Doorway states and the Bose-Hubbard model

A. N. Salgueiro, Chi-Yong Lin, A. F. R. de Toledo Piza, and M. Weidemüller

1 Instituto de Física, Universidade de São Paulo, CP 66318 CEP 05389-970, São Paulo, Brazil
2 Department of Physics, National Dong Hwa University Hua-Lien, Taiwan, R.O.C.
3 Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany

We use the concept of doorway states to solve the finite Bose-Hubbard model. This method allows for the inclusion of many-body correlations in a dynamically motivated hierarchical way, yielding useful approximations even within subspaces of the full Hilbert space of greatly reduced dimensionality. Moreover, we apply the doorway method to solve the problem of \( N \) bosons in a lattice, where the chemical potential, the on-site fluctuations, the visibility of the interference pattern arising from atoms in a one-dimensional periodic lattice and the width of the interference peak are calculated. Excellent qualitative agreement with exact numerical calculations as well as recent experimental observations is obtained.

PACS numbers: 03.75.Lm, 03.75.Hh, 03.75.Gg

I. INTRODUCTION

The physics of strongly interacting quantum systems has been subject of intense investigations since the early days of quantum mechanics. With the recent developments in the field of ultracold quantum gases, systems of strongly correlated bosonic and fermionic atoms with tunable interactions have become amenable to experimental studies \([6–9]\). Complete theoretical understanding of these coupled many-body systems is difficult, and only rare examples exist, for which analytical solutions for the ground state could be explicitly been given \([6]\). Of particular importance in this context is the Bose-Hubbard model, which can describe bosons or fermions in an optical lattice or in a double well potential. This model serves as a prototype system exhibiting a quantum phase transition \([12]\). Triggered by the recent observation of this phase transition from a superfluid to a Mott-insulating phase with bosonic atoms in one-dimensional (1D) and three-dimensional (3D) optical lattices \([2, 4, 13]\), the ground state and correlation properties of the Bose-Hubbard model have been extensively investigated by a large number of groups \([14–16]\). Complete theoretical understanding of these coupled many-body systems is difficult, and only rare examples exist, for which analytical solutions for the ground state could be explicitly been given \([6]\). The description generally has to rely upon approximation of numerical or analytical methods such as the density-group-renormalization \([7]\), quantum Monte Carlo approaches \([11]\), perturbative calculations \([27]\), and mean-field treatments \(e.g.,\) Gutzwiller ansatz \([8–10]\). In this context, it is necessary to introduce different methods which give the energy spectrum of a many-body hamiltonian and its respective eigenstates or at least the ground-state.

In this paper, we use the concept of doorway states to study bosons in a double well and bosons in an optical lattice. Both systems can be described by the Bose-Hubbard model. The method is based on the construction of doorway projectors as initially introduced by Feshbach in the context of scattering theory in Nuclear Physics to explain the appearance of intermediate structures in the cross section \([17]\). The main idea underlying this approach is a dynamically motivated decomposition of the full Hilbert space of the hamiltonian into a sequence of mutually orthogonal subspaces. The first subspace in the hierarchy is chosen on the basis of its particular relevance to the problem at hand and making use of the symmetries of the hamiltonian. In the original context of nuclear reactions this subspace spans the open channels. In the context of the Bose-Hubbard model, it spans the analytical lowest energy solutions of the pure hopping or the pure superfluid limiting cases, when one is interested in approximating the system ground-state. Subsequent subspaces are chosen as spanned by new state vectors generated from the action of the hamiltonian on each partially defined subspace. Formally, this is implemented by establishing a sequence of mutually orthogonal projectors \(P, D_1, D_2, \cdots\) such that \(P + \sum_i D_i\) is the identity operator and the hamiltonian has non-vanishing matrix elements only between states in consecutive members of the hierarchy. This hierarchy allows for dynamically controlled truncation schemes which may significantly reduce the computational effort. The advantage of the doorway approach is that it can be used as a numerical or analytical tool. The doorway method is also known as projection formalism and continued-fraction representation \([19]\). Moreover, this approach can be seen as a generalization of the several other schemes developed in different areas of many-body physics, such as the Lanczos method \([20]\) of Solid State physics, the resolvent method \([21]\) of Quantum Optics, and the Feshbach-Fano partitioning method \([22]\) of Quantum Chemistry. Note, in particular, that in each of these methods the subspaces are one-dimensional.

Usually it is much more difficult to obtain the eigenstates of a given hamiltonian rather than the eigenvalues of the energy. In this context, the way the doorway
method is constructed creates a reduced subspace where the Bose-Hubbard Hamiltonian can be projected. The projection of the Hamiltonian in this reduced subspace allows for the knowledge of part of the energy spectrum and its correspondent eigenstates. We are mainly interested in the ground-state of this system which features both the superfluid and Mott-insulator regimes. In this context, the energy spectrum with the same symmetry of the ground-state and the ground-state wavefunction of the Bose-Hubbard model is calculated. Furthermore, the correlation properties of a low density bosonic system in an optical lattice are calculated over the full range of coupling parameters and found to qualitatively describe the measurements of $^8$He, even though these experiments are inhomogeneous systems due to the presence of an external trap.

The paper is organized as follows. In section II a more formal presentation of the doorway approach is given. In section III the doorway approach is applied to solve $N$ bosons distributed in $M$ sites, described by the Bose-Hubbard model. In subsection III A we start with $M = 2$ sites and the doorway method is used to obtain the energy spectrum and the ground-state. In subsection III B the approach is applied to the more general case ($N$ boson distributed among $M$ sites), where experimental observables such as chemical potential, on-site variance and visibility are calculated.

II. DESCRIPTION OF THE DOORWAY METHOD

The doorway method consists in splitting the full Hilbert space of the many-body Hamiltonian $H$ into different subspaces which are accessed by the action of projectors on $H$. Let $P$ be the projector onto the subspace $\mathbb{P}$ generated by a set of state vectors which are relevant for the lowest order approximation to the system at hand. Specific choices in connection with Bose-Hubbard systems are discussed in the subsections below. $\mathbb{P}$ is in general multi-dimensional, so that $P = \sum_{i=1}^{k} |p_i\rangle \langle p_i|$ in terms of an orthonormal set of state vectors $\{|p_i\rangle\}_{i=1,\ldots,k}$. From $P$, it is possible to construct the basis which generates the first doorway subspace by the action of $|d_i^{(1)}\rangle \equiv (1 - P)H|p_i\rangle$ which have to be normalized. The second doorway subspace is defined by $|d_i^{(2)}\rangle \equiv (1 - P - D_1)H|d_i^{(1)}\rangle$, with $|d_i^{(1)}\rangle$ as the normalized first doorway state. The second doorway $|d_i^{(2)}\rangle$ has also to be normalized. The orthogonalization of the doorway states is done at each step. The procedure terminates when $(1 - P - D_1 - D_2 - \cdots - D_k)H|d_i^{(k-1)}\rangle = 0$ with $D_j = \sum_{i=1}^{k} |d_i^{(j)}\rangle \langle d_j^{(j)}|$ ($j = 1, 2, \ldots, n$) denoting the projectors onto the doorway spaces. The space $\mathbb{P} \oplus \mathbb{D}_1 \oplus \cdots \oplus \mathbb{D}_n$ then represents an irreducible subspace for the Hamiltonian containing the initial subspace $\mathbb{P}$. The crucial point is the choice of the most adequate starting state $|p_i\rangle$ to generate the initial subspace to obtain the solution in the most efficient way. The many-body Schrödinger equation is solved in this subspace

\begin{equation}
(E - H_{PP} - H_{PD} - \frac{1}{E - H_{D,1} - M_{i,2}} H_{D,P})|\psi\rangle = 0, \quad (1)
\end{equation}

where $H_{PP} = PHP$, $H_{D,1} = D_1$ and $H_{D,P} = D_i$ with $i, j = 1, 2 \ldots n$. Using the second equation recursively, one obtains a nonlinear problem within the $P$-subspace which determines the eigenvalues of the Hamiltonian in the full Hilbert space. All orders of interactions described by the Hamiltonian are taken into account inside this subspace. Therefore, the expansion is not perturbative in the couplings, but it represents the full solution in a subspace of lower (reduced) dimension. Once the solution is truncated, the diagonalization of the Hamiltonian happens within the used subspace (e.g. $\mathbb{P} \oplus \mathbb{D}_1 \oplus \cdots \oplus \mathbb{D}_{\text{last used}}$).

Information about the eigenstates of the system can be obtained by projecting the original Hamiltonian in the reduced subspace created by the doorway states, which can be either complete or truncated, depending on the physical system. In this case the quantities $\tilde{H}_{PP} = \langle P|H_{PP}|P\rangle$, $\tilde{H}_{D,1} = \langle D_1|H_{D,1}|D_1\rangle$, $\tilde{H}_{D,P} = \langle D_i|H_{D,P}|P\rangle$ are the matrix elements of the reduced Hamiltonian. In spite of the original doorway procedure giving no information about the eigenstates of the system, one can use the reduced subspace which is created by the doorway states to project the Hamiltonian in this reduced subspace, and then diagonalize it to obtain information about the eigenstates of the system.

III. DOORWAY METHOD APPLIED TO THE BOSE-HUBBARD MODEL

We apply the doorway method to a system of $N$ bosons in a 1D optical lattice of $M$ sites in the homogeneous case. The system is described by the Bose-Hubbard model

\begin{equation}
H = -J \sum_{j=1}^{M} (a_{j}^{\dagger}a_{j+1} + \text{h.c.}) + \frac{U}{2} \sum_{j} n_{j}(n_{j} - 1) \quad (2)
\end{equation}

which can be seen as a many-mode approximation for an ultracold gas of bosonic atoms occupying the lowest band in a periodic array of potential wells $\mathbb{D}_1, 2, \ldots$. The operators $a_{j}^{\dagger}$ and $a_{j}$ are the creation and annihilation operators, respectively, of a boson in the $j$-th site, and $n_{j}$ is the number of atoms at the lattice site $j$ ($j = 1, \ldots M$). The strength of the on site repulsion of two atoms on the lattice site $i$ is characterized by $U$. The parameter $J$ is the hopping matrix element between adjacent sites which characterizes the strength the tunneling term. A periodic boundary condition is included allowing for tunneling between the first and the last site of the lattice (site $M+1 = 1$).
site 1). In the case of $M = 2$ sites, the periodic boundary condition is already intrinsic.

In this paper, we consider the Bose-Hubbard Hamiltonian with periodic boundary conditions. Moreover, the Bose-Hubbard Hamiltonian with periodic boundary conditions conserves two important quantities: the total number of particles and the total quasi-momentum. As a consequence, its Hilbert space can be partitioned into $M$ decoupled subspaces corresponding to the values of quasi-momentum ($q=0,...,M-1$). Furthermore, the subspace with $q=0$ and, for even $M$, also the subspace with quasi-momentum $q=M/2$, can be further partitioned into symmetric and antisymmetric subspaces ("odd-even" symmetry) $^{[20]}$. The ground state of the system lies in the symmetric $q = 0$ subspace. Thus, the initial $\mathbb{P}$ subspace is chosen within this subspace. The full set of doorway subspaces constructed from the initial $\mathbb{P}$ subspace will finally span the symmetric part of the subspace with zero quasi-momentum, providing the full solution for the ground state. In order to define the $\mathbb{P}$ subspace, one can use the fact that the ground state of the system has two different limiting cases: the superfluid phase for $J \gg U$ where the particles are delocalized over the whole lattice, and the Mott-insulating phase for $J \ll U$ where the particles are localized with an equal number of atoms per site $n_0 = N/M$.

A. Two-site Bose-Hubbard model

To illustrate how the method works, we first apply the doorway method to the two-site Bose-Hubbard model, which corresponds to $N$ bosons in a double-well. First, the doorway method is used to construct the reduced subspace the two-site Bose-Hubbard Hamiltonian is projected. The projected Hamiltonian can be diagonalized. Analytical expressions for the matrix elements of the reduced Hamiltonian $\hat{H}_{pp}$, $\hat{H}_{pd_{i}}$, $\hat{H}_{dd_{i}}$, and $\hat{H}_{dd_{i+1}}$ are found. We start the doorway construction for the repulsive case using different $|p\rangle$ states, since there is a crucial difference between the ground state for $N$-even and $N$-odd. For $J = 0$, the $N$-even ground state is non-degenerate, $|p\rangle = |(N/2)(N/2)\rangle$, where the number of particles per site is an integer (Mott-insulator) while the $N$-odd ground state is degenerate $|p_{\pm}\rangle = 1/\sqrt{2}|((N+1)/2,(N-1)/2)\rangle \pm |(N-1)/2,(N+1)/2)\rangle$. In the first case $P$ is one-dimensional and in the second case $P$ is bi-dimensional. Now that $P$-projectors are defined, the doorway projectors can be built. For $N$-even the total doorway projector is given by $D = \sum_{i=1}^{l} D_{i}$, where $l = N/2$ and generator state of the doorway subspace is $|d_{i}\rangle = (1/\sqrt{2})|((N/2+i)(N/2-i))\rangle + |(N/2-i)(N/2+i))\rangle$, where $i$ is the number of particles one can remove or add to a particular site ($1 \leq i \leq N/2$). For $N$-odd the doorway projector is given by $D = \sum_{i=1}^{l}(D_{i} + D_{i-})$, where $l = (N-1)/2$ and the two unconnected type of generator states of the doorway subspace are related to the symmetric and antisymmetric subspace, namely $|d_{\pm}\rangle = (1/\sqrt{2})|((N + 1)/2 + i),((N - 1)/2 - i))\rangle \pm |((N - 1)/2 - i),((N - 1)/2 + i))\rangle$, where $i$ is the number of particles one can remove or add to a particular site ($1 \leq i \leq (N - 1)/2$). Now that we know all doorway projectors and $P$, the Bose-Hubbard Hamiltonian can be projected in the subspace generated by them and the matrix elements of the projected Hamiltonian $\hat{H}_{pp}$, $\hat{H}_{pd_{i}}$, $\hat{H}_{dd_{i-1}}$, and $\hat{H}_{dd_{i}}$, where $1 \leq i \leq n_{0} = l$, with $l = N/2$ for $N$ even and $l = (N - 1)/2$ for $N$ odd, can be calculated. For $N$-even,

$$\hat{H}_{pp} = \frac{U}{2}N(\frac{N}{2} - 1)|p\rangle\langle p|$$

$$\hat{H}_{pd_{i}} = -J\sqrt{N(N/2 + 1)}|p\rangle\langle d_{i}|$$

$$\hat{H}_{dd_{i}} = \left[\frac{U}{2}N(\frac{N}{2} - 1) + U|p\rangle\langle d_{i}|$$

$$\hat{H}_{dd_{i-1}d_{i}} = -2J\sqrt{N(N/2 + 1)}|d_{i-1}\rangle\langle d_{i}|$$

while for $N$-odd

$$\hat{H}_{pp} = \frac{|U|}{4}(N - 1)^{2} - \frac{J(N + 1)}{2}|p_{+}\rangle\langle p_{+}|$$

$$\frac{|U|}{4}(N - 1)^{2} + \frac{J(N + 1)}{2}|p_{-}\rangle\langle p_{-}|$$

$$\hat{H}_{dd_{i}} = \left[\frac{|U|}{4}(N - 1)^{2} + U(i + 1)|d_{i}\rangle\langle d_{i+1}| + |d_{i}\rangle\langle d_{i-1}|$$

$$\hat{H}_{dd_{i-1}d_{i}} = -(J/2)\sqrt{((N + 1)^{2} - 4i^{2})}|d_{i-1}\rangle\langle d_{i+1}|$$

Consequently the diagonalization of the reduced Hamiltonian can be performed. The doorway solution of the energy spectrum of the system is, of course, in perfect agreement with the exact diagonalization of the Hamiltonian. The doorway solution of the energy spectrum, which corresponds to the exact one, can be fully generated by considering $N/2 + 1$ ($N$ even or odd) doorways for the symmetric and $N/2$ ($N$ even) or $N/2 + 1$ ($N$ odd) doorways for the antisymmetric situation. It is well-known that the energy spectrum of this system is composed of regions with and without quasi-degenerate doublets $^{[22]}$ which is confirmed by the doorway solution. The degeneracy of the doublets is broken as the tunneling parameter increases. The same analysis can be extended to the case of attractive on-site interaction.

In the case considered here, the doorway method is optimized to give information about the eigenstates of the system, but the attention will be focus on the ground-state/first excited state and the last two excited states of the system. The general form of the ground state of this system with $N$-even number of particles as a function of the tunneling parameter is $|\psi_{g}\rangle = \alpha_{p}|p\rangle + \sum_{i=1}^{N/2} \alpha_{d_{i}}|d_{i}\rangle$. For this particular case, the ground-state is analogous to the Mott state for the two-site Bose-Hubbard model. This ground-state is an unique state. However, the ground state of the system with $N$ odd is
a degenerate doublet for $J/U = 0$. This degeneracy of the ground state is lifted as the tunneling parameter increases. Thus, one of the states of the quasi-degenerate doublet becomes the ground-state while the other state becomes the first excited state. The ground-state and the first excited state are given respectively by $|\psi_0\rangle = \alpha_p |P_+\rangle + \sum_{i=1}^{(N-1)/2} \alpha_{d,\sigma} |d_{\sigma}\rangle$ and $|\psi_1\rangle = \alpha_p |P_-\rangle + \sum_{i=1}^{(N-1)/2} \alpha_{d,\sigma} |d_{\sigma}\rangle$, as a function of the tunneling parameter. We compare the form of the wave-functions discussed above with the semi-classical solution. The semi-classical solution does not distinguish if $N$ is even or odd as the quantum one does. The semi-classical solution is always localized (see ref. [23]). It also does not make any difference if the on-site interaction is repulsive or attractive.

The last two excited states are a quasi-degenerate doublet, where one of the states of the doublet. For $J/U = 0$, the last two excited states are given by $|\psi_{e\pm}\rangle = 1/\sqrt{2} |0\rangle \pm |N\rangle \equiv \{d_{\text{last}}\}$ and for $J/U \neq 0$ new components are created in the states $|\psi_{e\pm}\rangle = \alpha p |P_\pm\rangle + \sum_{i=1}^{(N-1)/2} \alpha_{d,\sigma} |d_{\sigma}\rangle$. These excited states represent even-odd macroscopic superpositions (even and odd Schrödinger cat states). Nowadays, enormous effort has been put to create such states, since they are important to quantum information, spectroscopy and so on. Those states have been theoretically found before as the symmetry-preserving-class of solutions of the GP equation which preserves the symmetry [24]. It has been observed these even-odd macroscopic superpositions do not lose their strength until $J/U = 1$, and after that point, they start to disappear very quickly. To understand why they are more robust than any other states of spectrum, one has to look how the energy spectrum changes as a function of the tunneling parameter. These states are the last to be affected by the increase of tunneling parameter. It is the last degeneracy to be broken. even with a considerable vale of the tunneling parameter $J/U$.

\section*{B. Bose-Hubbard model for a lattice}

We extend the previous analysis to a more general case, the Bose-Hubbard model for a lattice ($M$-sites). Moreover, observables of one-body and two-body, such as chemical potential, variance and visibility are calculated with the help of the doorway method. For the commensurable situation ($N = n_0 M$) we choose $|p\rangle = |n_0\rangle^0 M$ corresponding to the ground state of the system in the pure Mott case ($U \gg J$), which generates a one-dimensional subspace $P$. If an extra particle is added to or removed from the system ($N \pm 1 = n_0 M \pm 1$) (non-commensurate situation), the initial multi-dimensional subspace $P$ is generated and has the form $P = \sum_{i=1}^{M} |p_i\rangle \langle p_i|$, where $|p_i\rangle = |(n_0 \pm 1)_i n_0^M\rangle$. Starting from these initial subspaces the correspondent doorway subspaces are constructed. For non-commensurate situation, however there is a simpler way to obtain only the ground-state, which is to start instead with the symmetric superposition $|p\rangle = \frac{1}{\sqrt{M}} \sum_{i=1}^{M} \{n_0 \pm 1\}_i n_0^M$. Furthermore, the doorway method gives the flexibility to choose another states as the starting point $|p\rangle$. Depending on the parameters of interest, one may also start from the pure superfluid state $(J \gg U)$ as the initial state $|p\rangle$ in the construction of the doorways, following the same procedure discussed in the section before. We will use this flexibility to study the on-site variance later. After finishing to generate the doorway subspaces, the part of the energy spectrum and the ground-state are obtained by solving by projecting the $M$-site Bose-Hubbard hamiltonian in the reduced subspace created by $P$ and doorway projectors. Unfortunately for this general case, it is not easy to obtain analytical expressions for the matrix elements of the reduced hamiltonian as in the previous case ($M = 2$). The exact ground-state of the system can be described in general as $|\psi_0\rangle = \sum_i a_i |d_i\rangle$, where $|d_0\rangle = |p\rangle$, where $n$ is the number of last generated doorway. One can check that the superfluid ground state $|\psi_{SF}\rangle \sim \left( \sum_{i=1}^{M} a_i \right) |0\rangle$ is asymptotically reached for $J/U \to \infty$.

The doorway method genuinely reduces the numerical effort to the diagonalization of the very small, but relevant part of the total Hilbert space. For small number of sites, it is possible to obtain numerically the full solution of the energy spectrum and ground state. However, for larger number of sites, it is not so easy to generate all doorways one needs to obtain the full solution because of numerical reasons, such as lack of available memory. In this context it is important to discuss the convergence of the method. A good measure for the convergence of the method is given by the "reliability" defined as $R = \sum_{i=0}^{n'} \langle \psi_0 | d_i \rangle^2$, where $|\psi_0\rangle$ being the exact ground state of the system obtained from the exact numerical diagonalization of the Bose-Hubbard Hamiltonian and $n'$ being the maximum number of doorways to generate the truncated solution. The meaning of the reliability can be understood in terms of the portion of the full symmetric subspace which has been covered by the truncated solution. The convergency of the method scales linearly with the number of particles for the commensurate and incommensurate cases. We have tested this convergency for cases we are able to obtain the exact solution. Fig.\textbf{1}a illustrates this convergency for $M = N = 5$, considering the truncated solution for $n = 2, 3, 2, 5, 16$ doorways. The convergency is then achieved after the fifth doorway $|d_5\rangle$ is created, showing the subspace spanned by the doorways already include the most relevant portion of the full symmetric subspace. For this particular case, the Hilbert space is of dimension $\left( \begin{array}{c} N+M-1 \end{array} \right) = 126$ whereas the symmetric zero quasi-momentum subspace has only dimension 16. The convergency of the method is surprisingly fast, since the recursive construction of the doorway states "automatically" creates the most efficient path into the irreducible subspace depending on the specific values of the parameters $U$ and $J$. 


Chemical potential: We derive the ground state energy and the chemical potential \( \mu_{N}/U = [E_{N}^{+} - E_{N}]/U \) as a function of the dimensionless tunneling parameter \( J/U \). Fig. 1(b) shows the chemical potential as a function of \( J/U \) comparing the exact solution of the Bose-Hubbard hamiltonian (dashed lines) with the result of the doorway method (solid lines) for the case of \( M = 5 \) sites. The distance between the apparent parallel lines of Fig. 1(b) is almost \( 1/M \), which vanishes in the thermodynamic limit \( (N, M \to \infty \; \text{and} \; N/M \text{finite}) \), characterizing the phase transition point where the two limiting curves \( \mu_{n0M} \) and \( \mu_{n0M+1} \) are the same. For convenience, the doorway method has only been applied to the limiting cases \( N = n0M \) and \( N = n0M \pm 1 \) where the determination of the corresponding initial states is described above. The curves inside the lobes are only shown for the exact calculation and they represent the evolution of the \( M \)-degenerate states of \( J = 0 \) as a function of the hopping parameter.

On-site number fluctuation: As a second application of the doorway method, we determine the on-site number fluctuation of the ground state \( \sigma_{i} = \sqrt{\langle n_{i}^{2} \rangle - \langle n_{i} \rangle^{2}} \) as a function of \( U/J \) and as a function of \( J/U \). The results are shown in Fig. 2. Depending on the regime, the most efficient construction of the doorways starts from either a pure superfluid state (left graph) or the Mott-insulator state (right graph). For small \( U/J \), the on-site fluctuations are found to decrease linearly starting from the initial value given by \( \sqrt{\frac{N}{2}(1 - \frac{1}{M})} \). At intermediate \( U/J \), the decrease curve changes slope in the region of the phase transition and finally approaches the dependence \( 2\sqrt{n0(n0+1)} \), which is identical to the perturbative result for the ground state wavefunction \( |\psi\rangle \approx |n0\rangle^{\otimes M} + \frac{1}{M} \sum_{\langle i,j \rangle} a_{i}^{\dagger}a_{j}^{\dagger}|n0\rangle^{\otimes M} \) with \( \langle i,j \rangle \) denoting the next neighbor sites. The results of the doorway method agree well with an analysis by Roth and Burnett based on the calculation of the superfluid fraction under twisted boundary conditions [14, 19]. Starting from the pure Mott-insulator state, we derive the on-site number fluctuations for \( J/U \ll 1 \) (right graph in Fig. 2). In the pure Mott phase, no correlations among the particles exist and the one-site number fluctuations vanish. As \( J/U \) increases, correlations are created resulting in a steady increase of the fluctuations. After the phase transition region is crossed, the fluctuations approach the asymptotic value for \( U/J = 0 \). It is instructive to compare the result with the commonly used Gutzwiller ansatz [3, 10] which, by construction, does not provide particle correlations and thus genuinely underestimates on-site fluctuations at small \( J/U \). The short-range correlations of the particles have to be included by additional perturbative terms [10]. Since the groundstate wavefunction constructed by the doorway method contains all relevant many-body correlations, the on-site fluctuations are rendered correctly for small \( J/U \) as well as for the region of the phase transition at intermediate values of the tunneling parameter.

Interference pattern and visibility: To demonstrate the efficiency of the doorway method for the determination of important experimental observables, the interference of atoms released from an optical lattice is modeled and the dependence of the visibility and the width...
of the first resonance peak of the matter-wave interference pattern on the parameter $J/U$ is derived. Comprehensive studies of these two quantities have recently been performed by Gerbier et al. \cite{18, 28} for 3D optical lattice and by Stöferle et al. as well as M. Köhl et al. for 1D optical lattice \cite{13}. The observed interference pattern is directly related to the Fourier transform of the single-particle density matrix $\rho_{ij} = \langle a_j^\dagger a_i \rangle$. Therefore, measurements of the visibility are particularly sensitive to short-range coherence induced by the tunneling of the particles. Following the derivation in Refs. \cite{14, 29}, the intensity is calculated for a one-dimensional lattice as

$$I = \frac{1}{M} \sum_{i,j=1}^{M} \exp(ik(r_i - r_j)) \langle a_j^\dagger a_i \rangle$$

where $k$ denotes the wave vector of the expanding matter wave after release from the lattice point $r_i$ or $r_j$, respectively. The result of the doorway method for $N = 8$ particles distributed over $M = 8$ sites, starting from the pure Mott state and taking nine doorways into account, is shown in Fig. 3. Periodic boundary conditions assure that limited size effects are minimized. Fig. 3(a) depicts the resulting intensity distribution for different tunneling parameters. One clearly sees the development of sharp multiple-beam interference maxima with increasing $J/U$, corresponding to a decrease of the well depth in the experiments. For very small $J/U$, the remaining weak modulation of the intensity distribution indicates small-scale correlations even deep in the Mott-insulator regime, as have been observed experimentally \cite{13, 18, 28}. The intensity pattern for small $J/U$ is well fitted by the result of perturbation theory for an infinite number of sites given by $I = 1 + 8J/U \cos(kd)$ (dashed line in Fig. 3) where $d$ is the separation of two adjacent lattice sites.

In Fig. 3(b) the visibility, defined as $V = (I_{\text{max}} - I_{\text{min}})/(I_{\text{max}} + I_{\text{min}})$, is plotted over a wide range of the parameter $U/J$. The power of the doorway method becomes apparent by the fact that all features of the visibility are correctly reproduced over the full range of $U/J$ by using a ground state wavefunction created by the superposition of few doorway states including the initial Mott-insulating state. For large $U/J$ (Mott-insulator regime), the visibility approaches the non-vanishing perturbative result $V = 4(n_0 + 1)J/U$ \cite{18, 28, 30} reflecting the persistence of short-range correlations. In the ballpark of the phase transition the visibility changes its analytical dependence on $J/U$ and finally reaches a value close to unity for small $U/J$. This graph qualitatively describes the experimental findings of Gebier et al. \cite{18}, even though the present model neglects the external trap and it is not 1D. A detailed investigation of the visibility in a 3D- inhomogeneous case can be found in Ref. \cite{31}.

Moreover, we can directly calculate the width of the first interference peak for different number of sites and compare with the experimental measurements of Refs. \cite{13} for 1D optical lattice. In Fig. 4 the width of the first interference peak is calculated using the doorway

FIG. 3: (a) Interference pattern of a matter waves released from a one-dimensional lattice for different values of the tunneling parameter $J/U$ for eight particles distributed over eight lattice sites. The intensity is plotted as a function of the accumulated difference in phase after the expansion. (b) Visibility of the interference pattern as a function of the inverse tunneling parameter $U/J$. The dashed lines in (a) and (b) show the result of perturbation theory for an infinite number of sites but finite average population per site $n_0 = 1$. 

![Graph showing interference pattern and visibility](image-url)
method for different number of sites ($M = 3, 4, 5, 6, 7, 8$). We observe that as the number of sites increases, the point the width curve starts to grow converges to a critical value which characterize the phase transition region. Our calculation describes qualitatively the results of refs. [13] until the phase transition point is reached. On the other hand, after this point is crossed we see in our model the finite size effects which does not show up in the experimental results. Moreover, we do not observe the presence of kinks neither in the visibility or in the width of the interference peak, since the external trap is neglected in the present model.

IV. CONCLUSIONS

In conclusion, we optimize the doorway states to solve the Bose-Hubbard model for interacting bosonic particle in a periodic lattice. The method is based on the successive construction of doorway states which genuinely takes profit of symmetries included in the hamiltonian. It naturally terminates when the full irreducible subspace containing the starting state is spanned by the doorway states. The intermediate doorway states depend on the interaction and tunneling parameters of Bose-Hubbard hamiltonian providing the closest approximation to the ground state. Therefore, the convergence of the method, as can be quantified by the “reliability” introduced in this paper, scales as the number of particles. All relevant correlations of the many-body system are included in the ground state wavefunction derived in this way, as was shown by calculating the energy spectrum, the on-site fluctuations and the expectation value for single-particle correlations. We have limited our discussion on a one-dimensional model to keep the calculational effort on a low level. Conceptually, there are no limitations for extending the method to 2D, 3D and to the inhomogeneous case. Other important observables currently under experimental investigation, such as two-particle correlations of Hanbury-Brown and Twiss type [32], can also be approached by the doorway method. Since the doorway method allows direct access to the many-body wavefunction of the system, it can be applied to other important systems involving many-body correlations such as fermionic gases coupled by Feshbach resonances or the fermionic variant of the Bose-Hubbard model. In addition, dynamical properties of the Bose-Hubbard model, such as many-body tunneling rates, may be investigated.

Acknowledgments

We thank W. Zwerger, A. Buchleitner, A. Malvezzi, T. Stöferle and T. Esslinger for enlightening discussions. In particular we thank T. Stöferle and T. Esslinger to provide us with their experimental data. A.N.S. is grateful to M. da Mata and is financially supported by FAPESP. M.W. acknowledges support by the DAAD in the framework of the PROBRAL programme. M.W. and A.N.S. thank L.G. Marcassa and V.S. Bagnato (USP São Carlos) for their hospitality. The work of C-Y.L. was partially supported by the National Science Council, ROC under the Grant NSC-94-2112-M-259-008 and by FAPESP. C-Y.L. thanks the hospitality of the members of Departamento de Física Matemática of USP, where this work was performed.

---

[1] M. W. Zwierlein et al., Nature 435, 1047-1051 (2005).
[2] C. Chin et al., Science 305, 1128 (2004).
[3] B. P. Anderson et M. A. Kasevich, Science 282, 1686 (1998).
[4] M. Greiner et al., Nature 515, 39 (2002).
[5] Michael Köhl et al., Phys. Rev. Lett. 94, 080403 (2005).
[6] E. H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963).
[7] S. R. White, Phys. Rev. Lett. 69, 2863 (1992); T. D. Kühner and H. Monien, Phys. Rev. B 58, R14741 (1998); S. Rapsch, U. Schollwöck and W. Zwerger, Europhys. Lett 46, 559 (1999) and references therein.
[8] D.S. Rokhar and B.G. Kotliar, Phys. Rev. B 44, 10328 (1991).
[9] D. Jaksch et al., Phys. Rev. Lett. 81, 3108 (1998).
[10] C. Schroll, Florian Marquardt and C. Bruder, Phys. Rev. A 70, 053609 (2004), and references therein.
[11] G. G. Batrouni et al., Phys. Rev. Lett. 89, 117203 (2002) and references therein;
[12] M. Fisher et al., Phys. Rev. B 40, 546 (1989).
[13] Thilo Stöferle et al., Phys. Rev. Lett. 92, 130403 (2004); M. Köhl et al., Appl. Phys. B 79, 1009 (2004).
[14] R. Roth and K. Burnett, Phys. Rev. A 67, 031602(R) (2003).
[15] R. Roth and K. Burnett, Phys. Rev. A 68, 023604
[16] W. Krauth, M. Cakarel, and J.-P. Bouchard, Phys. Rev. B 45, 3137 (1992); J.K. Freericks and H. Monien, Phys. Rev. B 54, 16172 (1996); D. van Oosten, P. van der Straten and H. T. C. Stoof, Phys. Rev. A 63, 053601 (2001); W. Zwerger, Journal Of Opta B: Quantum Semi-class. Opt. 5 S9-S16 (2003); H. P. Büchler et al. Phys. Rev. Lett. 90, 130401 (2003); A. F. R. de Toledo Piza, Brazilian Journal of Physics, 34, 1102 (2004).

[17] H. Feshbach, A.K. Kerman and R.H. Lemmer, Annals of Physics 41, 230 (1967).

[18] F. Gerbier et al., Phys. Rev. Lett. 95, 050404 (2005).

[19] G. Giuseppe Grosso and G. Pastori Parravivini, ”Solid State Physics” (Ed. Academic Press 2002) and references therein; Z. Ziegler, Phys. Rev. A 68, 053602 (2003).

[20] A good review about lanczos algoritum can be found at A. Malvezi, Braz. J. Phys 33, 55 (2003) and references therein; G. Giuseppe Grosso and G. Pastori Parravivini, ”Solid State Physics” (Ed. Academic Press 2002) and references therein.

[21] Claude Cohen-Tannoudji, Jacques Dupont-Roc, Gilbert Grynberg, ”Photons and Atoms: Introduction to Quantum Electrodynamics”, Ed. Wiley-Interscience, 1989.

[22] V. Brems et al., J. Chem. Phys. 117, 10635 (2002); V. Brems et al., J. Chem. Phys. 116, 8318 (2002); V. Brems et al., J. Chem. Phys. 104, 2222 (1996); V. Brems et al., J. Chem. Phys. 103, 4524 (1995).

[23] G. Milburn, J. Corney, E. M. Wright and D. F. Wall, Phys. Rev. A, 4318 (1997).

[24] Khan W. Mahmud, Heidi Perry and William P. Reinhardt, Phys. Rev. A 71, 023615 (2005).

[25] A.F.R. de Toledo Piza, Brazilian Journal of Physics, 34 n3B, 1102 (2004).

[26] A. R. Kolovsky and A. Buchleitner, Europhys. Lett. 68, 632 (2004).

[27] J. K. Freericks and H. Monien, Phys. Rev. Lett. B53, 2691 (1996).

[28] F. Gerbier et al., Phys. Rev. A 72, 053606 (2005)

[29] V. A. Kashurnikov, N. V. Prokof’ev, and B. V. Svistunov, Phys. Rev. A 66, 031601(R) (2002).

[30] Y. Yu, cond-mat/0505181 (2005).

[31] C. Kollath et al., Phys. Rev. A 69, R031601 (2004); P. Sengupta et al., Phys. Rev. Lett. 95, 220402 (2005).

[32] Simon Fölling et al., Nature 434, 481 (2005).