

Mixed phase and bound states in the phase diagram of the extended Hubbard model

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The paper examines part of the ground state diagram of the extended Hubbard model, with the on-site attraction $U < 0$ and intersite repulsion $W > 0$ in the presence of charge density waves, superconducting and η -superconducting order parameters. We show the possibility of the stabilization of the mixed state, with all three nonzero order parameters, in the model with nearest neighbor interactions. The other result of the paper is application of the exact solution of the Schrodinger equation for the two-electron bound state, as an additional bound for the phase diagram of the model, resulting in the partial suppression of the superconducting state of the s-wave symmetry, in favor of the normal state phase.

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INTRODUCTION

The Hubbard model is known for its universality. The model and its extensions have been used in research of magnetism, superconductivity and especially high temperature superconductivity (HTS), other various phases in the solid, charge orderings, phase separation etc., in materials like high temperature superconductors, bismuthates, Chevrel phases, amorphous semiconductors, heavy fermion materials, systems with alternating valence to name the few (for a review see, e.g., Ref.[1]). Despite intensive research the results concerning the model come mostly from different approximations or numerical simulations. The exact results are scarce and concern mostly specific situation of one dimension (1D) or specific band fillings or specific limits: zero bandwidth, infinite U or infinite d . We can mention the exact solution in 1D obtained by Bethe ansatz[2], Nagaoka ferromagnetism in repulsive, half-filled systems with one hole[3], flat band ferromagnetism[4], Lieb's ferrimagnetism[5], some bounds on correlation functions[6, 7, 8] and a statement of necessity of bound states for existence of extended s-wave superconductivity in 2D systems with low electron density n , by Randeria[9]. Let's also note that the mean-field BCS equations for superconductivity in the Hubbard model with effective attractive interaction between electrons, in the limit of vanishing electron density turn into Schrodinger equations, which can also be solved exactly[10].

An interesting, unresolved question concerning Hubbard model is: what happens, when we increase the strength of the interaction? What phases do we obtain? Or does the system prefer phase separation? That was the conclusion of the paper by Robaszkiewicz and Pawlowski[11]. By the broken symmetry Hartree-Fock approach they established that the attractive extended Hubbard model (with nearest neighbor – nn – density-density interactions of strength W added) in two dimensions for arbitrary electron density and moderate values of $|W|$ is superconducting in the ground state but becomes phase separated with increasing $|W|$ (except from $n = 1$, where the ground state is in charge density wave phase for any $W \geq 0$). In the case of $W < 0$ they obtained the phase of electron droplets and for $W > 0$ a phase separation between charge density waves (CDW) with $n = 1$ and a singlet on-site superconductivity (SS) (extended s-wave was not considered). The free energy of this phase separated state (PS[CDW/SS]) turned out to be lower than the energy of the homogenous mixed state (M(CDW+SS)). Stabilization of M state required longer than nn repulsive intersite interactions (W_2) or increasing $|U|$. For $U = -\infty$ PS and M states were degenerated even for $W_2 = 0$.

In this paper it will be shown that including η -pairing (superconducting pairing with singlet pairs with center-of-mass momentum π)[12, 13, 14] into the Hamiltonian stabilizes mixed phase, already with intersite interactions W restricted to the nn (in disagreement with Ref.[11]). It turns out that the phase separation PS[CDW/SS] exists only below certain critical value of W , above which the M phase can be stabilized.

LOW DENSITY LIMIT

It can be shown, that in the low density limit the BCS equations go over to the Schrodinger equation for the bound pair[10]. In the center-of mass coordinate system the wave function of the two particle bound state can be expanded as the sum of states with the definite relative momenta. Using that expansion we can obtain a set of self-consistent equations for the pair wave function in a position space, in terms of lattice Green functions[1, 15]. For the hypercubic lattices these equations were solved (see, e.g., [1]) and it has been found out that in one and two dimensions pairs

for $W = 0$ bind for any negative U , while in three dimensions there is critical value for W . In the cited reference the formula was given for the W_{cr} as a function of U :

$$\frac{|W_{cr}|}{2t} = \left[1 + \frac{2D}{U} \right]^{-1} + (C - 1)^{-1} \quad (1)$$

where $C = 1/N \sum_k (1 - \gamma_k/z)^{-1}$ is the Watson integral. In Ref.[1] this formula was given only for the case of $W < 0$ but in fact it is valid for any U and W . What's more, there exists analogic formula, applicable not only in the low density limit but for any electron density. It was derived from the Hamiltonian after Hartree-Fock linearization so it is not exact, but goes over into the exact Eq. (1) for $n \rightarrow 0$. The formula is given by:

$$W_{cr} = \frac{8t^2}{\mu(1-n) + 8tI - 2\mu^2/U}, \quad \text{where} \quad I = \int_{-1}^{\mu} x\rho(x) dx \quad (2)$$

or for the rectangular DOS[16]: $W_{cr}(1 + (n-1)^2(1 + 16t/U)) = -4t$.

PHASE SEPARATION

The energy of a phase separated state, E_{PS} , is calculated according to the formula:

$$E_{PS} = mE_+(n_+) + (1-m)E_-(n_-) \quad (3)$$

where $E_{\pm}(n_{\pm})$ are the values of $\langle H \rangle / N$ of the two separating phases at the $n = n_{\pm}$ corresponding to the lowest energy homogenous solution for a given phase. m and $(1-m)$ are fractions of the system occupied by the phases E_+ and E_- respectively. There is also a similar equation connecting charge densities in the two coexisting phases:

$$mn_+ + (1-m)n_- = n \quad (4)$$

A very useful is also Maxwell construction:

$$\frac{\partial E_-(n_-)}{\partial n_-} = \frac{E_+(n_+) - E_-(n_-)}{n_+ - n_-} \quad (5)$$

which is equivalent to the condition of minimization of E_{PS} respectively n_- with fixed n_+ and /

- let's note that Eq. (3) gives boundaries for E_{PS} . By the definition in Eq. (3), E_{PS} must be somewhere between $E_+(n_+)$ and $E_-(n_-)$. By the same reasoning that led us to the Eq. (7) we can say that the dependence of phase separated states on n should be strictly linear, with the same coefficients as in the Eq. (7). That's nothing else but the Maxwell condition restated
- the same considerations as above apply to the electron density: phase separated state can exist only for charge densities $n_- < n < n_+$. This is an important bound, which can be easily overlooked, as there are formal solutions for free energy of phase separated state also outside that range
- a simple implication of the preceding points, which we will call *Theorem 1*: we can not obtain a phase transition by changing n between two phase separated states having "a state in common" for the same fixed density n_+ , i.e. we can not have phase transition between states like PS1[CDW($n=1$)/phase1] and PS2[CDW($n=1$)/phase2]. The lines depicting F_{PS1} and F_{PS2} will begin in the same point and will extend in different directions.
- and last but not the least is the notion, that we have also bounds for homogenous phases: the phases can exist only for the positive compressibility, i.e. in the range of μ , for which $\partial\mu/\partial n > 0$

THE MODEL

We start from the extended Hubbard model:

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} W \sum_{ij} n_{i\sigma} n_{j\sigma'} - \mu \sum_i n_i \quad (8)$$

in standard notation. We use Hartree-Fock approach. In the mean-field Hamiltonian we retain charge density order parameter Δ_c and singlet superconductivity order parameters: Δ_0 and Δ_Q , for on-site and η -pairing respectively (see also Ref.[11]):

$$H_0 = \sum_{k\sigma} (\varepsilon_k - \bar{\mu}) c_{k\sigma}^\dagger c_{k\sigma} + \frac{1}{2} \sum_{k\sigma} (\Delta_c c_{k\sigma}^\dagger c_{k+Q\sigma} + h.c.) + \sum_k (\Delta_0 c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + h.c.) + \sum_k (\Delta_Q c_{k+Q\uparrow}^\dagger c_{-k\downarrow}^\dagger + h.c.) + C \quad (9)$$

where the order parameters are given by:

$$\Delta_c = \frac{1}{N} \sum_{k\sigma} (-zW + \frac{U}{2}) < c_{k+Q\sigma}^\dagger c_{k\sigma} > \quad (10)$$

$$\Delta_0 = \frac{U}{N} \sum_{k_2} < c_{-k_2\downarrow} c_{k_2\uparrow} > \quad (11)$$

$$\Delta_Q = \frac{U}{N} \sum_{k_2} < c_{k_2\downarrow} c_{-k_2+Q\uparrow} > \quad (12)$$

where z is number of nearest neighbors, $\bar{\mu} = \mu - (\frac{U}{2} + zW)n$, $W_k = W\gamma_k$, $\varepsilon_k = -t\gamma_k$, $\gamma_k = 2 \sum_{\alpha}^d \cos k_{\alpha}$, $\alpha \in (x, y, z)$ and $d = z/2$ is dimensionality of the hypercubic lattice; $\varepsilon_k \in < -\varepsilon_0, \varepsilon_0 >$ where $\varepsilon_0 \equiv D = zt$. In the following all values of dimension energy will be given in units of D and the simplest, zero temperature forms of the equations will be most often used. The constant C takes the form:

$$C = \frac{1}{4} (U + 2Wz)n^2 - \frac{|\Delta_c|^2}{U - 2Wz} - \frac{|\Delta_0|^2}{U} - \frac{|\Delta_Q|^2}{U} \quad (13)$$

After diagonalization we obtain Hamiltonian H_0 with two eigenenergies A_k^{\pm} :

$$A_k^{\pm} = \sqrt{\varepsilon_k^2 + \bar{\mu}^2 + \Delta_0^2 + \Delta_Q^2 + \Delta_c^2 \pm 2\sqrt{\varepsilon_k^2(\bar{\mu}^2 + \Delta_Q^2) + (\bar{\mu}\Delta_c - \Delta_0\Delta_Q)^2}} \quad (14)$$

In terms of the eigenstates of H_0 the free energy is given by the standard formula:

$$F_0 = -\frac{1}{\beta} \ln \text{Tr} \exp(-\beta H_0) + \mu N_e \quad (15)$$

what yields:

$$\frac{F_0}{N} = \bar{\mu}(n-1) + C - \frac{1}{\beta N} \sum_k \ln(4 \cosh \frac{\beta A_k^+}{2} \cosh \frac{\beta A_k^-}{2}) \quad (16)$$

The equations for the order parameters and chemical potential are obtained in a standard way, by minimization of the above expression. For the most general mixed, homogenous phase with all the order parameters present the equations take the form:

$$2(n-1) = \bar{\mu}(I_0 + J_2) + \Delta_c(\bar{\mu}\Delta_c - \Delta_0\Delta_Q)J_0 \quad (17)$$

$$\frac{-4\Delta_Q}{U} = \Delta_Q(I_0 + J_2) - \Delta_0(\bar{\mu}\Delta_c - \Delta_0\Delta_Q)J_0 \quad (18)$$

$$\frac{-4\Delta_0}{U} = \Delta_0I_0 - \Delta_Q(\bar{\mu}\Delta_c - \Delta_0\Delta_Q)J_0 \quad (19)$$

$$\frac{-4\Delta_c}{U - 2Wz} = \Delta_cI_0 + \bar{\mu}(\bar{\mu}\Delta_c - \Delta_0\Delta_Q)J_0 \quad (20)$$

where

$$I_0 = \frac{1}{N} \sum_k \left(\frac{1}{A_k^+} + \frac{1}{A_k^-} \right) \quad (21)$$

$$J_n = \frac{1}{N} \sum_k \left(\frac{1}{A_k^+} - \frac{1}{A_k^-} \right) \frac{\varepsilon_k^n}{\sqrt{\varepsilon_k^2(\bar{\mu}^2 + \Delta_Q^2) + (\bar{\mu}\Delta_c - \Delta_0\Delta_Q)^2}} \quad (22)$$

where A_k^\pm are given by Eq. (14). The equations for the mixed phases with smaller number of constituent phases (i.e., M(CDW+SS), M(CDW+SQ), M(SS+SQ)) as well as for pure phases can be obtained from Eqs. (17)-(22) by just dropping out respective order parameters. For the detailed form of the pure phase equations the reader is referred, e.g. to Ref.[11, 17].

RESULTS

The results were obtained using rectangular density of states (DOS) and $z = 4$ as an approximation for two dimensional square lattice. In Figs 1 (a) and (b) we plotted the results for the thermodynamical potentials. In (a) we have shown all the solutions for Gibbs energy (vs chemical potential), without applying yet the bounds for $n \pm$ or checking the sign of $\partial\mu/\partial n$. All homogenous phases are shown, except from η -pairing (denoted by SQ) and mixed M(SS+SQ) (SS denoting singlet, on-site superconductivity), which do not have solutions for $U > -2$. Nevertheless the phases: M(CDW+SQ), M(CDW+SS), upper branch of M(CDW+SS+SQ) (see lower inset) and upper branch of CDW for $n \neq 1$ must be excluded, because of the negative compressibility, connected with the downward curvature of these lines (compare also the upper inset - decreasing and increasing part of the plot corresponds to the opposite signs of compressibility and to the two branches of M(CDW+SS+SQ), from now on denoted as M3, in the main figure).

The remaining curves (and CDW one, for comparison) are a basis for plotting the free energy F - n diagram, shown in (b). The plot contains curves in the proper range of n , with all the bounds already applied. Apart from all the homogenous phases fulfilling the condition $\partial\mu/\partial n > 0$ (what corresponds to the downward curvature for $F(n)$) we can see also phase separated states indicated in (a) by Gibbs energy plots crossings: PS[CDW/SS], PS[CDW/NO], PS[M3/SS] (and PS[NO/NO], of slightly different nature). The states phase separated with CDW($n=1$) are connecting the point of energy E

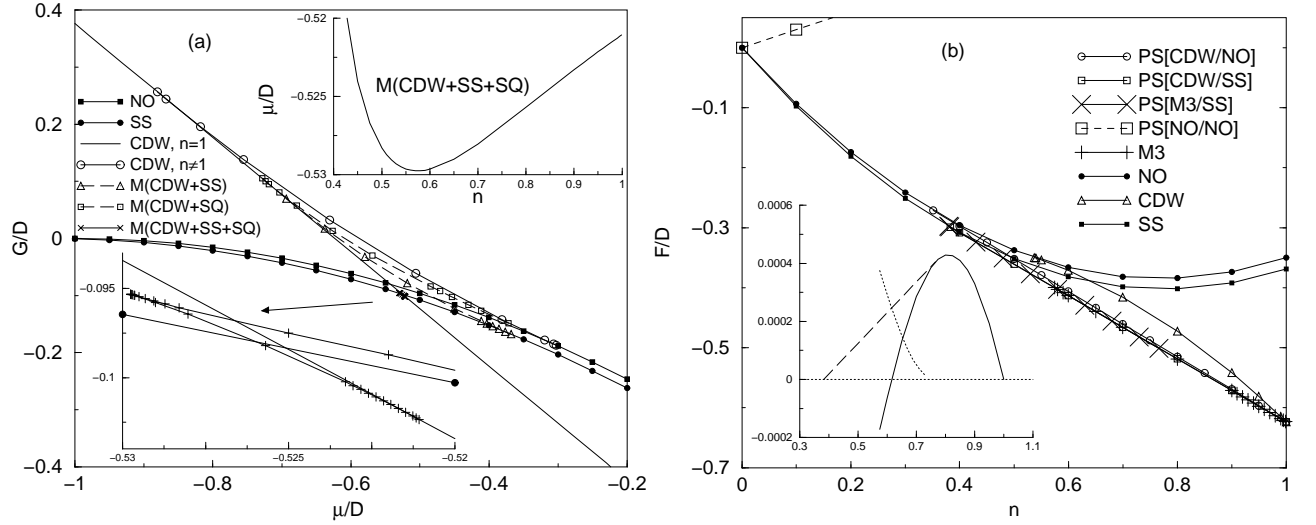


FIG. 1: (a) Gibbs energies G vs bare chemical potential μ , for $U = -1$ and $W = 0.2$. Lines are described in the figure. In the lower, left-hand corner in the inset, there is an enlargement of the area where the curves cross. In the inset in the upper right-hand corner there is plotted the dependence of chemical potential μ on charge density n in M3 phase. (b) The free energy F vs electron density n for $U = -1$ and $W = 0.2$. Lines are described in the figure. In the inset there are the differences of free energies plotted – full line: $F(\text{PS}[\text{CDW}/\text{SS}]) - F(\text{M3})$, dashed line: $F(\text{PS}[\text{CDW}/\text{SS}]) - F(\text{PS}[\text{M3}/\text{SS}])$, dotted line: $F(\text{M3}) - F(\text{PS}[\text{M3}/\text{SS}])$ for the range of n , where $\partial\mu/\partial n > 0$ for each phase. Horizontal dotted line is the just a guide for an eye.

is stabilized. Appearing of the M3 phase is connected with replacing PS[CDW/SS] by PS[M3/SS] phase, what is required by the Maxwell construction (see Eq. (5) and *Theorem 1*). With increasing $|U|$ the threshold and the extent of PS[CDW/SS] phase are decreased and, for large enough $|U|$, the M3 phase is stabilized for all $W > 0$ at $n = 1$, as shown in Fig. (2b). The area of PS[CDW/SS] disappears at all, in favor of mixed phase.

In both Figs (2a) and (2b) there is also a line "cutting off" the upper right-hand corner. This is the boundary for existence of bound pairs of extended s-wave symmetry, given by Eq. (2). In view of Randeria's notion[9], about necessity of such pairs for existence of superconductivity of this symmetry it can be used as an additional bound for the phase diagram[16]. Above these lines no superconductivity can survive so the NO phase enters diagram (to be

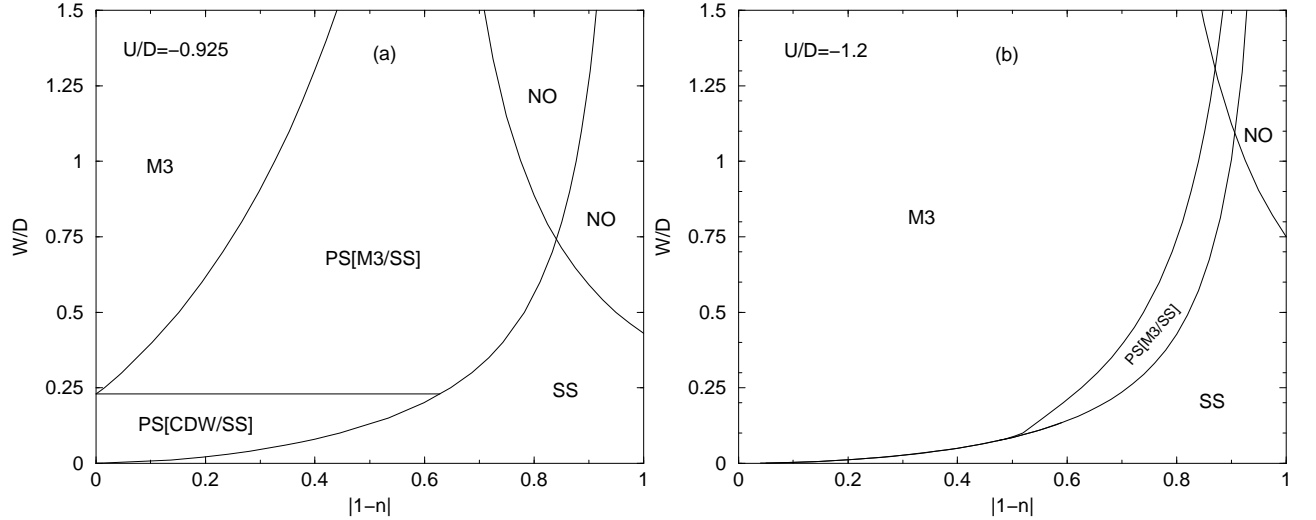


FIG. 2: Ground state phase diagram of model Eq. (9) calculated for the rectangular density of states for (a) $U = -0.925$ and (b) $U = -1.2$. For the $n = 1$ the ground state is CDW phase, a smooth limit of both $M(\text{CDW}+\text{SS}+\text{SQ})$ and PS[CDW/SS] phases.

sure of that we must consult again the free energy diagrams). Let's note, that it is only an approximation, as we did not calculate extended s-wave superconductivity but only on-site, pure s. Preliminary results show nevertheless that the parameter of extended superconductivity Δ_γ is two orders of magnitude smaller than Δ_0 along the boundary PS/SS state. Also η -pairing can have extended component, which will be stabilized by $W > 0$, due to negative sign at the extended part of the pairing potential, unlike the case of extended s-wave superconductivity with $Q = 0$. This fact will still enhance the main tendency outlined in this paper.

Inclusion of the normal Fock parameter into the calculations will bring about the increase of the bandwidth, thus effectively pushing the system into weak-coupling limit. It can cause the increasing of thresholds but should not change qualitatively the main results of this paper.

CONCLUSIONS

In the paper a phase diagram of the extended Hubbard model with attractive on-site and repulsive, nn, intersite interactions was analyzed in the Hartree-Fock approximation. A possibility of stabilizing the mixed phase in the model with short range, nn interactions only, was shown. Stabilization requires the existence of the three orderings: superconductivity, η -superconductivity and charge density waves. The extent of the mixed phase increases with increasing $|U|$.

The other result of the paper comes from the solution of the Schrodinger equation for bound pairs of extended s-wave symmetry. The area of the normal phase is introduced into the phase diagram due to this criterion.

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