Excitation spectrum of Mott shells in optical lattices

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Abstract
We theoretically study the excitation spectrum of confined macroscopic optical lattices in the Mott-insulating limit. For large systems, a fast numerical method is proposed to calculate the ground-state filling and excitation energies. We introduce many-particle on-site energies capturing multi-band effects and discuss tunnelling on a perturbative level using an effectively restricted Hilbert space. Results for small one-dimensional lattices obtained by this method are in good agreement with the exact multi-band diagonalization of the Hamiltonian. Spectral properties associated with the formation of regions with constant filling, so-called Mott shells, are investigated and interfaces between the shells with strong particle fluctuations are characterized by gapless local excitations.

1. Introduction
The equivalence of lattice sites is the foundation of solid state physics as it causes bands and lattice-periodic wavefunctions. Interesting physics emerges when the band is bent caused by the inhomogeneity of the system, e.g. in clusters, where bulk and surface electrons show a different physical behaviour. In optical lattices, the inhomogeneity comes naturally due to the finite waist of the lattice-establishing laser beams or due to an additional dipole trap. It has been shown in a series of pioneering work [1–3] that the bosonic Mott-insulator phase can be realized in optical lattices. Further measurements [4–6] have demonstrated that the situation is more subtle and Mott-insulator shells appear, i.e. plateaus with constant filling factors descending in integer steps from the centre of the trap. The existence of superfluid regions between the Mott shells has been theoretically predicted [7–12]. The system has previously been studied numerically, using quantum Monte Carlo [7–9] and DMRG [10], and analytically in [11, 12]. In addition to condensed matter aspects, the coexistence of compressible and incompressible regions has important implications on adiabatic heating in optical lattices [13].

We present a multi-band exact diagonalization study of small systems exploring the exact excitation spectrum and the precursor of shell formation. Based on this calculation we use a numerical method, which in the limit of deep lattices allows us to obtain an approximated energy spectrum and the exact occupation numbers. Thereby, we incorporate orbital changes by introducing a particle-number-dependent on-site interaction. The formation of shells, local excitation gaps and particle fluctuations are discussed, reflecting the strong inhomogeneity of the system. Our approach is suitable for optical lattices with millions of atoms in arbitrary spatial dimensions and allows a perturbative treatment of tunnelling. Compared to algorithms such as quantum Monte Carlo [7–9] and DMRG [10], this technique gives numerically inexpensive results for large 3D lattice systems in a specific parameter regime. We organize this paper as follows. Subsequent to the introduction of the system, we present results obtained by means of exact diagonalization followed by the numerical approach for vanishing tunnelling and a comparison of both results. Finally, we discuss consequences for two- and three-dimensional optical lattices including non-zero tunnelling.

The interaction of the ultracold bosonic atoms with mass \( m \) is modelled by a contact potential \( g \delta(\mathbf{r} - \mathbf{r}') \) with \( g = \frac{4\pi\hbar^2}{m}a_s \) and the \( s \)-wave scattering length \( a_s \). Using the bosonic field operator \( \hat{\psi}(\mathbf{r}) \), the Hamiltonian including the repulsive two-particle interaction reads

\[ H = -\frac{1}{2m} \sum_{\mathbf{r}} \left( \hat{\psi}^\dagger(\mathbf{r}) \right. \right. \cdot \nabla^2 \left. \left. \hat{\psi}(\mathbf{r}) \right) + \sum_{\mathbf{r}} g \delta(\mathbf{r} - \mathbf{r}') \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}') - \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}'} V(\mathbf{r} - \mathbf{r}') \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \]
\[ \hat{H} = \int d^3r \left( \hat{\psi}^\dagger(r) \left[ \frac{\hbar^2}{2m} + V_F(r) + V_C(r) \right] \hat{\psi}(r) + \frac{g}{2} \hat{\psi}(r) \hat{\psi}(r) \hat{\psi}(r) \hat{\psi}^\dagger(r) \right). \]  

where the periodic potential \( V_p \) of the optical lattice is given by \( V_{0,x} \cos^2(\pi x/a) + V_{0,y} \cos^2(\pi y/a) + V_{0,z} \cos^2(\pi z/a) \) with the lattice constant \( a \). The atoms experience an additional confinement potential \( V_C \) caused by the finite Gaussian beam waist \( W_0 \) of the laser beams and/or an additional dipole trap with the frequency \( \omega_d \). Using a harmonic approach, the confining potential in the \( x \)-direction is given by

\[ V_C = V_C \frac{x^2}{a^2}, \]

where \( V_C = \frac{1}{2} m \omega_{\text{eff}}^2 a^2 \) with \( \omega_{\text{eff}}^2 \approx \frac{4(V_{0,x}+V_{0,y})}{m W_0^2} + \omega_{\text{d},x}^2 \).

2. Exact diagonalization

For the exact diagonalization, the potential is truncated to a 1D lattice with \( m_1 = 10 \) and \( m_2 = m_3 = 1 \) sites by adding a smooth boundary [14]. As an example, we have chosen \(^{87}\)Rb atoms with \( a_0 = 100\alpha_0 \), where \( \alpha_0 \) is the Bohr radius, \( N = 10 \) particles, a lattice constant \( a = 515 \) nm and a transversal lattice depth \( V_{0,x} = 40E_R \), where \( E_R = \frac{\hbar^2}{2m a^2} \) is the recoil energy. The lattice depth in the longitudinal direction is \( V_{0,z} = 20E_R \), leading to a system deep within the Mott-insulator phase for a vanishing harmonic confinement (\( V_h = 0 \)). The potential of the 1D lattice is shown in figure 1(a), depicting the energy offsets \( \epsilon_i \) of the modelled chain, which are labelled \( \epsilon_0 = 0 \) for the two equivalent central sites and \( \epsilon_4 \) for the outermost sites. The parabolic shape of the confinement leads to large energy offsets of outer sites, although the offsets are small for central ones. At \( V_h = 0 \), the single-particle spectrum shows three discrete bands that comprise ten delocalized Bloch states each (corresponding to the number of sites), where the width of the lowest band is \( 4J \approx 2.4 \times 10^{-3}E_R \). For larger values of \( V_h \) the ‘band’ width is given basically by the offset of the outermost sites (see figure 1(a)). At \( V_h \gtrsim 0.4E_R \), the outermost site offset \( \epsilon_4 \gtrsim 8E_R \) causes the lowest two single-particle bands to overlap.

To calculate the many-particle spectrum by means of exact diagonalization, we limit the many-particle basis to 500 000 Fock states with lowest energy and freeze out the orbital degrees of freedom in the \( y \)- and \( z \)-directions. Afterwards, we calculate the matrix elements of (1) and obtain the 91 lowest eigenvalues (the ground state and the 90 states of the first band for \( V_h \rightarrow 0 \)). The exact diagonalization method includes particle correlations and the admixture of higher bands, i.e. orbital changes taking place for higher fillings [14], but is strongly limited to systems with few lattice sites. The many-particle spectrum is plotted in figure 1(b) (upper half) relative to the ground-state energy \( E_0 \) as a function of the harmonic confinement \( V_h \) using a logarithmic scale. For convenience,

\[ \hbar = \sum_i \hat{n}_i (\hat{n}_i - 1) / 2 + \epsilon_i \hat{n}_i, \]

and the localized occupation number basis \( |n_1, n_2, \ldots, n_M \rangle \) is an eigenbasis of the Hamiltonian, where \( M = m_1 m_2 m_3 \) denotes the number of sites. In principle, finding the ground state requires to calculate the total energy \( E = \langle \hat{H} \rangle \) of all possible basis states. The efficiency of this method is very limited due to the huge number of basis states \( (N+M-1)! \) for large lattices, where \( N \) is the number of particles. Following [11, 12], in the local density approximation an effective local chemical potential \( \mu(r) = \mu - V_C(r) \) can be introduced, and the ground state is then constructed via

3 Due to the symmetry of the potential, the two lowest bands contain nearly degenerate symmetric and antisymmetric states localized on two equivalent sites.

4 For certain system parameters \( (N, m_1, V_h) \) a degeneracy of the ground state can occur.
filling each lattice site up to the local chemical potential $\tilde{\mu}$ separately. Using the continuous limit, the chemical potential $\mu(N)$ is calculated analytically in [11] and numerically in [12]. The continuous limit is, however, only applicable to smooth confining potentials. In general, the self-consistent determination of $\mu(N)$ is tedious. We therefore suggest the following iterative algorithm for the solution of (3) directly.

\[ \mu_j(N) = n_j U + \epsilon_j \]

is calculated analytically in [11] and numerically in [12]. The continuous limit, the chemical potential $\mu_j(N)$ is presently minimal. This procedure gives the lowest energy occupation for any particle number $N$, since $\mu_j > 0$ and all sites are uncorrelated. The complexity of this algorithm is given by $O(NM)$, since each step adds one particle to one of the $M$ possible sites. This allows the calculation of the exact occupation numbers for a million particles, e.g. $N = M = 100^3$ within seconds on an ordinary desktop computer. This method is therefore considerably useful for the design and interpretation of experiments.

Compared with the exact diagonalization results for the 1D lattice, the crossover points can, in principle, be reproduced with this method but their positions are shifted. This effect is additionally enhanced for higher filling factors. To study this influence more quantitatively, we calculate the on-site few-particle interaction with exact diagonalization. Since the lattice depth is sufficiently deep, it is valid to approximate the lowest-band Wannier function $w_0(r)$ by the wavefunction of a single sinusoidal lattice site using hard boundary conditions. The correlationless Hubbard on-site interaction $U = g \int d^3r |w_0(r)|^4$ does not incorporate that particles tend to avoid each other for repulsive interaction. This causes broadening of the particle density and was addressed experimentally in [5]. Using the correct many-particle wavefunction $\Psi_n$ for $n$ particles, the expectation value of the on-site interaction becomes

\[ u(n) = \frac{8}{n(n-1)} \langle \hat{\psi}_r \hat{\psi}_r | \hat{\psi}_r \hat{\psi}_r \rangle, \]

which is normalized to the interaction energy per atom pair. The results that are depicted in figure 2 show that $u(n)$ determined by exact diagonalization deviates strongly from the Hubbard on-site interaction $U$. As expected, the interaction energy $u(n)$ decreases with an increasing number of particles per site. However, not only $u(n)$ changes when the modification of wavefunctions is taken into account. In fact, the admixture of correlated states and the broadening of the density change the expectation value of on-site kinetic and potential energy. The total on-site energy is the eigenvalue of the many-particle Schrödinger equation $\hat{H}_n \Psi_n = E_n \Psi_n$ restricted to single-site wavefunctions and using the full Hamiltonian (1) with $V_h = 0$. The normalized on-site energies $e(n) = 2(E_n - E_0^h)/n(n-1)$ are plotted in figure 2, where $E_0^h$ is the energy of the non-interacting system. It shows, that the total interaction lies energetically between $U$ and $u(n)$. Nevertheless, the deviation of $e(2)$ from the Hubbard $U$ is large. Using $U = e(2)$, the crossovers are still shifted noticeably for higher fillings (large $V_h$) comparing with the results of the 1D lattice (upper half of figure 1(b)). Therefore, we incorporate in our calculations the correct total interaction energy $e(n_j)$ for a single site with the occupation $n_j$. Please note that the optimization problem

**Figure 1.** (a) The periodic potential $V_p$ is superposed by a harmonic potential $V_C$ leading to site offsets $\epsilon_i$. The single-particle spectrum for $V_h = 0.06E_0^h$ containing discrete bands is plotted within the potential. (b) The many-particle energy spectrum (91 states) obtained by exact diagonalization (upper half) and for vanishing tunnelling (lower half) as a function of the harmonic confinement strength $V_h$. Additional states in the $J \rightarrow 0$ spectrum are plotted in grey. The energy scale is relative to the ground-state energy $E_0$ and the gap to the first excited state is depicted in grey.

**Figure 2.** A comparison of Hubbard on-site interaction $U$, the many-particle interaction energy $u(n)$ and the total on-site energy $e(n)$ per atom pair for $V_{hi} = V_0$ and $i = x, y, z$. The single-site many-particle wavefunction is determined by exact diagonalization for $n = 2$ particles (highest energy) to $n = 5$ particles (lowest energy).
remains the same if substituting the energy $\mu^+_j = n_j U + \epsilon_j$ for adding one particle by $\mu^+_j = e(n_j + 1) - e(n_j) + \epsilon_j$. In the lower half of figure 1(b), the energy spectrum for vanishing tunnelling ($J \rightarrow 0$) is shown using the corrected values of the on-site interaction. In this case, the crossover energies corresponding to the vanishing gaps for $J \rightarrow 0$ are in good agreement with the exact diagonalization of the 1D lattice. This result shows, in general, that the introduced filling-dependent on-site interaction $e(n_i)$ is appropriate to describe effects arising from orbital changes. The small remaining shift of the crossover energies in figure 1(b) is due to the ‘classical’ treatment of the states in our approach.

The energy gap can be obtained by removing one particle from site $j$ and adding it to site $k \neq j$. Finding the minimum excitation energy $\Delta E_{j,k}$ for all possible $j$ and $k$ has, in general, the complexity $O(M^2)$. The excitation energy is given by $\Delta E_{j,k} = \mu^+_j - \mu^-_k$, where

$$\mu^+_j = e(n_j + 1) - e(n_j) + \epsilon_j > 0,$$

for adding a particle on-site $j$ and

$$\mu^-_k = e(n_k - 1) - e(n_k) - \epsilon_k < 0,$$

for removing a particle from site $k$. Thus, it is sufficient to minimize $\mu^+_j$ and $\mu^-_k$ separately, which reduces the complexity to linear order in $M$. Finding the next excited state is more complicated, since this state may be an excitation of the ground state but also of the first excited state. For the calculation of the spectrum, a slightly modified Dijkstra algorithm can be used, where one considers the ground state as the node of a graph. This node is expanded according to all possible excitations. Iteratively, the node with the minimum energy, which is not yet expanded, is expanded. Consequently, the list of expanded nodes represents the states with the lowest energy. It is necessary, however, to check whether a created excited state is already a node in the graph, which is a major contribution to the complexity of the Dijkstra algorithm, but can numerically be highly optimized. Using this procedure, the resulting energy spectrum (lower half of figure 1(b)) reproduces well the basic features, i.e. the band gap, the overall shape and the density of states, of the exact calculation (upper half). Because of interactions, the degeneracy of states is lifted in the exact spectrum, so that the actual energies of many states are shifted.

4. Macroscopic lattices

Transferring the above results to macroscopic lattices is not straightforward. Enlarging the system’s size causes the differences in offset energies of neighbouring sites $\epsilon_j - \epsilon_k$ to decrease substantially when keeping the offset of the outermost sites fixed. This causes the width and the height of the energy lobes in the spectrum to decrease because a huge number of configurations become possible when increasing the number of particles and lattice sites. This process is drastically enhanced in 2D and 3D lattices, where practically the band gap vanishes for all confinement strengths $V_0$. The only exception is the real Mott-insulator phase, where the outermost sites have an offset smaller than $U$. In fact, the excitation spectrum of the total system becomes more or less continuous. This might appear contradictory to the insulating property at first glance but the system is inhomogeneous and only some of the atoms can perform gapless excitations. Therefore, local properties are more suited to describe the system, such as particle number fluctuations and the local excitation spectrum. It has already been pointed out [8-11] that the regions with fixed occupation number, the Mott-insulator shells, are surrounded by compressible shells for non-negligible tunnelling.

As an example, the occupation number distribution $n_i$ for $N = 10^6$ particles in a 3D lattice is depicted in figure 3(a). It shows the expected shell structure with filling factors from five (in the centre) to one. An advantage of the presented numerical algorithm is that it is also applicable to rapidly varying confinement potentials. It can thus be used to tailor more sophisticated shell configurations for experiments. Since the on-site interaction energy $U$ is relatively small compared to the depth of the lattice wells, the local filling factors can be adjusted without a stronger perturbation of the 3D lattice. Additional laser beams or magnetic fields can thus be used to obtain complex spatial distributions of atoms with specific filling factors. Figure 4(a) shows the occupation number distribution for an added periodic potential in the $x$-direction $V_C = V_{0x}^2/a^2 + U \cos^2(\pi x/a')$ with the periodicity $a' = 3a$ motivated by [15]. The superlattice structure leads to alternating local fillings. As a second example, an added hat-shaped ($-|x|$) potential causes two separate atomic clouds, shown in figure 4(b), that are in touch with each other at the origin.

5. Single-particle excitations and finite tunnelling

At the outer surface of each shell, almost gapless excitations are possible via the hopping of a particle to another site, whereas the inner surface can easily absorb particles. This is shown quantitatively in figure 5(a) (upper half), where $\Delta E^-_i = \mu^-_i + \min_j(\mu^+_j)$ is the minimal energy for removing
one particle from site $i$ and adding it to another site $j$. The minimal energy for adding one particle to site $i$ (and removing it from site $j$) is denoted as $\Delta E^+_i = \mu_+^i + \min_j (\mu_-^j)$ (lower half of figure 5(a)). The local excitation gap vanishes at the outer and inner surfaces and increases strongly within the shells. The excitation energies $\Delta E^\pm$ are explicitly shown for sites with $y = z = 0$ in figure 5(b). It reflects basically the harmonic shape of the confinement, so that $\Delta E^+_i$ and $\Delta E^-_i$ are positive and negative parabolas, respectively, subtracted by integer multiples of the on-site interaction. The situation changes drastically, if accounting only for excitations to nearest neighbours as shown in figures 5(c)–(d). Low energy excitations (either $\Delta E^+_i$ or $\Delta E^-_i$) can occur exclusively on sites directly at the boundary between different shells. Within the bulk the single-particle excitation gap is wide and nearly constant. Therefore, the nearest-neighbour tunnelling is, in general, strongly suppressed on these sites, where the system is a good insulator.

In the following, we use a perturbative approach to obtain particle fluctuations for finite tunnelling $J$. For each site $i$, the subsystem containing the site $i$ and all neighbouring sites is considered. The diagonalization of this subsystem with finite tunnelling $-J \sum_{\langle i,j \rangle} \hat{b}_i \hat{b}^\dagger_j$ allows an approximative calculation of the particle fluctuations $\Delta n_i = \sqrt{\langle \hat{n}_i^2 \rangle} - \langle \hat{n}_i \rangle^2$. For the example above, weak tunnelling causes finite fluctuations $\Delta n_j$ at the boundaries of the shells, which is shown in figures 3(b) and 4 for $J = 10^{-3} E_R$ and in figure 5(d) for $J = 5 \times 10^{-3} E_R$. Note that due to the finite cell size of the lattice, the results are not completely spherically symmetric. In accordance with the nearest-neighbour excitation energies, the fluctuations affect only sites directly at the surfaces. Because of the larger slope of the confinement and the lower filling, the tunnelling decreases for outer shells. Within the bulk of the Mott shells, small particle fluctuations can be observed due to the finite tunnelling. The fluctuations on the surface however enhance the tunnelling of the atoms next to the surface, which is not covered by this perturbative approach and would require a self-consistent calculation. The narrow energy gaps of particles close to the surface can, in principle, cause near-resonant tunnelling to non-nearest neighbours, so-called variable range hopping [16]. Due to the relatively strong $V_3$ (compared with $J$) and the regularity of the potential, only sites on the surface, which are dominated by nearest-neighbour hopping, have suitably low excitation energies.

The presented method provides the lowest energetic states (including particle-hole excitations) and is suitable to restrict the Hilbert space effectively. The obtained states can be used as a starting point for exact diagonalization, quantum Monte Carlo and dynamical mean-field calculations including tunnelling and finite temperatures. In particular, the diagonalization of the 1D lattice (figure 1(b)) could be transformed with much fewer basis states.

### 6. Conclusions

In summary, we have studied the excitation spectrum and exact site occupation numbers for confined optical lattices deep within the Mott-insulator regime. In good agreement with exact diagonalization for small 1D lattices, a numerical method was presented that allows for negligible tunnelling the exact treatment of macroscopic optical lattices with arbitrary shape of the confining potential. Adding slowly varying potentials to the optical lattice can give rise to complex filling structures. We have calculated the numerically exact many-particle on-site energies and have shown that introducing a filling factor depending on on-site interaction can be incorporated to cover orbital changes. For small systems, the many-particle spectrum contains lobes, whereas for macroscopic systems nearly gapless excitations are always possible at the boundaries of the Mott shells. Within a given Mott shell, the local excitation energy varies strongly leading to compressible sites close to the surface and incompressible inner sites. A perturbative treatment for finite tunnelling shows strong particle fluctuations at the boundaries between the shells, where the Mott-insulator gap vanishes. Finally, the presented
method can serve as a reduction scheme for the Hilbert space for further numerical treatments.

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