LETTER

Phase separation in fermionic systems with particle–hole asymmetry

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Abstract. We determine the ground-state phase diagram of a Hubbard Hamiltonian with correlated hopping, which is asymmetric under particle–hole transform. By lowering the repulsive Coulomb interaction $U$ at appropriate filling and interaction parameters, the ground state separates into hole and electron conducting phases: two different wavevectors characterize the system and charge–charge correlations become incommensurate. By further decreasing $U$ another transition occurs at which the hole conducting region becomes insulating, and conventional phase separation takes place. Finally, for negative $U$ the whole system eventually becomes a paired insulator. It is speculated that such behavior could be at the origin of the incommensurate superconducting phase recently discovered in the 1D Hirsch model. The exact phase boundaries are calculated in one dimension.

Keywords: solvable lattice models, phase diagrams (theory), Hubbard and related models (theory)

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One very debated issue in the context of correlated fermionic materials is the occurrence of phase separation (PS). For instance, in ultracold fermionic atoms trapped on optical lattices PS appears when the superfluid phase coexists with the normal phase [1, 2]; these systems may be investigated by means of the negative \( U \) Hubbard model [3]. Also, in high-\( T_c \) materials PS leads to the formation of one-dimensional stripes [4]. It is believed that the phenomenon could be a consequence of the interplay between antiferromagnetic order and hole propagation; as such, its appearance is investigated within the context of the \( t-J \) model [5]–[8], which describes the Hubbard model in the limit of strong repulsive Coulomb interaction. In the present letter we suggest a further scenario for the occurrence of PS in Hubbard-like systems, resulting from competition between conducting phases with different charge: in the hole-rich region the carriers are the electrons, while in the pair-rich region they eventually become the holes. In the absence of particle–hole symmetry, the proposed mechanism can generate incommensurability. The mechanism is proven to survive in dimensions greater than 1 for a simple case.

We study the bond-charge extended Hubbard Hamiltonian, which has been introduced to describe compounds containing extended orbitals [9]. It comes from assuming that the charge in the bond affects the effective potential acting on valence electrons; the extension of the Wannier orbitals and the hopping between them should vary with the charge. A generalization of that Hamiltonian is the \( U - X - X' \) Hamiltonian introduced in [10]. In the grand-canonical ensemble it is

\[
H_{BC} = - \sum_{\sigma=\uparrow,\downarrow,\langle ij \rangle} \left[ 1 - x(n_{i-\sigma} + n_{j-\sigma}) + x' n_{i-\sigma} n_{j-\sigma} \right] (c_{i\sigma}^\dagger c_{j\sigma} + H.c.) + u \sum_i n_i \uparrow n_i \downarrow - \mu \left( \sum_{i\sigma} n_{i\sigma} - N \right),
\]

where the lower case symbols denote that the coefficients of the interactions have been normalized in units of the hopping amplitude and the three-body interaction term \( x' \) appears as an effective interaction from the three band-model. Moreover \( N \) is the number of electrons on the \( D \)-dimensional \( L \)-site lattice \( \Lambda_D \). The model belongs to the class of Hubbard Hamiltonians with correlated hopping, which contains some integrable cases that have been widely studied in recent years (see [11] and references therein).

\( H_{BC} \) is, in general, not invariant under particle–hole transform. For this reason the model has been first proposed (for \( x' = 0 \)) in two dimensions, motivated by a theory of hole superconductivity [12]. It was investigated by means of a bosonization approach in [13] at half-filling for arbitrary (and weak) \( x \) and \( x' \). Also, a particle–hole invariant subcase of \( H_{BC} \), which takes place at \( x' = 2x \), has been previously discussed [14].

Recently, it has been proven [15, 16] that in 1D at half-filling \( H_{BC} \) displays a rich phase diagram already at \( x' = 0 \), quite different from that of the Hubbard model, and from that derived in the weak coupling limit [13]. In particular, at sufficiently low \( u > 0 \), and for an appropriate range of \( x \) values an unexpected incommensurate superconducting (ICSS) phase appears, which drives the usual transition to an insulating state to higher values of \( u \). Here we investigate the origin of such a phase by constructing the exact ground-state phase diagram of a particular subcase of (1) still asymmetric under particle–hole transform.

The Hamiltonian (1) can be written in terms of the Hubbard projectors, \( X_{\alpha\beta}^{\alpha\beta} = |\alpha\rangle_i \langle \beta| \); here, \( |\alpha\rangle_i \) are the states allowed at a given site \( i \), \( \alpha = 0, \uparrow, \downarrow, 2 \) (\(|2\rangle \equiv |\uparrow \downarrow\rangle\)).

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Phase separation in fermionic systems with particle–hole asymmetry

Figure 1. Phase diagram in the $u-t_x$ plane in $D=1$: the transition to the $U\infty$ region depends on the filling $n$, whereas the other transitions are independent of it. CPS and IPS denote the conventional and the incommensurate phase separation regions, respectively; PI stands for paired insulator. Full dots indicate the tricritical points.

Inserting the choice $x=1$ in $H_{BC}$, the resulting Hamiltonian $H \equiv H_{BC}(x=1)$ turns out to preserve the number of doubly occupied states $N_d = \langle \hat{N}_d \rangle = \langle \sum_j X_{j}^{22} \rangle$: $[H, \hat{N}_d] = 0$ for arbitrary $x'$, $D$ and $N$. In the following, we shall adopt such a choice. $H$ can then be written as

$$H = H_{01} + H_{12} - \mu(L - N),$$

where

$$H_{01} = - \sum_{\langle i,j \rangle} (X_i^{\sigma_0} X_j^{0\sigma} + \text{h.c.}) + \mu \sum_i X_i^{00}, \quad (2)$$

$$H_{12} = -t_x \sum_{\langle i,j \rangle} (X_i^{2\sigma} X_j^{2\sigma} + \text{h.c.}) + (U - \mu) \sum_i X_i^{22}, \quad (3)$$

with $t_x = 1 - x'$. We shall limit our analysis to the range $0 \leq t_x \leq 1$. By implementing the transformation $c_{i,\sigma} \to c_{i,\sigma}^\dagger$, it can be realized that the range is representative of the behavior of the model at any $t_x$ value. In the two limits $t_x = 0 (x' = 1)$ and $t_x = 1 (x' = 0)$ the Hamiltonian reduces to known cases, namely the infinite $U$ Hubbard model and the bond-charge Hubbard model at $x = 1$ [17], both integrable in one dimension.

On general grounds, we expect that, at large enough positive $u$, the ground state would contain the minimum number of doubly occupied sites. Hence it will coincide with that of the infinite $U$ Hubbard model (no doubly occupied sites) for $N \leq L$, and with its particle–hole counterpart for $N \geq L$. In figure 1 such a state is denoted as $U\infty$. Also, for large enough negative $u$, the number of doubly occupied sites will be maximized, so that for an even number of electrons the hopping term will be ineffective and the ground state would be a highly degenerate insulator consisting of $N/2$ pairs of electrons. In figure 1 this is denoted as PI (paired insulator). In order to investigate what happens between these two limits, let us think of the Hilbert space as factorized into three orthogonal subspaces:

$$\mathcal{H} = \mathcal{H}_{01} \oplus \mathcal{H}_{12} \oplus \mathcal{H}_\perp; \quad (4)$$

states with no doubly occupied sites belong to $\mathcal{H}_{01}$, states with no empty sites live in $\mathcal{H}_{12}$ and the remaining states stay in $\mathcal{H}_\perp$. $H_{10}$ does not act on doubly occupied sites present...
Phase separation in fermionic systems with particle–hole asymmetry

in $\mathcal{H}_\perp$ and annihilates states belonging to $\mathcal{H}_{12}$; hence, at given $N_d$ and $N$, it reaches its minimum in $\mathcal{H}_{01}$. Analogously, $H_{12}$ does not act on empty sites present in $\mathcal{H}_\perp$ and annihilates states in $\mathcal{H}_{01}$, hence reaching its minimum in $\mathcal{H}_{12}$. So that, at any given $N$ and $N_d$, the absolute minima of both $H_{10}$ and $H_{12}$ (and consequently of $H$) are reached in the space orthogonal to $\mathcal{H}_\perp$. We can then rewrite the ground-state energy $E_{gs}$ in the form

$$E_{gs} = \min_{|\psi\rangle \in \mathcal{H}} \langle \psi | H | \psi \rangle = \min_{|\psi\rangle \in \mathcal{H}_{01} \oplus \mathcal{H}_{12}} \langle \psi | H | \psi \rangle,$$

(5)

where the minimum has to be taken with respect to $N_d$, the constraint $L - N = N_e - N_d$ is implemented through the chemical potential and $N_e = \sum_i n_i^0$ is the (conserved) number of empty sites. More explicitly, one could look for a ground state of the form

$$|\psi(N_e, N_d)\rangle_{gs} = a|\psi_{01}(N_e')\rangle + \sqrt{1 - a^2}|\psi_{12}(N_d')\rangle,$$

(6)

where $a$ is a further variational parameter, and $N_e = a^2 N_e'$ and $N_d = (1 - a^2) N_d'$. Here $|\psi_{01}(N_e')\rangle \in \mathcal{H}_{01}$ and $|\psi_{12}(N_d')\rangle \in \mathcal{H}_{12}$ are the ground states of $H_{01}$ at given $N_e'$ and $H_{12}$ at given $N_d'$, respectively. The corresponding energies are recovered from those of the infinite $U$ Hubbard model, $E_{gs}^{\infty}$. In fact, the spectra of $H_{01}$ and $H_{12}$ are the same: up to a multiplicative factor $t_x$, and to the conserved quantities $N_e, N_d$, they coincide with the spectrum of the infinite $U$ Hubbard model. Explicitly

$$E_{gs} = a^2 E_{gs}^{\infty}(N_e') + (1 - a^2) [t_x E_{gs}^{\infty}(N_d') + a N_d'] - \mu (N_d - N_e + L - N).$$

(7)

By minimization of $E_{gs}$ with respect to $\mu$ one obtains that the actual value of $a^2$ is given by

$$a^2 = \frac{L - N + N_d'}{N_e' + N_d'}.$$  

(8)

The case $a^2 = 1$ ($a^2 = 0$) corresponds to the $U\infty$ phase described above for $N \leq L$ ($N \geq L$), with $N_e' = L - N$ ($N_d' = N - L$). Apart from these limits, the system is always separated into two phases, characterized by $N_e', N_d'$, and $\mu$ values which minimize $E_{gs}$ as given by (7), at given $t_x$ and $u$. Such values do not depend on the actual filling $N$: $\mu$ implies that the chemical potential is constant with the filling.

Since $t_x \leq 1$, independently of the actual value of $E_{gs}^{\infty}$ (and $D$), one could expect three different behaviors to emerge from the minimization equations within the PS phase, depending on the filling and the interaction parameters.

(i) $N_e' < N_d' < L$: both the coexisting phases are conducting. They are characterized by different Fermi momenta $k_F^{(e)}$ and $k_F^{(d)}$, which can be inferred from those of the corresponding infinite $U$ model, and are, in general, not commensurate between each other. For this reason we characterized the phase as IPS, incommensurate phase separation. Later on we shall discuss how such incommensurability reflects on some physical feature.

(ii) $N_e' < N_d' = L$: only the hole-rich region is conducting, whereas the other phase is a paired insulator. The system is characterized by the Fermi momentum $k_F^{(e)}$ of the conducting electrons, i.e. that of the infinite $U$ Hubbard model at a filling $L - N_e' < N$.

We denote such a phase as CPS (conventional phase separation).
(iii) $N_e' = N_d' = L$: both phases are insulating. In this case we are in one of the infinitely many (in the thermodynamic limit) degenerate ground states characterizing the PI phase.

A further interesting limiting case, not discussed above though contained in the minimization equations, occurs when $N_e' = N_d' \neq L$. In such a case both phases are conducting as in (i), but they are characterized by the same Fermi momentum, $k^{(e)}_F = k^{(d)}_F$. This is the case for $t_x = 1$. The latter is the already mentioned bond-charge Hubbard model at $x = 1$ [17] and manifests particle–hole invariance. This example illustrates how in our scheme the IPS phase, intended as the appearance of two not commensurate modulations, is in fact associated with the presence of particle–hole asymmetry.

In order to make the above predictions more quantitative, we now turn to the discussion of the 1D case. In that case the ground-state energy per site of the infinite $u$ Hubbard model is known exactly. In the thermodynamic limit it is

$$E_{gs}^{\infty}(n) \frac{L}{L} = -\frac{2}{\pi} \sin(\pi n), \quad (9)$$

with $n$ average per-site filling, $n \equiv (N/L)$.

When inserted into $E_{gs}/L$, as given by (7), the above information allows for an explicit derivation of the ground-state phase diagram, shown in figure 1. This is achieved by solving the minimization equations with respect to $n_e'(L/N')$ and $n_d'(L/N')$, which in turn fix $k^{(e)}_F = \pi(1 - n_e')$ and $k^{(d)}_F = \pi(1 - n_d')$.

Interestingly, the same phase diagram and ground-state energy can also be obtained by generalizing the approach developed in [18] for studying PS in the extended Hubbard model for $V \to \infty$, with $V$ neighboring sites diagonal Coulomb interaction. At a given filling, the ground state can be thought of as an island of $N_d + Z$ singly and doubly occupied sites inserted into a chain of $L - N_d - Z$ singly and empty sites. Such a choice allows us to maximize the number of available low energy momenta. In the thermodynamic limit, minimizing the energy of that state with respect to $N_d$ and $Z$ gives precisely the same phase diagram obtained here in figure 1. It turns out that the following relations hold:

$$n_e' = \frac{1}{\pi} \arccos \left( \frac{\mu}{2} \right), \quad n_d' = \begin{cases} \frac{1}{\pi} \arccos \left( \frac{u - \mu}{2t_x} \right) & \text{IPS} \\ 1 & \text{CPS} \end{cases} \quad (10)$$

The solutions $n_e' = 1 - n (a^2 = 1)$ below half-filling, and $n_d' = 1 (a^2 = 0)$ above half-filling, are obtained for $u > u_c(n, t_x)$ (see below). These identify the U$$\infty$ phase. In particular, at $n = 1$ a charge gap $\Delta_c$ opens and the phase becomes insulating: for $u \geq u_c(1, t_x) = 2(t_x + 1), \Delta_c = u - u_c$.

For $a^2 \neq 0, 1$ the solution to the minimization equation is

$$n_e' = \frac{1}{\pi} \arccos \left( \frac{\mu}{2} \right), \quad n_d' = \begin{cases} \frac{1}{\pi} \arccos \left( \frac{u - \mu}{2t_x} \right) & \text{IPS} \\ 1 & \text{CPS} \end{cases} \quad (10)$$

Minimizing $E_{gs}$ is thus reduced to solving the following transcendental equation in $\mu$:

$$\mu = \frac{1}{n_e' + n_d'} (-2t_x \sin \pi n_d' + un_d' + 2 \sin \pi n_e'), \quad (11)$$

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with \( n_e' \) and \( n_d' \) as specified in (10). Let us denote the solution by \( \tilde{\mu}(u, t_x) \). The actual value of \( \tilde{\mu}_1 \) in the IPS phases is limited by the constraint

\[
\tilde{\mu}_1 \in \max(-2, u - 2t_x), \min(2, u + 2t_x), \tag{12}
\]

whereas in the CPS phase \( \mu \) becomes independent of \( t_x \) and \( \tilde{\mu}_C(u) \) is the solution of (11) for \( n_d' = 1 \). In fact, all the transition curves can be characterized by the value of \( \tilde{\mu} \) along them:

1. \( U \infty \rightarrow \text{IPS, CPS} \)

\[
\tilde{\mu}(u, t_x) = \begin{cases} 
-2\cos(\pi n) & n \leq 1 \\
\; u + 2t_x\cos(\pi n) & n \geq 1.
\end{cases} \tag{13}
\]

2. IPS \( \rightarrow \text{CPS} \), \( \tilde{\mu}_1 = \tilde{\mu}_C \); the transition occurs at \( \tilde{t}_x = [\tilde{\mu}_C(u) - u]/2 \), implying \( n_d' = 1 \).

3. finally at CPS \( \rightarrow \text{PI} \), \( \tilde{\mu}_C = -2 \).

When passing from \( \mu \) to \( n \), one realizes that only the two transitions 1 do depend on the filling, whereas the others are independent of it. At transition 1 the explicit value of \( u_e(n, t_x) \) is obtained by solving equation (13) for \( u \). Transition 2 takes place at \( t_x = \tilde{t}_x \); transition 3 occurs at \( u = -4 \). As an example, we report the critical curves in figure 1 in the \((u, t_x)\) plane at two different filling values. For \( u \leq 2 \), depending on \( n \), two tricritical point (T1) are recognized, characterized by the merging of \( U\infty \), IPS and CPS phases: one (not shown) occurs at \( n = 2 \), whereas the other one occurs at the same \( u \) value and at a filling \( n_{T1} \leq 1 \). Analytical calculations show that \( u_{T1} = -2(\cos[\pi n_{T1}] + t_x) \), \( n_{T1} \approx (1/\pi)\arccos[(3t_x - 1)/(1 + t_x)] \). Increasing \( t_x \) progressively drives the system to a particle–hole symmetric diagram. For \( t_x = 1 \) \( n_{T1} = 0 \), which is the particle–hole counterpart of the tricritical point in \( n = 2 \). The critical curves in the \((u, n)\) plane (not shown) highlight that particle–hole asymmetry \( (t_x \neq 1) \) favors the IPS phase at filling greater than half, in which case it survives at appropriate positive \( u \) values up to \( n = 2 \). Figure 1 also shows that the infinite \( U \) Hubbard model \( (t_x = 0) \) exhibits CPS for \( u \leq 2 \) if doubly occupied sites are allowed.

In order to clarify the meaning of the different modulations in the IPS phase, we also give in figure 2 the charge–charge correlations \( C(r) = \langle (n_i - n)(n_{i+r} - n) \rangle \) at half-filling (upper part), and their Fourier transform \( N(q) = \sum_r e^{iq}C(r) \) (lower part). Since \( C(r) \) can be evaluated exactly (see, for instance, [19]), we can also provide an analytic expression for \( N(q) \), which is

\[
N(q) = C(0) + (\delta(q) - 1) d_{PS} - a^2\gamma_{k_F}(q) - (1 - a^2)\gamma_{k_F}(q). \tag{14}
\]

Here \( \delta(q) \) is the Dirac delta and \( d_{PS} = (1 - n + n_e')(n - 1 + n_d') \) is the constant responsible for the divergent contribution in \( q = 0 \) characteristic of phase separation: at given \((u, t_x)\) it becomes zero for \( n < n_i \equiv 1 - n_e', \) or \( n > n_h \equiv 1 + n_d' \). Moreover

\[
\gamma_k(q) = \frac{1}{4\pi^2} R[L_2(e^{i(q+2k)}) + L_2(e^{-i(q-2k)}) - 2L_2(e^{iq})], \tag{15}
\]

with \( k = k_F^{(e)}, k_F^{(d)} \) and \( L_2(z) \), denoting the dilogarithm of \( z \) (\( R[\cdot] \) being the real part of \([\cdot] \)), describes the \( q \) dependence of density correlations. Equations (14) and (15) show how in the IPS phase two wavevectors do characterize \( N(q) \), namely \( q^{(e)} = 2k_F^{(e)} \) and \( q^{(d)} = 2k_F^{(d)} \) respectively, where \( k_F^{(e)} \) is the Fermi wavevector for electrons.
Phase separation in fermionic systems with particle–hole asymmetry

Figure 2. (a) Equal-time density correlations $C(r)$ versus distance $r$ at $u = 1$ and $t_x = 0.6$; the dashed line represents the slope $1/r^2$. (b) $N(q) - d_{PS}$ at $t_x = 0.3$, $u = 0$ and three different fillings: from top to bottom $n = 0.5$ (blue), $n = 1$ (pink), $n = 1.7$ (violet).

$q^{(d)} = 2k_F^{(d)}$, as shown in the lower part of figure 2, whereas in the CPS phase, since $k_F^{(d)} = 0$ and $\gamma_0(q) = 0$, only one feature characterizes $N(q)$, namely the wavevector of the single fermion problem corresponding to a filling $n = 1 - n'_e$. It can be recognized that the above type of ground-state phase diagram could explain different features displayed by the non-integrable 1D Hirsch model discussed in [16]. At variance with the present model, in that case the model still had arbitrary $t_x$ ($t_x = 2x - 1$) but also $x' = 0$, implying the appearance of a further term in the Hamiltonian. The numerical solution did show incommensurate charge–charge correlations (and superconductivity) at appropriate values of $u$ and $t_x$, always missing particle–hole invariance. Also, by suitably varying $u$ and $t_x$ at half-filling, the system could first pass from an insulating phase, characterized by flat density correlations, to a conducting phase in which those correlations acquire a modulation; then to the ICSS phase in which further modulations occur. We suggest that the two latter phases could be identified with our CPS and IPS phases, respectively. As an example, in figure 2 we report $C(r)$ at $u$ and $t_x$ values identical with those used for the Hirsch model in figure 3 of [16]. The resemblance of the two figures is convincing.

In this letter, we have shown how the appearance of incommensurate characteristic wavevectors in strongly interacting fermionic systems could be related to the occurrence of phase separation, in the case the system is not symmetric under particle–hole transform. Recently the occurrence of incommensurate modulations in charge correlations was observed also in a Hubbard-like model including next-nearest-neighbor hopping [20]. Since that model is particle–hole asymmetric, we suggest that IPS could occur in that case.

The mechanism could also be a natural candidate for explaining PS in unbalanced mixtures of cold fermionic atoms [1,2]. In this case the PI phase should be interpreted...
as the (unpolarized) superfluid phase and the CPS phase should be identified with the coexistence of the superfluid with the (polarized) Fermi gas.

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