Phase diagram of harmonically confined one-dimensional fermions with attractive and repulsive interactions

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We construct the complete \( U-\mu \) phase diagram for harmonically confined fermionic atoms with repulsive and attractive interactions. (\( \mu \) is the chemical potential and \( U \) the interaction strength.) Our approach is based on density-functional theory, and employs analytical expressions for the kinetic and correlation energy functionals. For repulsive interactions our calculations confirm previous numerical studies, and complement these by closed expressions for all phase boundaries and characteristic lines of the phase diagram, and by providing an explanation and solution for difficulties encountered in earlier density-functional work on the same system. For attractive interactions we propose a new and accurate interpolation for the correlation energy, and use it to extend the phase diagram to \( U < 0 \).

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The field of strongly correlated low-dimensional fermions has a long history and multifarious applications in condensed-matter physics. More recent experimental progress in the field of confined ultracold atoms \[1, 2, 3, 4\] has further widened the scope of this already very rich field by introducing, e.g., an unprecedented degree of control over the confining potential, and the possibility to continuously tune the particle-particle interaction from repulsive to attractive — which is not easy for cold atoms, but unachievable for electrons. After much progress on bosonic atoms and their condensation, more recently fermionic atoms have come under intense study.

In the present paper we focus on one particular model for optically confined fermionic atoms, the one-dimensional Hubbard model. The parameters characterizing this model and spanning its phase diagram are the on-site interaction \( U \) \[5\] and the filling factor \( n = N/L \), where \( N \) is the number of particles and \( L \) the number of lattice sites. For systems in which \( n \) is spatially varying, such as in the presence of a confining potential, it is more useful to specify the chemical potential \( \mu \) instead, which is a constant throughout the system. Hence, we are interested in the phase diagram of the one-dimensional Hubbard model in \( U-\mu \) space. Our aim is to map out this phase diagram, identify the physics governing each possible phase, and to provide analytical expressions for all phase boundaries.

The \( U > 0 \), i.e., repulsive, part of this phase diagram has recently been studied also by Liu et al. \[6\], who used a half-numerical half-analytical local-density approximation (LDA). Rigol et al. \[7\] obtained essentially the same \( U > 0 \) phase diagram from fully numerical Quantum Monte Carlo simulations. An interesting feature that emerged in these works is the appearance of mixed Mott-insulator Luttinger-liquid phases, characterized by spatially separated incompressible and compressible regions in the optical trap, and plateaus in the density profiles coinciding with the incompressible regions. Xinlong et al. \[8\] have recently studied the case of negative \( U \), i.e., attractive interactions, where the physics is dominated by Luther-Emery-type pairing correlations and the spontaneous formation of atomic density waves. However, the Kohn-Sham-type density-functional calculations of Ref. \[8\] do not allow one to map out the entire phase diagram, because the self-consistency cycle does not converge in the mixed metal-insulator phases at \( U > 0 \).

In the present paper we use an analytical local-density approximation both for the kinetic energy (in the spirit of Thomas-Fermi theory) and for the correlation energy (in the spirit of the Bethe-Ansatz LDA proposed in Ref. \[9\]) to obtain the \( U-\mu \) phase diagram. For repulsive interactions our results coincide with those obtained numerically in Refs. \[3, 4\]. However, as our approach is entirely analytical, we obtain closed expressions for the various phase boundaries, which previously had to be extracted numerically. Moreover, our present work also covers the case of attractive interactions, \( U < 0 \), thus mapping out the entire physically relevant phase diagram.

To make our paper self-contained we start by briefly describing and comparing the various approximation schemes employed. Density-functional theory (DFT) \[10, 11\] shows that the total energy of a many-body system in an arbitrary potential can be written

\[
E[n] = T_s[n] + \frac{1}{\beta} \sum_{i=1}^{N} V(n_i) + E_{xc}[n],
\]

where \( T_s \) is the kinetic energy of noninteracting particles, \( E_H \) is the Hartree energy (i.e., the mean-field approximation to the interaction energy), \( V \) is the potential energy (arising from the spatial distribution of the nuclei in solid-state and molecular applications of DFT, and from the optical confining potential for atoms in optical traps), and \( E_{xc} \) is the exchange-correlation energy \[12\]. The local-density approximation to any energy component \( F \) is defined by \( F^{LDA} = \int df(n)_{n \rightarrow n(\tau)} \) in the con-
tinum, and \( F_{\text{LDA}} = \sum_i f(n)|\rightarrow n_i \) on a lattice, where \( f \) denotes the per-volume or per-site value of \( F \) in a spatially uniform (homogeneous) system.

Although DFT is mostly applied to \textit{ab initio} electronic-structure calculations in solid-state physics and quantum chemistry [11, 12], its formal framework is sufficiently general to permit application also to wide classes of model Hamiltonians [13, 14], and, in particular, to the Hubbard model [2] 14, 15. A Bethe-Ansatz based LDA functional for the correlation energy of the one-dimensional Hubbard model was proposed in [6] and applied to Mott insulating phases [16] and superlattice structures [17]. These works employed a parametrization of the per-site ground-state energy of the spatially uniform Hubbard model, \( e(n, U) \), which was constructed [6] to recover exactly known results at \( U = 0 \), \( U \rightarrow \infty \) and \( n = 1 \), and to be close to data obtained from numerical solution of the Bethe-Ansatz (BA) [18] equations inbetween [19]. For \( 0 \leq n \leq 1 \)

\[
e(n, U) = -\frac{2\beta(U)}{\pi} \sin \left( \frac{\pi n}{\beta(U)} \right)
\]

and for \( 1 \leq n \leq 2 \)

\[
e(n, U) = (n - 1)U - \frac{2\beta(U)}{\pi} \sin \left( \frac{\pi(2 - n)}{\beta(U)} \right)
\]

Here \( \beta(U) \) is obtained from

\[
-\frac{\beta}{\pi} \sin \left( \frac{\pi}{\beta} \right) = -2 \int_0^\infty \frac{J_0(x)J_1(x)}{x(1 + e^{U/x^2})} dx =: -2I(U),
\]

and \( J_m \) is the \( m \)’th order Bessel function. The difference between the \( n < 1 \) and the \( n > 1 \) branch is responsible for a derivative discontinuity of \( E_c \) and the opening of a Mott gap at \( n = 1 \) [16, 18].

To perform analytical calculations for attractive interactions, our first task is to extend this construction to \( U < 0 \). The construction of a parametrization of the per-site energy is not unique, but a convenient and accurate choice is

\[
e(n, U) = \frac{Uni}{2} - 4I(|U|) \sin \left( \frac{2\pi n}{2} \right).
\]

This expression by construction satisfies the following exactly known properties of \( e(n, U) \) for negative \( U \) : (i) \( e(n = 0, U) = 0 \), (ii) \( e(n = 1, U) = -4I(|U|) + U/2 \), (iii) \( e(n, U) = 0 \) \( \rightarrow (-4/\pi) \sin(\pi n/2) \), (iv) \( e(n, U \rightarrow -\infty) \rightarrow Un/2 \), (v) \( \partial e(n, U)/\partial |U| = U/2 \), and (vi) \( e(2 - n, U) + U(n - 1) = e(n, U) \). Note that unlike 24 \( c \) and 24, the \( U < 0 \) expression [25] is particle-hole symmetric and [property (iv)], and defined on only one branch.

The Kohn-Sham approach treats \( T_s \) exactly, by means of single-particle orbitals, and approximates \( E_c \), e.g., by the BA-LDA of Ref. [4].

\[
E_{\text{K-S-LDA}}[n, U] = T_s[n] + V[n] + E_H[n, U] + \sum_i e_c(n_i, U).(6)
\]

where for a spin-unpolarized system \( E_H[n, U] = (U/4) \sum_i n_i^2, \) and \( V[n] = \sum_i V_i n_i \) is the potential energy in the confining potential \( V_i \). \( T_s(n) = e(n, U = 0) \) is the per-site kinetic energy of noninteracting particles, and the difference \( e(n, U) - e_H(n, U) - t_s(n) \) is the correlation energy.

The total-energy LDA (TLDA), employed below, uses an LDA both for the kinetic and the correlation energy, so that

\[
E_{\text{TLDA}}[n] = \sum_i t_s(n_i) + V[n] + E_H[n] + \sum_i e_c(n_i, U) (7)
\]

\[
= \sum_i e(n_i, U) + V[n], \quad (8)
\]

where the second equality follows because the Hartree energy is a local functional for an on-site interaction. Note that the TLDA approach is different from the Thomas-Fermi approximation (TFA), which also employs an LDA for \( T_s \), but takes \( E_c = 0 \).

We now proceed to characterize the phase diagram. To this end we employ the TLDA, which is more accurate than the TFA, and unlike KS procedures can yield closed analytical results. The density profile is obtained from minimizing the energy functional under the constraint of fixed total particle number. Hence

\[
\frac{\delta(E - \mu N)}{\delta n_i} = \frac{\partial e(n_i, U)}{\partial n_i} + V_i - \mu = 0. \quad (9)
\]

From the above parametrizations [24, 25] and [26] of \( e(n, U) \) we obtain the Euler equations

\[
-2 \cos \left( \frac{\pi n_i}{\beta} \right) + V_i - \mu = 0 \quad 0 \leq n_i < 1 \quad (10)
\]

\[
U + 2 \cos \left( \frac{\pi(2 - n_i)}{\beta} \right) + V_i - \mu = 0 \quad 1 < n_i \leq 2 \quad (11)
\]

for \( U > 0 \), and

\[
\frac{U}{2} - 2\pi I(|U|) \cos \left( \frac{\pi n_i}{2} \right) + V_i - \mu = 0 \quad (12)
\]

for \( U < 0 \). Note that at \( n_i = 1 \) the expression \( e(n, U) \) for \( U > 0 \) is not differentiable and no Euler equation is obtained. The three Euler equations [10] - [12] have a complex solution space with a rich structure, which we now proceed to analyse.

Let us first consider \( U > 0 \). In the low-density region far from the trap center the solution of Eq. [10] is \( n_i = \frac{\beta}{\pi} \arccos \left( \frac{V_i - \mu}{2} \right) \). However, this solution only belongs to the interval \([0, 1]\) if

\[
V_i - 2 \leq \mu \leq V_i - 2 \cos \left( \pi/\beta \right). \quad (13)
\]

Closer to the center of the trap \( n_i > 1 \), and the relevant branch of the solution is [11], leading to \( n_i = 2 - (\beta/\pi) \arccos((\mu - V_i - U)/2) \), provided that

\[
V_i + U + 2 \cos \left( \pi/\beta \right) \leq \mu \leq V_i + U + 2. \quad (14)
\]
Note that the conditions (13) and (14), which guarantee that the solution found does indeed pertain to the density interval it is obtained from, do not necessarily match continuously. In particular, if
\[
U + 2 \cos \left( \frac{\pi}{\beta} \right) > -2 \cos \left( \frac{\pi}{\beta} \right)
\] (15)
there are values of \( \mu \) for which neither of the two branches of the Euler equation has a solution. The actual density in this situation is then the one for which the Euler equation has a solution. The actual density is obtained from Eq. (12). Since there is only one branch, the criterium for a valid solution is
\[
\frac{U}{2} + V_i - 2\pi I(|U|) \leq \mu \leq \frac{U}{2} + V_i + 2\pi I(|U|)
\] (16)
for \( \mu \) inside this interval the solution of (12) is
\[
\left( \frac{2}{\pi} \right) \arccos \left( \frac{U_i + U/2 - \mu}{2\pi I(|U|)} \right)
\]
For \( \mu < \frac{U}{2} + V_i - 2\pi I(|U|) \) the solution is \( n_i = 0 \) and for \( \mu > \frac{U}{2} + V_i + 2\pi I(|U|) \) it is \( n_i = 2 \). Typical density profiles in this region (not shown) are of the same type as for \( U > 0 \), with possible plateaus at \( n = 0 \) and \( n = 2 \). The absence of any possible plateaus with \( n = 1 \) is due to the absence of a derivative discontinuity of \( E_c \). The atomic density waves found from Kohn-Sham calculations in Ref. 8 are not reproduced by the TLDA, showing that observation of these oscillations (just as Friedel oscillations) require an exact (orbital) treatment of the single-body kinetic energy. The expressions for the phase boundaries obtained with TLDA can be used to analytically construct the full \( U-\mu \) phase diagram, shown in Fig. 3. For a harmonic confining potential of the form \( V_i = k_i^2 \) region II (characterized by a central plateau with \( n = 1 \), i.e., a local Mott-insulator-like state) is bounded by \( k - 2 \cos(\pi/\beta) < \mu < U + 2 \cos(\pi/\beta) \). Region III (two lateral plateaus with \( n = 1 \)) is bounded by \( U + 2 \cos(\pi/\beta) < \mu <
FIG. 3: The $U$-$\mu$ phase diagram. See main text for details.

$k + U/2 + (U/4 + \cos(\pi/\beta))^2/k$, and region V (a central band-insulator-like plateau with $n = 2$) by $\mu > U + 2 + k$. Region IV is the set of points satisfying simultaneously the criteria for region III and V, i.e., has lateral plateaus with $n = 1$ and a central plateau with $n = 2$. Region I (purely metallic without any plateaus, except for, possibly, sites with $n = 0$ at the wings of the trap) is the set of points with $\mu < -2$ that do not belong to any other $U > 0$ region. In the TFA ($E_c \equiv 0$) the $U > 0$ phases II, III and IV disappear, and the dividing line between phase I and V becomes $\mu = U + 2 + k$. Phases II, III and IV thus owe their existence to correlation. Region VI is the $U < 0$ extension of region V and characterized by a plateau at $n = 2$ in the trap center. It is bounded from below by $\mu = k + U/2 + 2\pi I(U)$ . Region VII, finally, is the $U < 0$ extension of region I and characterized by the absence of any plateaus except for, possibly, sites with $n = 0$ at the wings of the trap.

Special values of $U$ and $\mu$ can be used to further classify the possibilities: For $\mu < \mu^*$, where $\mu^*(U > 0) = -2$ and $\mu^*(U < 0) = U/2 - 2\pi I(-U)$, the only solution is $n_i = 0$ at all sites, i.e., an empty system (hatched region in the phase diagram). For $0 < U < U^*$ the intervals permitting solutions of [13] and [14] overlap, and no $n = 1$ plateaus can appear, leaving only phases I, V and VI. (In this situation, at isolated sites, an $n > 1$ and an $n < 1$ solution can coexist.) For $U^* < U < U^{**}(k)$, where $U^{**}(k)$ is the solution of $(U/4 + \cos(\pi/\beta))^2 = k(U/2 + 2)$, there cannot be a phase IV (i.e., plateaus at $n = 1$ and $n = 2$) and instead there appears a reentrant metallic phase of type I above phase III.

In summary, we have constructed the complete $U$-$\mu$ phase diagram of one-dimensional interacting harmonically confined fermions. For $U > 0$ we confirm earlier numerical results, but complement them by providing analytical expressions for the phase boundaries. The TLDA approach also provides an explanation why Kohn-Sham calculations do not work in the metal Mott-insulator phase-separated state (with plateaus at $n = 1$) and provides an alternative way for obtaining density profiles in this region. For $U < 0$ we propose, in Eq. (5), a simple analytical parametrization of the Bethe-Ansatz solution, which we use, within TLDA, to extend the phase diagram to attractive interactions.

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