Phase diagram of the extended Bose–Hubbard model

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\textbf{Abstract.} By means of the density matrix renormalization group technique, we accurately determine the zero-temperature phase diagram of the one-dimensional extended Bose–Hubbard model with on-site and nearest-neighbor interactions. We analyze the scaling of the charge and of the neutral ground-state energy gaps, as well as of various order parameters. In this way we come to an accurate location of the boundaries between the superfluid and the insulating phases. In this last region, we are able to distinguish between the conventional Mott insulating and density-wave phases and the Haldane insulator phase displaying long-range string ordering, as originally predicted by Dalla Torre \textit{et al} (2006 \textit{Phys. Rev. Lett.} 97 260401).

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1. Introduction

Over the last decade, ultracold atomic gases loaded in optical lattices were successfully established as an excellent setup to probe the equilibrium, as well as the out-of-equilibrium physics of strongly correlated quantum systems. The great advantages of these experimental setups are essentially related to two aspects. On the one hand, they have a very high degree of flexibility: in addition to the ability to address different geometries, and to deal with bosonic and with fermionic species, they also admit the possibility of manipulating the underlying Hamiltonian system parameters to a large extent. Moreover, the remarkably high degree of isolation from any environmental source of decoherence opened up entirely new scenarios in the observation of genuinely many-body quantum phenomena [1].

The paradigm model to describe cold bosonic atoms trapped in an optical lattice is obtained by combining the kinetic energy in the lowest band with the on-site repulsion arising for sufficiently deep lattices. This leads to the celebrated Bose–Hubbard model (BHM) [2]. The rich physics of the BHM stems from the competition between the kinetic energy $J$, which is gained by delocalizing particles across the lattice in an extended Bloch state, and the repulsive on-site interaction $U$, which disfavors having more than one particle per site. When the kinetic energy term dominates, the system is in a coherent superfluid (SF) phase; on the other hand, repulsive interactions tend to favor a Mott insulating (MI) phase [3].

The recent advances in manipulating magnetic atoms and molecules with a large dipole momentum make it possible to achieve longer-range interactions, which can be accurately tuned as well, thus permitting us to probe the interplay between strong correlations and charge-ordering effects [4]. Dipolar bosons confined in optical lattices are typically described by an extended version of the BHM, the so-called extended Bose-Hubbard model (EBHM), which includes a two-body non-local repulsive term typically decaying as $r^{-3}$ with distance $r$.

Interestingly, the presence of long-range interactions noticeably enriches the phase diagram of the BHM, for example leading to a stabilization of a peculiar insulating phase, named the bosonic Haldane insulator (HI). This gapped phase presents some analogies with the well-known Haldane phase in integer spin chains [5]; it does not break the translational symmetry of the lattice and is characterized by an underlying hidden order, that is, a non-trivial ordering of the fluctuations that appear in alternating order separated by strings of equally populated sites of arbitrary length [6–8]. More recently, a mean field analysis suggested the existence of various supersolid phases and a series of non-trivial density-wave (DW) states with an increased ground-state degeneracy, which can be stabilized in the strong coupling regime, but with a relatively weak on-site interaction [9]. It has also been shown that the presence of disorder in the on-site potential [10], as well as occupation-dependent hopping and pair tunneling terms arising from dipolar interactions [11], can drive important modifications in the phase diagram, leading to the stabilization of a plethora of novel quantum phases, such as structured insulating states, Wigner crystals or pair supersolids.

The aim of this paper is to work out the zero-temperature phase diagram of the pure one-dimensional (1D) EBHM, by means of the numerical density matrix renormalization group (DMRG) technique [12], in order to accurately determine the phase diagram first proposed in [6, 7] and extend their preliminary results. This method has already revealed its great potentialities in the study of ground states of 1D strongly correlated bosons on a lattice, providing very accurate results for these kinds of systems (see, e.g., [13–18] and references therein).
This paper is organized as follows. In section 2, we introduce the model we are going to study, and qualitatively discuss the various emerging quantum phases. We then present, in section 3, all the relevant quantities we will address: (i) three kinds of local and non-local correlators, which will enable us to locate all the different phases identifying suitable order parameters; and (ii) the ground-state charge and neutral energy gaps, which will serve to discriminate critical phases as well as insulating quantum phase transition (QPT) points. A phase diagram of the model is shown in section 4, followed by a detailed discussion of the finite-size scaling of the various order parameters (section 4.1) and of the charge and energy gap (section 4.2), up to a few hundreds of sites. Finally, in section 5, we draw our conclusions.

2. The model

In the following, we will focus on the 1D EBHM, with on-site and nearest-neighbor repulsive interactions. The sharp cutoff of the $r^{-3}$ interaction range, although presenting quantitative differences with the standard long-range EBHM, does not qualitatively alter its physics:

$$
\mathcal{H} = -J \sum_j \left( b_j^\dagger b_{j+1} + \text{h.c.} \right) + \frac{U}{2} \sum_j n_j (n_j - 1) + V \sum_j n_j n_{j+1}.
$$

Here $b_j^\dagger$, $b_j$ are creation and annihilation operators of bosons on site $j$, $J$ denotes the hopping strength, while $U$ and $V$ are the on-site and the nearest-neighbor interaction strengths. Hereafter we set the energy scale by taking $J = 1$, and work in units of $\hbar = 1$.

We will concentrate on the model in equation (1) at zero temperature and at integer filling $\bar{n}$, which is known to exhibit quite a rich phase diagram with various quantum phases, ranging from the SF for low $U$, $V$ interaction strengths, to insulating phases in the opposite regime. Depending on the relative strength of $U$ and $V$, a Mott insulator (MI) or a DW state can form, the first one establishing with large values of $U$, while the second one with large $V$. In between the two conventional insulating phases, a peculiar gapped phase emerges: the HI.

The phase diagram and phase transitions of such a kind of model describing bosons loaded in optical lattices with short-range interactions have been addressed since a long time ago [3]. Emphasis was put on the experimentally accessible SF–MI transition [19]. In the 1D case and with a constant integer filling, the transition is of the Berezinskii–Kosterlitz–Thouless type and was extensively analyzed with DMRG in [13, 14]. The same authors also demonstrated that, in the presence of nearest-neighbor interactions, there is no normal or supersolid phase, but a direct phase transition from the DW to the SF phase occurs. Only a few years ago, by means of a mean field theory describing low-energy excitations in the continuum limit, in [6, 7] it was realized that extended interactions can stabilize a further HI phase, possessing hidden order that is revealed by non-local string correlations. In those papers the DMRG was employed to extract some preliminary quantitative results and draw the resulting phase diagram in one dimension. Further DMRG calculations have also been used to address closely related effective spin-1 chains, including finite-size scaling studies [20, 21] and the effects of trapping potentials [22], and to study the entanglement spectrum in order to probe the degeneracies in the HI phase [23].

Here we numerically probe the EBHM over all its parameter space, corroborating the investigations reported in the literature and providing an accurate description of its complete phase diagram at integer filling. In order to locate the different quantum phases of equation (1)
we resort to the DMRG algorithm with open boundary conditions\(^2\). Our code is based on a variational ansatz using matrix product states, in the restricted subspace of integer filling [12].

### 3. Correlation functions, order parameters and energy gaps

The nature of the different quantum phases emerging in the EBHM, as well as all the QPT points determining the various phase boundaries, are revealed by the behavior of certain two-point correlation functions. The following three correlators are able to univocally distinguish between all the emerging quantum phases:

\[
C_{\text{SF}}(r) = \langle b_j^\dagger b_{j+r} \rangle,
\]

\[
C_{\text{DW}}(r) = (-1)^r \langle \delta n_j \delta n_{j+r} \rangle,
\]

\[
C_{\text{string}}(r) = \langle \delta n_j e^{ir \sum_{k \leq j < j'} \delta n_k} \delta n_{j+r} \rangle,
\]

where \(\delta n_j = n_j - \bar{n}\) denotes the boson number fluctuations from the average filling (hereafter we will always consider the case \(\bar{n} = 1\)).

The long-range off-diagonal order, typical of SF states, manifests itself in a power-law decay to zero of \(C_{\text{SF}}(r)\); on the other hand, in the insulating phases the absence of such an ordering is characterized by an exponential suppression of \(C_{\text{SF}}(r)\) with \(r\). The large-\(r\) limit of the second correlator, \(C_{\text{DW}}(r)\), identifies a staggered diagonal order which naturally emerges in the DW phase: at \(\bar{n} = 1\), large values of \(V\) in equation (1) tend to stabilize such an ordering, by inducing a pattern \(
\cdots - 2 - 0 - 2 - 0 - \cdots
\) for the occupation number. Such phases are then characterized by a finite DW order parameter \(O_{\text{DW}} \equiv \lim_{r \to \infty} C_{\text{DW}}(r)\). Finally, the two-point correlator \(C_{\text{string}}(r)\) contains a non-local string correlation function accounting for the number of bosons that are present in between the two points. For large values of \(r\), this has been shown to define an order parameter for the HI, namely \(O_{\text{string}} \equiv \lim_{r \to \infty} C_{\text{string}}(r)\), which is distinguished from the usual MI through such a highly non-local ordering. In contrast, in the incoherent MI phase all the correlation functions in equations (2)–(4) vanish exponentially.

In addition to the previously defined correlation functions, we also analyze the energy gap. The nature of the different quantum phases, as well as all the QPT points, is indeed sensitive to it. In particular, we will focus on the neutral \((\Delta E_n)\) and on the charge \((\Delta E_c)\) gaps, respectively defined as

\[
\Delta E_n = E^{(1)}_L - E^{(0)}_L,
\]

\[
\Delta E_c = E^{(0)}_{L+1} + E^{(0)}_{L-1} - 2E^{(0)}_L,
\]

where \(E^{(k)}_m\) indicates the energy of the \(k\)th excited state (\(k = 0\) labeling the ground state, \(k = 1\) the first excited state and so on) for a system with a given number of \(m\) bosons in \(L\) lattice sites\(^3\). In practice, we run our DMRG simulations in the canonical ensemble. The charge gap is evaluated by running three instances of DMRG, each of them separately targeting the ground

\(^2\) The choice of open boundary conditions is popularly used in the DMRG community, and is dictated by the fact that it has been proven that they perform more efficiently than periodic boundaries [12]. We will take special precautions for border effects emerging in our simulated finite-size systems.

\(^3\) The case \(m = L\) corresponds exactly to the integer filling sector \(\bar{n} = 1\), in which the neutral gap is evaluated. The charge gap in equation (6) expresses the difference in the energy costs \(\Delta E^{(0)}_L\) to add and subtract a single particle from the ground state at unitary filling, i.e. \(\Delta E_c = \Delta E^{(0)}_c - \Delta E^{(0)}_c = (E^{(0)}_{L+1} - E^{(0)}_L) - (E^{(0)}_{L-1} - E^{(0)}_L)\).
state of \( n = \{L, L \pm 1\} \) particle number sectors \([13, 14]\). The neutral gap is extracted by running only one instance of DMRG, in which both the ground state and the first excited state are targeted\(^4\).

Unfortunately, the charge gap \( \Delta E_c \) only detects particle and hole excitations, and is able to locate the superfluid-to-insulator transition, as well as the MI–HI QPT point. On the other hand, the HI phase can display another type of excitation, which in energy goes below the particle–hole excitation and is revealed only by the neutral gap \( \Delta E_n \). It turns out that the presence of such low-energy neutral modes becomes crucial for the identification of the HI–DW transition, as we will explicitly show later.

In the next section, we will discuss in detail our results. We first show the phase diagram of the EBHM, distinguishing between the various quantum phases of the model. Then we will present our data on the order parameters and ground-state energy gaps.

### 4. Phase diagram

We start the discussion of our results by presenting the phase diagram of equation (1) in the \((U, V)\)-plane. Our DMRG simulations were performed for systems with open boundary conditions up to \( L = 400 \) sites, keeping at most \( m = 500 \) states, and working in a canonical ensemble with a fixed number of bosons. Due to computational reasons, for a filling \( \bar{n} = 1 \) we admitted a maximum of \( n_{\text{max}} = 3 \) bosons per site. We checked that the location of the phase boundaries is not qualitatively affected by the values of the various cutoffs\(^5\).

Figure 1 summarizes the results of our investigation. As we stated before, model (1) has four different quantum phases. For large \( U \) values, the system is always insulating. In order to distinguish between MI, HI and DW phases, we carefully analyzed the string and the DW order parameter, \( O_{\text{string}} \) and \( O_{\text{DW}} \), respectively. An accurate finite-size scaling of the \( O_{\text{string}} \) data allowed us to draw the black line (data are shown as circles) in figure 1. A similar analysis was also performed on \( O_{\text{DW}} \), producing the red curve in the figure (red squares). For further details of the specific situation with \( U = 5 \), see section 4.1. We performed a cross-check of such obtained phase boundaries by looking at the charge and the neutral energy gaps (see section 4.2), obtaining minimal values for the gaps at the QPT points.

For small values of \( U \) and not too large \( V \), the system enters a critical SF phase, characterized by long-range off-diagonal order. We located the SF by looking at the charge energy gap (blue diamonds). While for small \( V \) values the determination of the SF–insulator boundary is quite accurate at relatively small sizes \( L \approx 300 \) (where, by increasing \( U \), at some critical point the charge energy gap undergoes a sudden increase), this becomes harder for larger \( V \). The dashed line in the figure has been plotted as a guide to the eyes, and is an interpolation between the blue data in the small-\( V \) region and the red DW boundary at large values of \( V \). As a matter of fact, despite the relatively low numerical accuracy that we were able to achieve in that region, our data are indeed compatible with the presence of an SF phase below the HI, for small \( U \) values and \( 1.5 \lesssim V \lesssim 3 \), in agreement with the findings of \([10]\).

\(^4\) In general, fixing the system size and the bond-link dimension, the evaluation of \( \Delta E_c \) is much faster and more accurate than that of \( \Delta E_n \), since only the ground state has to be addressed.

\(^5\) We also performed simulations fixing \( n_{\text{max}} = 2 \), thus mapping the problem into a spin-1 Heisenberg Hamiltonian with a single-site uniaxial anisotropy, and explicitly found a phase diagram with the same qualitative features as those depicted in figure 1. We, however, noted important quantitative changes, with the HI phase being shifted at lower values of \( V \), and the DW phase enlarged.

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4.1. Scaling of the order parameters

In order to determine the HI–DW and the MI–HI phase boundaries, we respectively looked at the correlation functions in equations (3)–(4). In particular, we computed the string and the DW order parameters by extracting the large-$r$ limit of such correlators. To minimize border effects due to open boundaries, we computed the average expectation values of all the two-point correlators between spins in the middle part of the chain, discarding the outer $L/4$ sites on both sides. We also studied the dependence on the system size by performing a finite-size scaling up to $L = 400$ system sites.

An example of such an analysis is shown in figure 2, where we fixed the on-site interaction strength $U = 5$, and varied $V$. Both the HI order parameter (filled symbols, on the left part of the main panel) and the DW order parameter (empty symbols, on the right of the main panel) are plotted as a function of $V$ and for different sizes ranging from $L = 50$ to $L = 400$. The MI–HI phase transition is located at the point where $O_{\text{string}}$ becomes finite, which is estimated to be at $V_{\text{MI} - \text{HI}} \approx 2.95 \pm 0.05$ (dashed black vertical line). On the other hand, the HI–DW phase transition occurs where a finite $O_{\text{DW}}$ appears, that is, at $V_{\text{HI} - \text{DW}} \approx 3.525 \pm 0.05$ (dashed red vertical line).

Finite-size effects are clearly visible in the figure. In the inset, we show how the two order parameters approach the zero value very close to the QPT. Namely, we plotted $O_{\text{string}}$ (black circles) and $O_{\text{DW}}$ (red squares), respectively, at $V_{\text{MI} - \text{HI}} = 2.95$ and $V_{\text{HI} - \text{DW}} = 3.525$. In both cases, we obtained an exponential decay of $O$ with the system size $L$. 

Figure 1. Ground-state phase diagram of the 1D EBHM in the $(U, V)$-plane, with a maximum admissible number of 3 bosons per site. The boundaries between the different phases have been calculated by analyzing the string order parameter (MI–HI—black circles), the DW order parameter (HI–DW—red squares) and the charge energy gaps of the system (SF–MI—blue diamonds). The dashed blue line is an interpolation of the continuous blue curve and the red points at large $V$ values.
4.2. Scaling of the energy gaps

Further analysis of the QPT points has been performed by looking at the neutral and the charge energy gaps, $\Delta E_c$ and $\Delta E_n$ (see equations (5) and (6)). In addition to corroborating the results obtained from the order parameters scaling analysis as we will show in figures 4 and 6, the closure of the energy gaps discriminates between the SF and the insulating phase. This is a method of locating the SF boundaries, which reveals more accurately than directly looking at the off-diagonal ordering. As a representative example, in figure 3 we show the behavior of the charge energy gap in the proximity of the SF–MI transition of model (1) as long as $U$ is increased to a critical value (see blue diamonds in figure 1). Namely, we plotted $\Delta E_c$ as a function of $U$ for a fixed value of $V$ and for a system of $L = 400$ sites. The SF–MI QPT is revealed by a sudden growth of $\Delta E_c$ at a critical value $U^*$, which is estimated to be $U^* \approx 3.33$ at $V = 0$ and $U^* \approx 2.3$ at $V = 1$.\(^6\) We remark that, at the sizes that are typically studied, it is easy to discriminate between a power-law decay of $C_{\text{SF}}(r)$ deep in the SF phase and its exponential decay deep in the MI, as is clearly shown in the two insets of figure 3. Nonetheless, this becomes much trickier in the proximity of the phase boundaries and would require very large sizes to distinguish between the two behaviors [14].

\(^6\) The value $U^* \approx 3.33$ corresponds to the quantum critical point for the SF–MI transition in the 1D BHM at filling $\rho = 1$, which has been thoroughly investigated in the literature (see, for example, [14]).
Figure 3. Ground-state charge energy gap $\Delta E_c$ as a function of $U$, for two different values of $V$. The two insets display the correlation function $C_{SF}(r)$ as a function of $r$, deep in the SF phase (left inset—P1 at $V = 1$, $U = 0.5$) and deep in the MI phase (right inset—P2 at $V = 1$, $U = 4$). The dotted lines show the complementary cases (P2 in the left inset and P1 in the right inset), and are plotted in order to better highlight the different power-law versus exponential behavior. Data are for a system of $L = 400$ sites. The outer 100 sites have been discarded so as to minimize boundary effects.

We point out that we are always interested in the bulk energy gaps, even if our DMRG method preferably works with open boundary conditions. Unfortunately, the appearance of edge states in the HI phase can interfere with the determination of the bulk gaps. For this reason, we lifted the excitations at the borders by forcibly requiring to have zero particles on the leftmost site of the chain and two particles on the rightmost site. This corresponds to applying some strong field at the edges. Such a bias also breaks the ground-state degeneracy of the DW phase, thus stabilizing the numerical algorithm at large values of $V$.

4.2.1. Ground-state charge energy gap. In figure 4, we show the charge energy gap as a function of $V$ and for different numbers of sites $L$ after fixing the on-site interaction strength $U = 5$ (the same value as in figure 2). The non-monotonic behavior, with a minimum gap that closes for $L \to \infty$, indicates the presence of an insulating QPT between an MI phase on the left side and an HI phase on the right side.

A finite-size scaling of the obtained results is performed in figure 5. In the left panel, we plot the corresponding value of $V$ where the gap reaches its minimum, as a function of the system size. By linearly fitting our numerical data as a function of $1/L$, we are able to extrapolate a value at the thermodynamic limit that is equal to $V_{\text{min}}^{L \to \infty} \approx 2.98$. Under numerical accuracies, this is in agreement with the value $V \approx 2.95$ of the MI–HI QPT point that was found from the analysis of $O_{\text{string}}$ at $U = 5$. The right panel clearly shows that the minimum charge energy gap $\Delta E_c$, which is reached at the MI–HI transition, drops to zero as a power law with the size, following the behavior $\Delta E_c \sim 1/L$. This kind of behavior at the QPT transition can be explained within the conformal field theory approach, where it has been proven that finite-size corrections to the energies of low-lying gapless excitations behave as $1/L$ [24, 25].
4.2.2. Ground-state neutral energy gap. Let us now concentrate on the neutral gap $\Delta E_n$, which is plotted in figure 6 for the same Hamiltonian parameters of figure 4. Besides the QPT between the MI and the HI located at $V \approx 3$, another critical point at $V \approx 3.5$ emerges, separating the HI and the DW phase (see also figure 1). In the MI phase and in part of the HI phase, the particle and hole excitations (detected by $\Delta E_c$) are the lowest-energy excitations. As is seen from the figure, this is no longer the case for $V > V^* \approx 3.3$, starting from the middle of the Haldane phase. The presence of a marked cusp at $V^*$ indeed indicates a modification in
the nature of the lowest excitation, which becomes of a different kind. The charge gap is not able to detect such an excitation, and the transition to the DW phase, occurring at $V > V^\ast$. In contrast, the non-monotonic behavior of the neutral gap at $V^\ast$ and its dependence on the size clearly indicate it through a gap closure.

In the inset of figure 6, we analyze the behavior of the minimum neutral gap at the HI–DW transition, showing that, similarly to the minimum charge gap at the MI–HI transition, it drops to zero with the size as $1/L$ [24, 25].

Finally we remark that, for the finite sizes we considered, the neutral gap does not perfectly coincide with the charge gap at $V < V^\ast$. This slight discrepancy is barely visible from a direct comparison of figures 4 and 6, and comes from boundary effects which are more important for small sizes, and split the difference in the energies of the first charge and neutral excitations. Differences are also induced by the bias added to lift the border excitations.

5. Conclusions

In this paper, we worked out an accurate phase diagram of the extended BHM in one dimension using the DMRG algorithm with open boundary conditions. We located the SF, as well as the MI, the DW and the HI phases, by performing an up-to-date finite-size scaling with systems of up to $L = 400$ sites. Our analysis involved the order parameters for the HI and the DW and the study of the ground-state charge and neutral gaps. We point out that it would be tempting to analyze also the bipartite fluctuations of the boson number in a sub-block of the whole lattice system; this method can be employed within standard DMRG simulations and without any additional computational effort. Being able to clearly distinguish between critical and gapped
phases, it could provide more accurate data for the location of the SF region at large values of $V$ \cite{18,26}.

Besides giving rigorous predictions for future investigations of strongly correlated quantum phases in cold gases of dipolar atoms, our quantitative study is also relevant in the context of quantized transport through adiabatic pumping \cite{27}. The model we discussed here indeed supports two distinct insulating phases separated by a critical point: the MI and the HI. One can open a gap at such a point by breaking the inversion symmetry of the system (for example, via a correlated tight-binding hopping for the bosons). Therefore, by suitably tuning the various parameters of the Hamiltonian, it is possible to adiabatically encircle the MI–HI critical point. As a consequence, the non-trivial topology of the isolated gapless point inside the loop would induce the transport of a single boson through the chain \cite{28}.

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