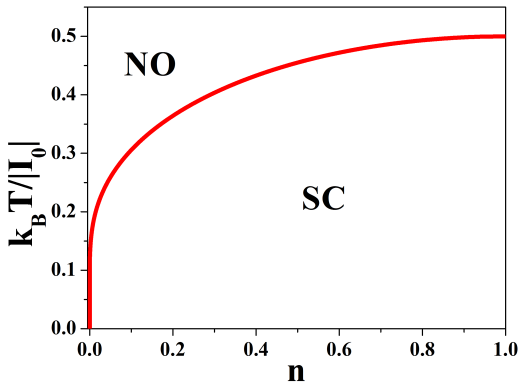

FIG. 1. Phase diagram for $|W|, |J| < |I|$, $U = 0$, $I_0 = zI$.

T. The $k_BT/|I_0|$ vs. n phase diagram of the model is shown in Fig. 1 ($I_0 = zI$). The analytical result for the SC–NO boundary as a function of n can be obtained as $k_BT_{SC}/|I_0| = (n-1)\ln^{-1}(n/(2-n))$ [2, 3] ($n < 1$). The structure of the diagram as a function of μ is the same as of the diagram obtained for $W = 0$ and $J = 0$ [3]. For $W = 0$ and any J, on the SC–NO transition line the relation $\bar{\mu}/I_0 = n - 1$ occurs (generally always in the SC phase), but for $W \neq 0$ the relation $\mu(n)$ is not so simple (cf. Refs. [3, 8, 9, 21–24]).

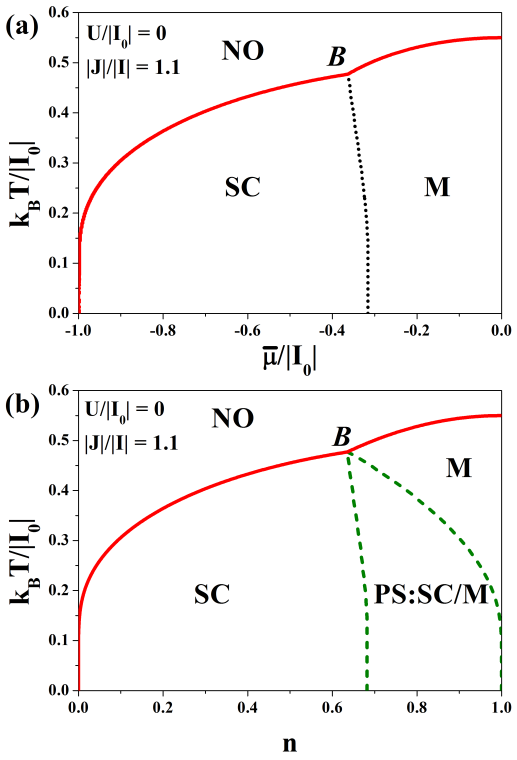

FIG. 2. Phase diagrams for $|J|/|I| = 1.1$ ($U = 0$, $W = 0$, $\bar{\mu} = \mu - U/2$). Details in text.

A. Superconductivity and magnetism

First, let us discuss the competition between I and J interactions. Following discussion of phase diagrams is valid for $|W|/|I| < 1$, but $W \neq 0$ changes the thermodynamical characteristics and the locations of phase boundaries only on diagrams as a function of μ (not as a function of n).

In particular, the phase diagrams for $|J|/|I| = 1.1$ ($W = 0$) are shown in Fig. 2. For that case there are three homogeneous phases (SC, M, NO) on the phase diagrams. The transitions SC–NO and M–NO with increasing temperature are second-order ones and their temperatures decrease with increasing $|\bar{\mu}|$ and $|n-1|$. The analytical equations for temperatures T_{SC} and T_M of these transition, respectively, as a function of n can be derived (in their ranges of occurrence): for T_{SC} it was given above in the beginning of Sec. II, whereas for T_M it is obtained as $k_BT_M/|J_0| = n(2-n)/2$. The SC–M transition is first-order (for fixed μ) and thus the PS:SC/M state is stable in the define range of n. The first-order SC–M as well as the "third-order" SC–PS and PS–M transition temperatures increase with $|\bar{\mu}|$ and $|1-n|$, respectively. All transition lines merge at a bicritical point, denoted as **B** on the diagrams. Notice that the MIX1:SC/M phase (a coexistence of SC and M in homogeneous phase, $\Delta_{\vec{q}}, m^{\alpha}_{\vec{q}} \neq 0$) does not appear on the diagrams at any $T \geq 0$.

For $|J|/|I| = 1$ the SC and M phases are degenerated for $n = 1$ ($\bar{\mu} = 0$), whereas for $n \neq 1$ the SC phase is stable. The case of $n = 1$ for arbitrary $U/|I_0|$ has been analyzed in Ref. [25], whereas the behaviour of the system at $T = 0$ have been investigated in Ref. [9]. With increasing $|J|$, the **B**-point moves along the SC–NO boundary toward larger $|\bar{\mu}|$ ($|1-n|$). The region of the M phase stability is extended, whereas the region of the SC phase occurrence is reduced by increasing the ratio $|J|/|I|$. The location of the **B**-point can be determined from the equation $T_{SC} = T_M$. Moreover, for higher $|J|/|I|$ the structure of the diagram can also change. Exemplarily, for $|J|/|I| \gtrsim 1.34$ the M–NO transition can also be first-order (if it occurs at $k_BT/|J_0| < 1/3$, for fixed μ) [25], the multicritical point changes its type (there can be more than one multicritical point on the diagram), and the PS:M/NO state can also occur (cf. also [26–28]). For $|J|/|I| > 2$ the region of the SC phase occurrence vanishes totally. The detailed analyses of this problem will be explored further in a subsequent publication.

B. Superconductivity and charge orderings

Next, we will discuss the diagrams of the model for $|W|/|I| > 1$ and $|J| < |I|$. The examples of the phase diagrams for $W/|I| = 1.1$ and $|J| < |I|$) are presented in Fig. 3. For the case $W/|I| > 1$ there are three homogeneous phases (SC, CO, NO) on the phase diagrams and the structures of the diagrams are similar to those discussed in previous section. The transitions to the

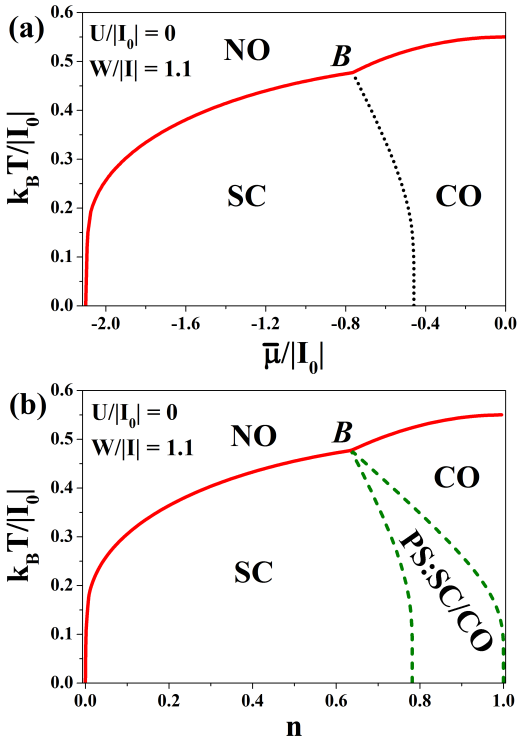

FIG. 3. Phase diagrams for $W/|I| = 1.1$ and $|J|/|I| < 1$ ($U = 0$, $\bar{\mu} = \mu - U/2 - W_0$, $W_0 = zW$). Details in text.

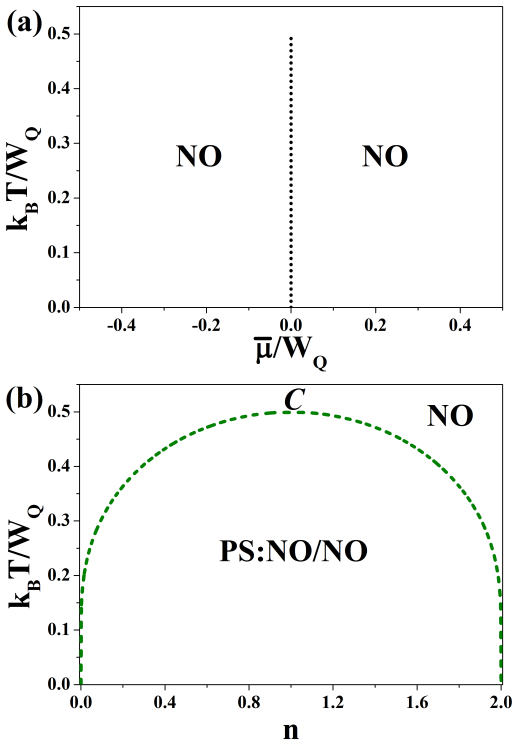

FIG. 4. Phase diagrams for $W/|I| < -1$ and $|J|/|I| < 1$ ($U = 0$, $\bar{\mu} = \mu - U/2 - W_0$, $W_Q = -zW$). Details in text.

NO phase with increasing temperature (i.e. SC–NO, CO–NO) are second-order ones and their temperatures decrease with increasing $|\bar{\mu}|$ and $|n-1|$ [8]. The analytical equations for temperatures T_{SC} and T_{CO} of these transition, respectively, as a function of n can be derived (in their ranges of occurrence): for T_{SC} it was given above in the beginning of Sec. II, whereas for T_{CO} it is obtained as $k_B T_{CO}/W_0 = n(2-n)/2$. The transition between two ordered phases is first-order (for fixed μ) and the PS:SC/CO state is stable in the define range of n. The first-order SC–CO as well as the "third-order" SC–PS and PS–CO transition temperatures increase with $|\bar{\mu}|$ and $|1-n|$, respectively. Similar as in previous case all transitions lines merge at a bicritical point **B**. Moreover, at $T = 0$ the PS:SC/CO state is degenerated with the MIX2:SC/CO phase (a coexistence of SC and CO in homogeneous phase, $\Delta_{\vec{q}}, n_{\vec{Q}} \neq 0$), but at any $T > 0$ that degeneration is removed [8, 9, 29].

With increasing $W > 0$, the **B**-point moves along the SC–NO boundary toward larger $|\bar{\mu}|$ ($|1-n|$). Its location can be determined from the equation $T_{SC} = T_{CO}$. The region of the CO phase stability is extended, whereas the region of the SC phase occurrence is reduced, by increasing the ratio $W/|I|$. For $W = |I|$ there homogeneous phases: SC, CO and MIX2 are degenerated at $n = 1$ [1, 8, 9], but the SC phase has a lowest energy for $n \neq 1$.

For $W/|I| < -1$ only the NO phase and the PS:NO/NO state (in define range of n) are present on phase diagrams. The diagrams for $W/|I| < -1$ are shown in Fig. 4 (cf. also Refs. [8, 9, 24]) and they do not change with decreasing $W < 0$. The first-order NO–NO transition line (vertical one for fixed $\bar{\mu} = 0$) ends at critical point **C** located at $k_B T/W_Q = 0.5$. The analytical result for the PS:NO/NO–NO boundary as a function of n can be obtained as $k_B T_{PS}/W_Q = (n-1)\ln^{-1}(n/(2-n))$ ($W_Q = -zW$, $n < 1$). For $W/|I| = -1$ the SC phase and the NO phases (the PS:NO/NO state) are degenerated for any $\bar{\mu}$ (for any n, respectively).

III. CONCLUSIONS AND FINAL REMARKS

In conclusions, we note that the analysis of the model considered ($U = 0$) shows that the superconductivity can coexists with magnetism (for $|J|/|I| > 1$) and charge orderings (for $W/|I| > 1$) in the states with phase separation (PS:SC/CO and PS:SC/M, respectively) and the mixed homogeneous phases (MIX1, MIX2) do not appear on the phase diagrams at $T > 0$. In particular, we have derived that transitions between the superconducting phase and other ordered phases (the SC–CO and SC–M transitions) are of the first order for fixed chemical potential μ and it leads to the occurrence of the phase separation (PS:SC/CO and PS:SC/M, respectively) in the definite ranges of electron concentration n.

Notice that repulsive $U > 0$ [3, 5] or external magnetic field [4, 6] can change the SC–NO transition into first-order one (for fixed μ) and the phase separation state

PS:SC/NO can occur in the define ranges of n. Moreover, $U < 0$ favors the SC phase, whereas $U > 0$ favors the M phase. The CO phase for $W > 0$ as well as the PS:NO/NO state for $W < 0$ can exist for both signs of U and sufficiently large $|W|/|I|$ (if $U \gg 0$ these states can be stable only for $n \neq 1$), cf. e.g. Refs. [21–24].

In this paper we have not considered the case of $|J| > |I|$ and $|W| > |I|$. The analysis of the interplay between J and W interactions [30–32] is beyond the goal of this work and will be presented elsewhere.

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