Ground-state properties of the one-dimensional Hubbard model with pairing potential

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Abstract

We consider a modification of the one-dimensional Hubbard model by including an external pairing potential. We determine the grand-canonical zero-temperature phase diagram using both finite and infinite density matrix renormalization group algorithm based on the formalism of matrix product states and matrix product operator, respectively. By computing various local quantities as well as the half-system entanglement, we are able to distinguish between Mott, metallic and superconducting phases. We point out the compressible nature of the Mott phase and the fully gaped nature of the many-body spectrum of the superconducting phase, in the presence of explicit U(1)-charge symmetry breaking.

Keywords: density matrix renormalization group, Hubbard model, entanglement entropy
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1. Introduction

Long-range quantum correlations often fully characterize the nature of a quantum phase in many-particle systems. An abrupt change of correlations typically occurs at quantum phase transitions [1]. As a quantitative measure

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of quantum correlations, the entanglement entropy plays a central role, potentially able to signal quantum phase transitions or to characterize critical gapless phases [2].

To define the entanglement entropy [3], one bipartites the quantum system into two parts $A$ and $B$. One then introduces a density matrix $\rho = |\Psi\rangle\langle\Psi|$ of a pure quantum state $|\Psi\rangle$, and obtains the reduced density matrix $\rho_A = \text{Tr}_B \rho$ by tracing out the subsystem $B$. The entanglement entropy is the von Neumann entropy, which is given by $S_A = -\text{Tr}(\rho_A \ln \rho_A)$. Since we will consider zero-temperature properties in the following, we will compute entanglement properties using the ground-state as wavefunction $|\Psi\rangle$.

In order to find the ground state in quantum many-particle systems, the density matrix renormalization group [4] (DMRG) method is suitable, especially in one dimension. The connection between DMRG and tensor networks was first recognized by the quantum information community [5]. A detailed reformulation of DMRG in terms of matrix product states (MPS) was reviewed by Schollwöck [6]. The generalization of MPS to handle two-dimensional systems was carried out, and the projected entangled pair state (PEPS) was introduced [7]. For critical systems, the multi-scale entanglement renormalization ansatz (MERA) is useful [8]. When a Hamiltonian has translational invariance, we can use the so-called infinite DMRG (iDMRG) [9], in which we assume that the matrices in the MPS are identical. Without entering into too much details, let us simply mention that we update a few matrices and environments to converge to the ground-state $|\Psi_0\rangle$ with the iDMRG method.

Since experimentalists can design ultracold many-fermion systems loaded on quasi one-dimensional optical lattices [10], the one-dimensional fermion Hubbard model has become a physical reality. Quite interestingly, the attractive Hubbard model which is the simplest model to describe pairing and superconductivity in a fermionic system can also be realized [11]. In our case, the repulsive Hubbard model with an additional pairing potential, providing a tendency to form nearest-neighbor singlet pairs, could also be realized in fermionic systems, for instance by proximity effect with a singlet superconductor.

The purpose of this paper is to compute the ground-state phase diagram of the one-dimensional Hubbard model with a (singlet) pairing potential. To do so, we apply two standard algorithms (finite and infinite DMRG) separately to optimize the matrices in the MPS. The results obtained by both methods are consistent with each other. By changing the chemical
potential, a quantum phase transition occurs between gapless and gapped phases, as can be measured from the scaling of the entanglement entropy.

2. Model and method

We consider a simple generalization of the Hubbard model on a one-dimensional (1D) lattice:

\[
H = -t \sum_{\langle ij \rangle} (c_{i\uparrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{j\downarrow} + c_{j\downarrow}^\dagger c_{i\uparrow} + c_{j\uparrow}^\dagger c_{i\downarrow}) \\
+ U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) \\
- \Delta \sum_{\langle ij \rangle} (c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + c_{i\downarrow}^\dagger c_{j\uparrow} + c_{i\downarrow} c_{j\uparrow} + c_{j\uparrow} c_{i\downarrow}),
\]

(1)

where \( c \) and \( c^\dagger \) are the usual spin-1/2 fermion annihilation and creation operators, \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \) is the local spin-resolved density and \( \langle ij \rangle \) stands for nearest neighboring sites on the 1D chain. We fix the hopping strength \( t = 1 \) (as unit of energy) and vary the other three parameters: the on-site Coulomb repulsion \( U \), the chemical potential \( \mu \), and the pairing strength \( \Delta \). The role of the chemical potential is to control the average number of fermions in the system. Note that the (bond) singlet pairing potential does not conserve the particle number so that the model only has SU(2) spin symmetry. Physically, such a potential may account for the proximity effect of a nearby singlet superconductor. Without pairing potential, i.e. for \( \Delta = 0 \), we recover the standard one-dimensional (repulsive) Hubbard model which will be used for benchmark calculations as it is exactly solvable [12, 13].

Let us make some additional remarks about the symmetries of this model. Half-filling will correspond to \( \mu = 0 \) obviously and the phase diagram will be symmetric under \( \mu \leftrightarrow -\mu \). Moreover, when \( \mu = 0 \), applying a particle-hole symmetry only on odd sites (\( d_{2i,\sigma} = c_{2i,\sigma} \) and \( d_{2i+1,\sigma} = c_{2i+1,\sigma}^\dagger \)) amounts to exchanging the hamiltonian parameters as \( (t, U, \mu = 0, \Delta) \leftrightarrow (\Delta, U, \mu = 0, t) \), i.e. exchanging the role of \( t \) and \( \Delta \).

In the non-interacting case \( (U = 0) \), the model is quadratic so that it can be diagonalized in Fourier space using a Bogoliubov transformation to get

\[
H_0 = \sum_k E_k (\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k)
\]

(2)
with a dispersion $E_k = \pm \sqrt{(\varepsilon_k - \mu)^2 + (\Delta \cos k)^2}$ where $\varepsilon_k = -2t \cos k$ is the tight-binding dispersion. In particular, for a generic filling (i.e. a generic $\mu$ value), we have a one-dimensional superconductor with a finite gap. Indeed, there is no U(1) symmetry breaking in this model (since the particle number conservation is *explicitly* broken) and, hence, no emergent zero-energy Goldstone modes. On general grounds, we expect that this superconducting phase will persists in some range of the phase diagram, even in the presence of a finite repulsive $U$. Note also that, in this gapped superconducting phase, the compressibility is finite though.

Since the Hamiltonian has translation symmetry, we construct the corresponding matrix product operator (MPO), which acts on matrix product state (MPS). By performing the usual matrix multiplication, we can check that the following MPO does represent our Hamiltonian:

\[
\begin{pmatrix}
1 & c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger & c_{i\uparrow} & c_{i\downarrow} & U(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) - \mu(n_{i\uparrow} + n_{i\downarrow}) \\
0 & 0 & 0 & 0 & 0 & -tc_{i\uparrow} - \Delta c_{i\downarrow}^\dagger \\
0 & 0 & 0 & 0 & 0 & -tc_{i\downarrow} + \Delta c_{i\uparrow}^\dagger \\
0 & 0 & 0 & 0 & 0 & tc_{i\uparrow} + \Delta c_{i\downarrow} \\
0 & 0 & 0 & 0 & 0 & tc_{i\downarrow} - \Delta c_{i\uparrow} \\
0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}
\]  

(3)

where we omit the boundary operators. Obviously, we need to take care of ordering for fermions when we carry out iDMRG by acting with the MPO on the MPS.

Let us assume that the physical index $\sigma_i$ labels the state on the $i$-th site. For the Hubbard model, $\sigma_i = (\alpha_i, \beta_i)$, where $\alpha_i(\beta_i) = 0$ or $1$ means that there is a vacancy or occupation of the spin-up (down) fermion at the $i$-th site, respectively. The state of the Fock space for a $L$-lattice system is thus written in terms of the creation operators $c_{i\uparrow}^\dagger$ and $c_{i\downarrow}^\dagger$ as follows:

\[
|\sigma_0 \cdots \sigma_{L-1}\rangle = (c_{0\uparrow}^\dagger)^{\alpha_0}(c_{0\downarrow}^\dagger)^{\beta_0} \cdots (c_{L-1\uparrow}^\dagger)^{\alpha_{L-1}}(c_{L-1\downarrow}^\dagger)^{\beta_{L-1}}|0\rangle.
\]  

(4)

It is important to maintain the order of the fermions in the state of the Fock space to handle the minus sign caused by the exchange of fermion. We adopt the order of spin-up first and spin-down next as above.

\[\text{In the many-body spectrum, the ground-state is unique and there is a finite gap } 2|\mu| \text{ for the first excitation.}\]
For iDMRG with a two-site unit cell, two tensors, $A$ and $B$, in the MPS are repeated as $\cdots ABABAB \cdots$ with the usual matrix multiplication. The tensors, $A_{ab}^\sigma$ and $B_{cd}^\rho$, have three indices, among which the physical index $\sigma$ and $\rho$ takes a value from 0 to 3 for our model. For the degree of freedom of the internal bond, the indices $a$ (left) and $b$ (right) for $A$ range from 0 to $\chi - 1$, where $\chi$ is the dimension of the internal bond. The Schmidt coefficients between $A$ and $B$, and between $B$ and $A$, are denoted by $\lambda^{AB}$ and $\lambda^{BA}$, respectively. Thus, a state in the space of matrix product states is written as

$$|\Psi\rangle = \sum_{\cdots \sigma \rho \nu \eta \cdots} \text{Tr}(\cdots A_{ab}^\sigma \lambda_{bc}^{AB} B_{cd}^\rho \lambda_{de}^{BA} A_{ed}^\nu \lambda_{de}^{AB} B_{de}^\eta \cdots)|\cdots \sigma \rho \nu \eta \cdots\rangle,$$

where Tr means that the indices of the internal bonds $a, b, c, d, \cdots$ are summed up. The thermodynamic limit will be reached when the bond dimension $\chi$ goes to $\infty$.

Regardless of the $t$, $U$, $\mu$, and $\Delta$ values used in our calculations, we have observed a smooth convergence. Our numerical DMRG results show that the ground-state solutions fall into two classes: MPS are either of the form $\cdots ABABAB \cdots$ (i.e. unit cell of two sites that we will identify as a Mott phase) near half-filling ($\mu = 0$), or uniform $\cdots AAAAAA \cdots$ further away from half-filling, that we will identify as metallic or superconducting phases, for $\Delta = 0$ or non-zero, respectively.

### 3. Numerical results

We will present data obtained using the infinite DMRG (with a two-site unit cell) as well as the finite-size algorithm for chain length up to $L = 512$. After computing the ground state $|\Psi\rangle$, we compute local quantities such as the bond energy and the local densities and we also use the half-chain entanglement entropy to determine if the system is critical and, if so, what is its central charge.

By contraction of the Hamiltonian bond operator with the ground-state MPS, we obtain the bond energy. Close to half-filling, since the MPS has an ABAB form, we obtain alternating bond energies on even and odd bonds. We have observed however that the modulation seems to vanish for $\chi \rightarrow \infty$. To be more quantitative, we determine the half-chain entanglement entropy.
Figure 1: The entanglement entropy difference $\Delta S$ versus the bond energy difference $\Delta E$ for $\chi = 80, 90, 100, 110, 120, 130$. We set $t = 1$ and $U = 4$. The linear fits are compatible with a zero intercept, i.e. $\Delta S$ and $\Delta E$ are proportional.

The Schmidt coefficients $\lambda_a$ are obtained when we perform a singular value decomposition (SVD) to find the matrices $A$ and $B$ in the MPS. Normalization of $\sum_{a=0}^{\chi-1} \lambda_a^2 = 1$ guarantees $\langle \Psi | \Psi \rangle = 1$. For the $\cdots ABABAB \cdots$ solution, we obtain two different values of the entanglement entropy: $S_o$ with $\lambda^{AB}$ on the odd bonds and $S_e$ with $\lambda^{BA}$ on the even ones.

The calculation shows that, close to half-filling, both the bond energy and the entanglement entropy have a finite modulation. In such a case, the energy difference $\Delta E = E_e - E_o$ and the entropy difference $\Delta S = S_o - S_e$ are proportional to each other [14]. In Fig. 1, we present the $\chi$-dependence.
of $\Delta E$ versus $\Delta S$. The numerical results confirm that $\Delta S$ is proportional to $\Delta E$ to a very high accuracy of $10^{-6}$. We conclude that $\Delta S = 0$ and $\Delta E = 0$ in the thermodynamic limit of $\chi = \infty$, as expected.

In order to determine the Mott transition, characterized by a change in the compressibility, we compute the (average) ground state energy $E = (E_e + E_o)/2$ vs the chemical potential $\mu$ starting from $\mu = 0$. On the other hand, we can also compute the ground-state energy in the uniform solution by decreasing $\mu$ (starting from large values). In each iDMRG calculation, the tensors of the initial environment are given by the previous solution of the different $\mu$. First, as a benchmark, we plot in Fig. 2 the evolution of the ground state energy for $\Delta = 0$, where we find a level-crossing at a critical $\mu_c$. In the thermodynamic limit, corresponding to $\chi \to \infty$, our extrapolation of $\mu_c$ is quite close to the exact value $\mu_+$ found using the Lieb-Wu method \cite{12,13} and it corresponds to the well-known second-order phase
transition between an incompressible Mott phase and a metallic one.

We also compute the density, i.e. the expectation value of the occupation number $n = \langle n_{i,\uparrow} + n_{i,\downarrow} \rangle$, as a function of $\mu$ as shown in Fig. 3 for several values of the pairing strength $\Delta$ and $U = 4$. For $\Delta = 0$, we do observe an incompressible phase around $\mu = 0$ and a transition point identical to the previous one, see Fig. 2. For $\Delta > 0$, the compressibility (which is the slope of $n$ vs $\mu$) is always finite but we do observe a sudden change for some critical $\mu_c$, which we identify as the phase transition between Mott and superconducting phases.

As a concluding remark about this section, we have observed that the critical $\mu_c$ varies with the pairing strength $\Delta$ so that we can summarize the numerical results in the phase diagram shown in Fig. 4. On top of our numerical data, we provide a qualitative sketch of the full phase diagram but it is difficult numerically to determine what happens for large $\Delta$ at $\mu = 0$. In this region, we can use the partial particle-hole transformation that was discussed in Sec. 2. Indeed, for $\mu = 0$, the model with parameters
\((t = 1, U, \Delta)\) at large \(\Delta\), which is difficult to analyze, is equivalent to the one at \((t = \Delta, U, \Delta = 1)\) which is simply a tight-binding chain with small perturbation. In this case, we do expect a Mott phase with a very small gap \([13]\), hence a very small Mott region.

![Numerical phase diagram of the one-dimensional Hubbard model](image)

**Figure 4**: Numerical phase diagram of the one-dimensional Hubbard model at \(t = 1\) and \(U = 4\), as a function of the chemical potential \(\mu\) and the singlet pairing potential \(\Delta\), obtained from iDMRG (magenta squares) and DMRG (purple circles, \(L = 128\)). The red line is a guide to the eyes. The region of the Mott-insulating phase shrinks for smaller \(U\).
Figure 5: Half-chain entanglement entropy versus $\mu$ for several values of the pairing $\Delta$. We have set the parameters to $t = 1$, $U = 4$ and $\chi = 100$.

4. Entanglement entropy scaling

It is well-established that block entanglement entropy scaling can be used to determine if the ground-state is gapped or critical. In the later case, the central charge of the underlying Conformal Field Theory (CFT) can also be computed [15]. In Fig. 5, we present the half-chain entanglement entropy $S = (S_o + S_e)/2$, which is obtained from iDMRG. In agreement with our local measurements from the previous section, we do observe a rather flat plateau region around $\mu = 0$, at least for $\Delta$ not too large, corresponding to the Mott phase obtained from the compressibility data. Note that the size of the plateau is decreasing with $\Delta$ so that it is still difficult to determine the physics for large $\Delta$ at $\mu = 0$.

In addition, using a conformal scaling with $\chi$,

$$S = \frac{1}{\sqrt{\frac{12}{c} + 1}} \ln \chi + \tilde{s},$$
Figure 6: Entanglement entropy versus $\ln(\chi)$ for two values of $\mu$, fixing $U = 4$ and $\Delta = 2$. For $\mu = 0.6$, $S$ saturates at large $\chi$, in agreement with a gapped superconducting behavior. At $\mu = 0$, the data can be fitted as $S = 0.22 \ln(\chi) + \tilde{s}$, in agreement with the conformal scaling with central charge $c = 1$ (see text).

one can determine the central charge $c$ in all critical phases with a constant $\tilde{s}$. In Fig. [6] we present the finite-$\chi$ scaling of the half-chain entanglement entropy for several $\Delta$ and $\mu$. For parameters $U = 4$, $\Delta = 2$ and $\mu = 0.6$, we observe the saturation of $S$ at large $\chi$, a behavior characteristic of a fully gapped phase as expected for the superconducting one. In contrast, for the model with $U = 4$, $\Delta = 2$ and $\mu = 0$, the above conformal scaling is well realized providing the central charge is set to $c = 1$, as expected for a Mott phase with a single gapless spin mode.

In order to provide a complementary quantitative analysis, we have used finite-size DMRG algorithm keeping up to $m = 4000$ states and with a discarded weight below $10^{-8}$. For a finite-system with open boundary conditions, conformal field theory predicts that, in a critical region, the
block entanglement entropy $S$ should follow the universal scaling behavior:

$$S = \frac{c}{6} \ln d(x/L) + \tilde{s}. \quad (7)$$

where $c$ is the central charge, $d(x/L) = \pi/L \sin(x\pi/L)$ is the conformal block size of size $x$, and $\tilde{s}$ is a non-universal constant.

In Fig. 7, we present the finite-size scaling of the entanglement entropy for $U = 4$ in all different regions. In the metallic phase ($\Delta = 0$, $\mu = 2$), we measure a large central charge $c \simeq 2$ corresponding to two gapless modes (one in the charge channel, one in the spin channel) as expected. For $\Delta = 2$ and $\mu = 2$, we are in the fully gapped superconducting phase. Last, in the Mott phase at or close to half-filling (for instance $\Delta = 2$ and $\mu = 0$), we observe a smooth crossover from a large central charge $c \simeq 2$ at small distance to a proper $c = 1$ at large distance, as expected from a single gapless spin mode, as found for instance in the pure Hubbard model with $\Delta = 0$. Indeed, it is well-known that, for the pure Hubbard model at half-filling, the charge gap is exponentially small ($\sim \exp(-t/U)$) while it becomes of order $U$ at large $U$ [13]. Similarly, there is a corresponding length scale (proportional to the inverse of the gap) that governs this crossover.

In conclusion on this section, our finite-size DMRG calculations have confirmed that the charge channel is always gapped for finite $\Delta$. However, we have distinguished the Mott phase from the fully gapped superconducting one by its gapless $c = 1$ spin mode.

5. Conclusion

In summary, we have used both the finite-size and infinite DMRG to obtain the ground-state of the one-dimensional Hubbard model with an additional singlet pairing potential. Such a model would be relevant for a strongly correlated chain with some proximity coupling to a singlet superconductor. We have computed local quantities as well as entanglement properties in order to establish the full phase diagram, including Mott, metallic and superconducting phases.

Our study has revealed a particularly interesting feature of the Mott and superconducting phases, connected to the existence of a potential breaking explicitly particle number conservation. In that case, the inverse of the compressibility $\kappa$ is no longer related to the many-body charge gap $\Delta_C$, as $\kappa^{-1} \sim L \Delta_C$, so that $\Delta_C$ and $\kappa$ could be simultaneously non zero in the thermodynamic limit $L \to \infty$. Such a remarkable feature is exemplified by the
Figure 7: Entanglement entropy scaling versus the conformal size of the block for $U = 4$ and various parameters $\Delta$ and $\mu$, obtained from DMRG on chains of length $L$. (a) $\Delta = 0$ and $\mu = 2$ in the metallic phase; (b) $\Delta = 2$ and $\mu = 0$ in the Mott phase; (c) $\Delta = 2$ and $\mu = 2$ in the superconducting phase.
Mott and the superconducting phases which are both simultaneously gapped (in the charge sector) and compressible. The Mott phase can however be characterized by the existence of a gapless spin mode (described by a $c = 1$ CFT) while the superconducting phase is fully gapped.

It would be an interesting prospect to extend this study to two-dimensional systems, using for instance PEPS formulation that does not suffer from the negative sign problem.

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