Analytical Mean-Field Approach to the Phase Diagram of Ultracold Bosons in Optical Superlattices

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Abstract—We report a multiple-site mean-field analysis of the zero-temperature phase diagram for ultracold bosons in realistic optical superlattices. The system of interacting bosons is described by a Bose–Hubbard model whose site-dependent parameters reflect the nontrivial periodicity of the optical superlattice. An analytic approach is formulated based on an analysis of the stability of a fixed point of the map defined by the self-consistency condition inherent in the mean-field approximation. The experimentally relevant case of the two-period one-dimensional superlattice is briefly discussed. In particular, it is shown that, for a special choice of the superlattice parameters, the half-filling insulator domain features an unusual loophole shape that the single-site mean-field approach fails to capture.

1. INTRODUCTION

Although originally introduced for liquid helium in confined geometries [1], the Bose–Hubbard (BH) model proves successful in describing ultracold atoms trapped in optical lattices [2]. In this framework, the sites of the ambient lattice correspond to the local minima of the effective optical potential created by counterpropagating laser beams, and the height of the potential barriers between adjacent minima, which is proportional to the laser intensity, determines the hopping amplitude in the BH model. Such a direct relation allows for unprecedented experimental control of the model parameters and plays a key role in experiments aimed at revealing the superfluid–insulator transition characterizing the BH model [3].

In general, the superposition of simple optical lattices with commensurate lattice constants gives rise to confining potentials characterized by a richer periodicity—the so-called superlattices [4]. Reference [5] reports on a recent experiment in which a simple 1D optical superlattice is created by superimposing two 1D optical lattices [6] and a cigar-shaped magnetic potential providing for confinement in the transverse direction. Each of these optical lattices is created by the interference pattern of two laser beams crossing at a given angle. The lattice constants, determined by the crossing angle, are chosen to be \( d_1 \) and \( d_2 = 3d_1 \), so that the supercell of the resulting optical potential contains three local minima. Following this scheme, a 1-periodic 1D superlattice—i.e. a lattice characterized by a 1-site supercell—can be created by a suitable adjustment of the crossing angles determining \( d_1 \) and \( d_2 \).

Following the tight-binding-like approach of [2], a system of ultracold alkali atoms confined in a 1D optical superlattice comprising \( M \) sites is described by the following BH Hamiltonian:

\[
H = \sum_{k=1}^{M} \left[ \frac{U}{2} n_k (n_k - 1) - (\mu - v_k) n_k - t_k (a_k^+ a_{k+1} + a_{k+1}^+ a_k) \right],
\]

where \( a_k^+ \), \( a_k \), and \( n_k = a_k^+ a_k \) are, respectively, the boson creation, annihilation, and number operators relevant to the site labeled \( k \). As for the Hamiltonian parameters, \( U > 0 \) accounts for on-site repulsion (proportional to the atomic scattering length), \( \mu \) is the grand canonical chemical potential, \( v_k \) is the local potential at site \( k \), and \( t_k \) is the hopping amplitude between adjacent sites \( k \) and \( k + 1 \). The \( l \)-site periodicity of the superlattice yields

\[
t_{k+l} = t_k = t \tau_{ks}, \quad v_{k+l} = v_k = v v_k,
\]

where \( s = 0, \ldots, M/l - 1 \) labels the supercells and \( t, v \) are scaling coefficients directly related to the intensity of the laser beams that give rise to the optical potential.

As is well known, in the homogeneous case \( l = 1 \) Hamiltonian (1) is characterized by the superfluid–insulator quantum phase transition [1]. In more detail, the competition between the on-site repulsion and the kinetic energy—proportional to \( U \) and \( t \), respectively—gives rise to a zero-temperature phase diagram in the \( \mu/U-t/U \) plane consisting of an extended superfluid phase and a series of adjacent Mott-insulator lobes. In the latter, the system is remarkably characterized by a commensurate population, i.e., by an integer filling. Several numerical and analytical approaches have been adopted for the study of such a zero-temperature phase diagram. We refer the reader to [7] for a brief review of such techniques.
Recently, some attention has been devoted to the phase diagram of superlattice BH models [8–11]. In general, incompressible Mott domains are expected to occur in correspondence with critical fractional filling. In the case of 1D \( l \)-periodic superlattices, such critical fillings are integer multiples of \( l^{-1} \). Furthermore, it has been shown that, when the local potentials \( v_j \) are not all different from each other, some of the Mott domains exhibit an unusual loophole shape [12].

In this paper, we study the zero-temperature phase diagram of Hamiltonian (1) by adopting a multiple-site mean-field approach, thus generalizing the technique introduced in [13]. The latter provides satisfactory qualitative results for the quantum phase transition occurring in the homogeneous case, but fails to predict the loophole insulator domains that may appear in the case of superlattices [10]. We mention that a two-site mean-field approach is adopted in [7] for the study of homogeneous lattices. We furthermore show that, in general, the zero-temperature phase diagram can be worked out by analyzing the stability of a particular fixed point of the map defined by the mean-field self-consistency condition [10]. Many such analyses can be carried out analytically based on a perturbative expansion of the spectrum of the mean-field Hamiltonian. This allows one to determine the phase diagram by solving a numerical problem that is much less demanding than the standard iterative procedure used to deal with the original self-consistency equations. Furthermore, in some special cases, entirely analytical results can be obtained. In particular, our method provides for an analytical description of the boundaries of such a loophole domain.

2. MULTIPLE-SITE MEAN FIELD

In the simple case of the usual lattice, \( l = 1 \), qualitative information about the zero-temperature phase diagram of Hamiltonian (1) can be obtained by making use of the single-site mean-field approach introduced in [13]. Denoting by \( \langle \cdot \rangle \) the expectation value in the ground state, it is assumed that, for every \( k \),

\[
a_k a_k^+ = \langle a_k \rangle a_k^+ + a_k^\dagger \langle a_k^\dagger \rangle - \langle a_k^\dagger \rangle \langle a_k^+ \rangle. \tag{3}
\]

This allows one to recast Hamiltonian (1) as the sum of \( M \) single-site Hamiltonians, \( \mathcal{H} = \sum_{k=1}^{M} \mathcal{H}_k \), where

\[
\mathcal{H}_k = \frac{U}{2} n_k (n_k - 1) - \mu n_k - t(\alpha_{k+1} + \alpha_{k-1})(a_k + a_k^* - \alpha_k)
\]

and the so-called superfluid parameters are to be determined self-consistently as

\[
\alpha_k = \langle a_k \rangle = \langle a_k^\dagger \rangle. \tag{5}
\]

After the translational invariance characterizing the system is taken into account, \( \alpha_k = \alpha_{k+1} = \alpha \), the Hamiltonians in Eq. (4) are decoupled and become formally identical. The original problem thus reduces to the study of one single-site Hamiltonian. In this framework, the Mott-insulator domains in the \( \mu/U-l/U \) phase diagram are characterized by the vanishing of the superfluid order parameter. Indeed, in this case it is easy to check that the local density of bosons \( \langle n_k \rangle \) is pinned at an integer value and the system is incompressible.

In inhomogeneous structures translational invariance is lost, and the single-site Hamiltonians in Eq. (4) are coupled by self-consistency conditions (5). This single-site mean-field approach gives fairly satisfactory qualitative results for superlattices whose supercell features local potentials \( v_l \) that are all different from each other [10], but it fails to capture the loophole-shaped insulator domains that appear when some of these potentials are equal [12].

A more structured approach that takes into account the nontrivial periodicity of a \( l \)-periodic superlattice involves adopting approximation (3) every \( l \)th site. By doing so, Hamiltonian (1) becomes the sum of identical \( l \)-site Hamiltonians, one for each supercell, and, as in the single-site approach, the original problem reduces to the study of one such supercell Hamiltonian. Dropping the supercell index, the latter reads

\[
\mathcal{H} = \sum_{k=1}^{l} \left[ \frac{U}{2} n_k (n_k - 1) - (\mu - v_k)n_k \right]
\]

\[
- \sum_{k=1}^{l-1} t_k (a_k a_{k+1}^* + a_{k+1}^* a_k) - t_l \alpha_l (a_1 a_1^* + a_l a_l^*) - 2 \alpha_l \alpha_1,
\]

where

\[
\alpha_j = \langle a_j \rangle = \langle a_j^\dagger \rangle, \quad j = 1, l. \tag{7}
\]

This approach is expected to give satisfactory results if approximation (3) is adopted for the hopping terms characterized by the lowest hopping amplitude, \( t_l < t_h \).

\[1\] The superfluid parameters defined in Eq. (5) are real, since the boson operators in Eq. (4) have a real representation on the usual Fock basis.
As in the single-site approximation, the Mott-insulator phase is characterized by vanishing superfluid parameters: \( \alpha_1 = \alpha_l = 0 \). In this situation, the mean-field Hamiltonian \( \mathcal{H} \) commutes with the total number of bosons (in the supercell), \( \sum_{k=1}^M n_k \). Hence, the expectation value of the latter on the ground-state is fixed to an integer value determined by the Hamiltonian parameters and, quite interestingly, the filling of the system is a fixed point of the map in Eq. (8) for any value of the superfluid parameters.

The most standard approach to the mean-field problem defined by Eqs. (6) and (7) consists of an iterative numerical procedure. In more detail, the superfluid parameters appearing in multiple-site Hamiltonian (6) at a given iteration are determined evaluating Eq. (7) on the ground state of the previous iteration. The procedure is arrested when the value of the superfluid parameters does not change significantly between two subsequent iterations.

3. ANALYTICAL APPROACH

The standard iterative procedure illustrated above shows that solving the self-consistency problem in Eqs. (6) and (7) amounts to finding a stable fixed point of the map

\[
\begin{align*}
\alpha'_1 &= F_1(\alpha_1, \alpha_1) \\
\alpha'_l &= F_l(\alpha_1, \alpha_l),
\end{align*}
\]

where \( F_j(\alpha_1, \alpha_l) \equiv \langle a_j \rangle \), \( j = 1, l \). Note that the choice \( \alpha_1 = \alpha_l = 0 \), corresponding to the Mott-insulator phase, is a fixed point of the map in Eq. (8) for any value of the Hamiltonian parameters \( \mu, U, \{ t_k \}, \{ v_k \} \). Indeed, as we mentioned in the previous section, in this situation the ground state of the system belongs to a fixed-number subspace and the expectation values in Eq. (7) necessarily vanish. This means that the insulator domains are characterized by choices of the Hamiltonian parameters that make the fixed point \( \alpha_1 = \alpha_l = 0 \) stable. According to the standard criterion, this happens when the absolute values of the eigenvalues of the Hessian matrix

\[
\begin{pmatrix}
\partial_{\alpha_1} F_1(\alpha_1, \alpha_l) & \partial_{\alpha_l} F_1(\alpha_1, \alpha_l) \\
\partial_{\alpha_l} F_l(\alpha_1, \alpha_l) & \partial_{\alpha_l} F_l(\alpha_1, \alpha_l)
\end{pmatrix}
\]

are smaller than 1.

Note that the Hessian matrix is completely determined by a first-order expansion of \( F_j \) in the parameters \( \alpha_1, \alpha_l \), which can in turn be obtained from a first-order expansion of the ground state of \( \mathcal{H} \) in the same parameters. Since the term \( t_l a_l a_l \) in Eq. (6) does not contribute first-order corrections to the ground state of \( \mathcal{H} \), it can be discarded without loss of generality. After this, the desired first-order approximation can be obtained using \( t_l \) as the perturbative parameter, since it multiplies all of the first-order terms in \( \alpha_l \) and \( \alpha_l \) appearing in Eq. (6):

\[
\begin{align*}
\mathcal{H} &= \mathcal{H}_0 + t_l V, \\
V &= -\alpha_l (a_l + a_l^+) - \alpha_l (a_1 + a_1^+).
\end{align*}
\]

Since the unperturbed Hamiltonian \( \mathcal{H}_0 \) commutes with the total number of bosons (in the supercell), its eigenstates belong to fixed-number subspaces. Denoting by \( |\psi_0\rangle \) such eigenstates and by \( \epsilon_k \) the relevant eigenvalues, the first-order approximation to the ground state of \( \mathcal{H} \) is \( |\psi\rangle = |\psi_0\rangle + t_l |\psi_1\rangle \), where \( |\psi_0\rangle \) is the unperturbed ground state and

\[
|\psi_1\rangle = \sum_{k \neq 0} \frac{\langle \phi_0 | V | \phi_0 \rangle - \epsilon_k | \phi_0 \rangle}{\epsilon_0 - \epsilon_k}.
\]

This means that

\[
F_j(\alpha_1, \alpha_l) = \langle \psi | a_j | \psi \rangle = \langle \phi_0 | a_j | \phi_0 \rangle + \langle \psi_1 | a_j | \psi_0 \rangle = \langle \phi_0 | a_j + a_j^+ | \psi_0 \rangle - \alpha_1 c_{j1} + \alpha_l c_{j1},
\]

where

\[
c_{jk} = t_l \sum_{k \neq 0} \frac{\langle \phi_0 | a_j + a_j^+ | \phi_0 \rangle - \epsilon_k | \phi_0 \rangle}{\epsilon_0 - \epsilon_k}.
\]

Therefore, as we have mentioned, the Hessian matrix in Eq. (9) is determined in terms of the coefficients appearing in first-order approximation (13) and defined in Eq. (14), and the condition for the stability of fixed point \( \alpha_1 = \alpha_l = 0 \) is

\[
|c_{11} \pm \sqrt{c_{11}^2} \sqrt{c_{11}^2} | \leq 1.
\]

Since the coefficients in Eq. (14) depend on the Hamiltonian parameters in Eqs. (1) and (2) through the eigenvalues and eigenstates of \( \mathcal{H}_0 \), inequality (15) allows one to determine the regions of the \( \mu/U - t/U \) plane pertaining to the Mott-insulator phase. According to the above discussion, within such a phase the (integer) number of bosons in each supercell is

\[
N = \langle \phi_0 | \sum_{k=1}^C n_k | \phi_0 \rangle
\]

and corresponds to the fractional filling \( f = N/l \).

Note that the study of the phase space by inequality (15) is much less demanding than the standard iterative procedure briefly illustrated in the previous section. Indeed, for a given choice of the Hamiltonian parameters, the latter involves the iterative diagonalization of a matrix whose size is \( \sum_{k=0}^{C} d_k \), where \( d_k = (k+l-1)!/k!(l-1)! \) is the dimension of the subspace relevant to \( k \) bosons in \( l \) sites and \( C \) provides a cutoff for the (in principle) infinite Hilbert space of the problem.
Conversely, no iterative procedure is required for the study of inequality (15). Indeed, it is sufficient to diagonalize only the three (independent) blocks of \( \mathcal{H}_0 \) relevant to the total numbers of bosons \( N-1, N, \) and \( N+1 \), where \( N \) is the cell population characterizing the Mott domain under investigation. Furthermore, as we illustrate in the following, in some simple cases inequality (15) can be studied in a completely analytical way.

4. RESULTS: \( l = 2 \) SUPERLATTICE

In this section we consider the realistic case of a \( l = 2 \) 1D superlattice, which can be created as in [5] by superimposing two homogeneous 1D optical lattices with lattice constants \( d_1 \) and \( d_2 = 2d_1 \). The insulator domains relevant to the lowest fractional fillings (dark gray), as evaluated by means of a numerical study of inequality (15), are displayed in the figure for the parameter choice \( U = 1.0, \tau_1 = 1.0, \tau_2 = 0.3, \nu_1 = 0.00 \), and, from the top to the bottom panel, \( \nu_2 = 0.12, 0.06, 0.03, 0.00 \). Note that the width at \( t/U = 0 \) of the half-filling insulator domain equals the energy offset between the sites of the same supercell, \( \nu_2 - \nu_1 \) [10]. As the latter vanishes, the insulator domain assumes an unusual loophole shape [12].

In this special case, \( \nu_1 = \nu_2 \) (bottom panel of the figure), the study of inequality (15) involves the diagonalization of \( 2 \times 2 \) matrices and can be carried out in a completely analytical way. After some calculations, it is possible to show that the loophole-domain border is determined by the following equation:

\[
0 = 3\tau_1^2(\tau_1 + \tau_2)t^3 + [U(2\tau_2 - \tau_1) + \mu(5\tau_1 + 2\tau_2)]\tau_1 t^2 +\mu^2(\tau_1 - \tau_2)t + U\mu^2 - \mu^3. \tag{16}
\]

A simple analysis shows that the loophole domain disappears when no positive \( t \) satisfies the preceding equation for \( \mu = 0 \), i.e., when \( \tau_1 < 2\tau_2 \). However, this is an artifact introduced by the mean-field approximation, which is known to provide at best qualitative information. As is shown in [12], the loophole domain can be proven to exist for any \( \tau_2 \neq \tau_1 \) by resorting to the exact mapping between the hard-core limit \( (t/U \ll 1) \) of Hamiltonian (1) and the model for spinless noninteracting fermions on the same superlattice.

5. CONCLUSIONS

In this paper, we introduce a multiple-site mean-field approach to the study of the zero-temperature phase diagram for ultracold bosons in realistic one-dimensional superlattices. A perturbative expansion in the hopping amplitudes between neighboring supercells allows one to recast the self-consistency constraints involved in this approach into a problem that requires a numerical effort much less demanding than the usual iterative procedure.

Relying on such a multiple-site mean-field approach, we supply some explicit results for the experimentally relevant case of a two-periodic superlattice. In particular we show that, as the energy offset between the sites of the supercell decreases, the superfluid phase clamps around the half-filling insulator domain, which assumes an unusual loophole shape for a vanishing energy offset. Our multiple-site mean-field approach shows that this “clamping effect” of the superfluid phase likewise occurs around all of the fractional-filling insulator domains of the \( l = 2 \) superlattice. Similar and even more complex “clamping effects” can be shown to occur on more structured superlattices [12].

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