Excitations of Bose-Einstein condensates in optical lattices

K. Braun-Munzinger,* J. A. Dunningham, and K. Burnett
Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford, OX1 3PU, United Kingdom
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In this paper we describe numerical simulations of the response of atoms confined in an optical lattice in the region of a quantum phase transition. We use the increase in the number variance of atoms as the diagnostic of excitations produced by tilting the lattice. We show that this locally determined quantity is a good indicator of the resulting coherence changes as observed in recent experiments. This is found to hold for commensurate and noncommensurate filling of the lattice, implying that our results should hold for a wide range of conditions. In accordance with this view, we find that the qualitative features of our results are in good agreement with recent experiments. We do, however, find extra features in the excitation spectra that may well be of use in future experimental studies. We also show that the variation of the spectra with the duration of the perturbation is a useful diagnostic of the atom dynamics that take place during the tilt.

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I. INTRODUCTION

Interest in the properties of atomic Bose-Einstein condensates (BECs) in optical lattices, both theoretical [1–3] and experimental [4–7], has been growing rapidly. Part of this interest comes from the possibility of studying the physics of a strongly correlated atomic system for a wide range of the relevant parameters. In particular, the observation of the superfluid (SF) to Mott insulator (MI) transition has caused a great deal of excitement. Atomic arrays in optical lattices also promise a potentially significant route to the physical implementation of quantum information processing [8].

The experimental feasibility of adding a linearly varying component to the lattice potential has opened up a new way to study the SF to MI phase transition. In this paper we present numerical simulations of this technique that enable us to compare the effect of such tilting on states with various degrees of reduced number fluctuations. Our focus is on the region of the phase transition where the repulsion between atoms is larger than the hopping amplitude and strong number squeezing results.

We shall first give a brief description of the Bose-Hubbard model and the numerical method we use to simulate the behavior of the atoms in the presence of a tilt. We then present the results from the numerical evolution for a range of initial states. These include simulations for different numbers of sites as well as numbers of atoms per site. We shall argue that the change in the number variance for atoms on a typical site is a robust indicator of the lattice response for a wide range of systems. This change in number variance is, of course, closely related to the change in phase coherence between sites on the lattice observed in recent experiments. We are thus able to see that the response of our model lattices is in good agreement with the observations reported in those experiments.

II. BOSE-HUBBARD MODEL AND THE ENERGY GAP

The system we simulate in this paper consists of a BEC transferred to a one-dimensional lattice. The behavior of this system is described by the Bose-Hubbard model [9,10], i.e.,

$$H = \sum_j E_j \hat{n}_j + \frac{1}{2} U \sum_j \hat{n}_j(\hat{n}_j - 1) - J \sum_{\langle j,k \rangle} \hat{a}_j^\dagger \hat{a}_k. \qquad (1)$$

Here, $\hat{a}_j$, $\hat{a}_j^\dagger$ stand for the bosonic annihilation and creation operators, $\langle j,k \rangle$ denotes summation over nearest neighbors, $\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j$ is the bosonic number operator, and E_j is the energy for site j. J is the hopping constant and U is the on-site repulsive interaction constant. For numerical simplicity, we consider modestly sized lattices with between four and eight sites and average occupation numbers $n_{\text{av.occ.}}$ of up to three atoms per site. Experiments that demonstrate the SF to MI transition typically involve many more lattice sites than this [4–7]. By considering the evolution of what we expect to be locally determined quantities such as number variance, we should, however, be able to minimize the effects of finite size on our results. This, in turn, should allow us to gain some insight into the behavior of larger lattices than we are able to treat numerically. When comparing results for different numbers of lattice sites, we find that they show remarkably similar behavior, encouraging us in our use of the number variance as an indicator of lattice response. While we focus on a one-dimensional system, we believe that our results have implications for three dimensions as the phenomena we see are of a generic nature.

We study our system by solving the coupled equations of motion for the components of the wave functions in the number state basis using an embedded fifth order Runge-Kutta approximation [11]. The initial states for the simulations are the eigenstates of the Hamiltonian given in Eq. (1) for different values of U/J. These number squeezed states are then probed by tilting the lattice in our simulations. This tilting is implemented by adding a linearly varying component E_{tilt} to the on-site energy E_j. Our measure of change is the number variance V, defined as

$$V = \langle (\hat{n}_i)^2 \rangle - \langle \hat{n}_i \rangle^2, \qquad (2)$$

where $\hat{n}_i$ is the number operator for site i and $\langle\ \rangle$ denotes the expectation value. We compute this number variance V after

*Electronic address: k.braun-munzinger1@physics.ox.ac.uk

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the potential gradient has been applied for a time τ_{perturb}.

Excitations in the MI phase were measured experimentally (e.g., in [4]) via changes in the interference patterns observed in the distribution of atoms released from the lattice. These excitations, caused by tilting the lattice, show up in the increased width of the main interference peaks found when the system is taken back into the SF phase [4]. In other words, excitations were observed through changes induced in the phase coherence across the lattice. Deep in the insulator state there is no phase coherence and correspondingly zero number variance. Excitations give rise to an increase in number variance and that is what we see in our simulations. For further discussion of the use of number variance in the theory of BEC and the relationship between phase coherence and number variance see [10,12,13]. We should note that the number variance may also be measured experimentally by studying the collapse and revival times of the relative quantum phase between sites [14–16].

In our simulations we wished to examine the change in the response to the tilt in the region of the quantum phase transition. One of the main indicators of the onset of the MI state is, of course, the appearance of an energy gap. When present, it implies that atoms can only move between sites if they are given sufficient energy. Tilting a lattice changes the relative potential energy of the sites and hence the energy available for a hop. Accordingly, if the energy difference between sites is made comparable to the energy gap, atomic hopping should occur. When the energy difference between sites produced by the tilt matches the energy gap, the hopping will be resonant. Such resonant production of a particle-hole excitation is observed both in experiments [5,7] and in the simulations we present. In the SF phase, there is no gap in the excitation spectrum and a flow of atoms will result for all values of the tilt.

For an infinite one-dimensional lattice, mean field and quantum Monte Carlo calculations indicate that the phase transition is located at $U/J \approx 5.8$ [2,17,18]. In a lattice of finite size, the phase transition is not sharp, which translates into a gradual onset of the energy gap. In Fig. 1, we plot energy eigenvalues for the values of U/J studied in our simulations: close to the phase transition ($U/J=6$), we see indeed that no gap is observable. As expected, states further into the Mott insulator regime ($U/J=20$ and $U/J=50$) show a definite gap, even though bands are still broadened. Consequently, the simple Mott insulator picture with an energy gap of approximately U cannot explain all excitations possible for these ranges of eigenstates. In support of this, we observe a broad smooth curve superimposed on Mott insulator peaks that goes away with increasing U/J (see, for example, Fig. 2). Recent experimental results for lattices with about 100 sites show a similar broad background [7].

In the next section, we will present and discuss the results of our numerical simulations.

III. RESULTS OF THE NUMERICAL SIMULATIONS

As explained above, we use states with a range of different degrees of number squeezing as the initial states in our simulations and apply a tilt for a time τ_{perturb}. We then determine the number variance V for the resulting wave function of atoms in the lattice.

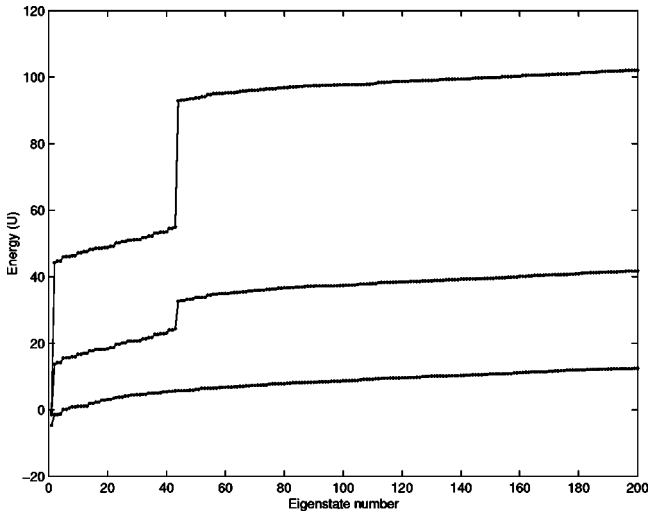

FIG. 1. The first 200 eigenstates for $U=6, 20,$ and 50 (bottom to top) and $J=1$, six lattice sites, and $n_{\text{av.occ.}}=1$.

The results of the simulations for various initial states and durations of tilt are shown in Figs. 2–5. What features do we expect to observe? For a perfectly squeezed state in an infinite lattice, we would expect to find resonances at integer multiples of the interaction energy U, i.e., for Un_1. We suppose that such resonances correspond to n_1 particle-hole pairs being created in adjacent sites. In addition, we also expect to see resonances for fractions of the interaction energy, i.e., U/n_2, where n_2 is an integer. This effect should correspond to the creation of a particle-hole excitation in two sites n_2 sites apart (i.e., in site i and site $i+n_2$).

We find that even for rather small lattices the location of peaks is in good agreement with these arguments for an in-

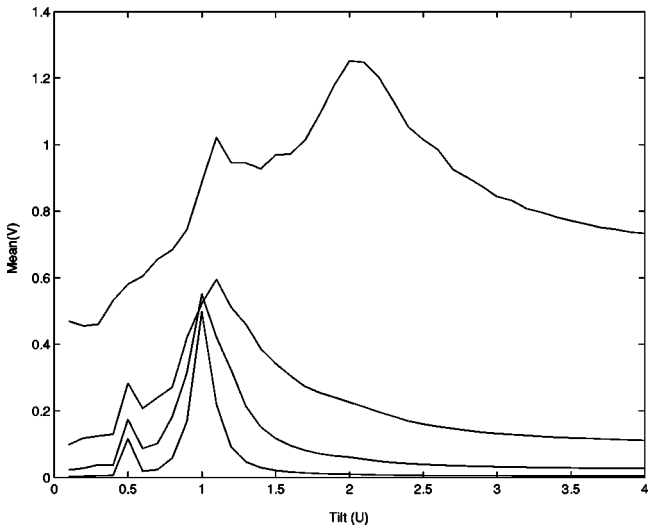

FIG. 2. Dependence of the excitations on the degree of number squeezing of the initial state. With increased squeezing [plots are for $U=6, 10, 20,$ and 50 (top to bottom), $J=1$ (constant), four lattice sites, $n_{\text{av.occ.}}=1$, and $\tau_{\text{perturb}}=5/J$], resonance effects become noticeably narrower and the background decreases. The mean variance (y axis) is dimensionless.

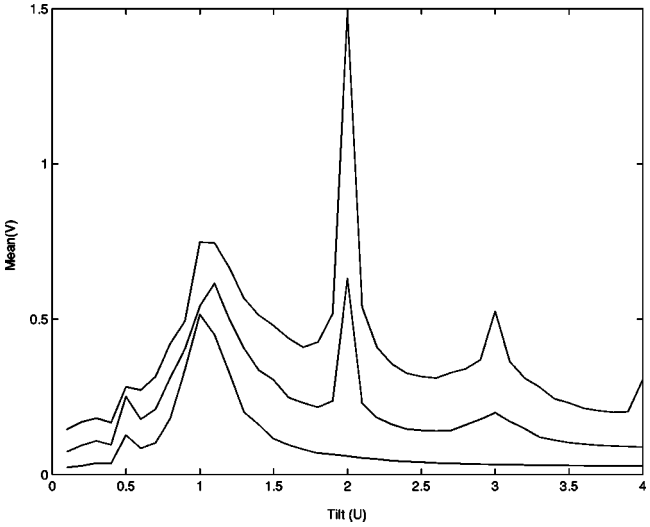

FIG. 3. Excitation pattern for $\tau_{\text{perturb}}=2/J$, $U=20$, $J=1$, four lattice sites, and $n_{\text{av.occ.}}=1,2,$ and 3 (bottom to top). The mean variance (y axis) is dimensionless.

finite lattice as can be seen, for example, in Fig. 3, which shows excitations for filling factors of one, two, and three for four lattice sites. All these plots show one-particle-hole excitations at $E_{\text{tilt}}\approx 1\,U$ and $E_{\text{tilt}}\approx 0.5U$. For $n_{\text{av.occ.}}\geqslant 2$, two-, three-, and even four-particle-hole excitations appear.

There is a slight shift of the maximum of the resonance at $E_{\text{tilt}}\approx 1\,U$ for excitations near the phase transition (see, for example, Fig. 2). We found this shift for all numbers of lattice sites we considered. This is most likely due to the combination of a broad continuous spectrum with the discrete peaks we discussed above. We note that the experimental spectrum has an appearance consistent with this interpretation [7].

When studying the time dependence of our simulations (plotted in Fig. 6), we find that the time taken to establish the

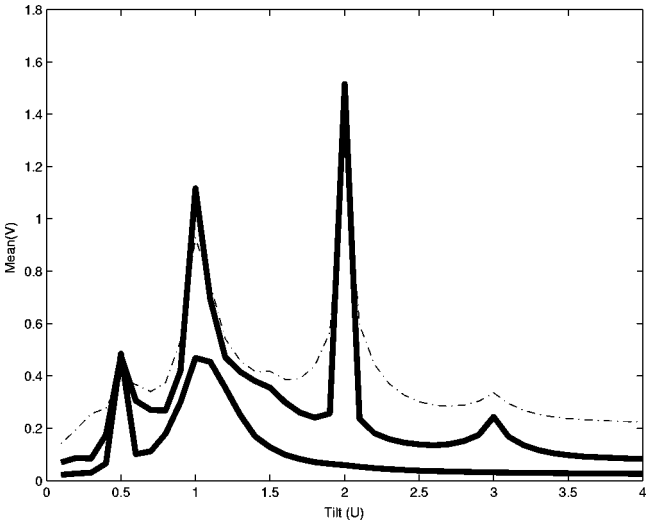

FIG. 4. The thick black lines are for commensurate filling (upper $n_{\text{av.occ.}}=2$, lower $n_{\text{av.occ.}}=1$), while the thin broken line shows results for $n_{\text{av.occ.}}=1.8$. There are five lattice sites, $\tau_{\text{perturb}}=5/J$ and $U=20$, $J=1$. The mean variance (y axis) is dimensionless.

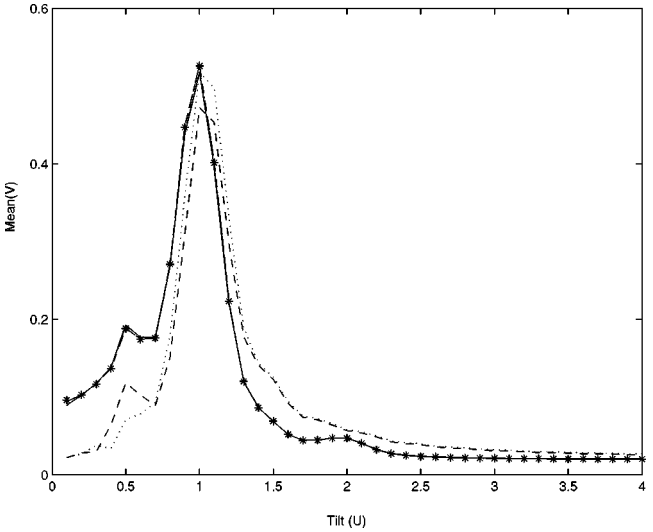

FIG. 5. Results for $U=20$, $J=1$ and $\tau_{\text{perturb}}=1/J$ for four to eight lattice sites and $n_{\text{av.occ.}}=1$. (Dots) four sites; (dashes) five sites; (solid line) six sites; (dash-dot) seven sites; (stars) eight sites. The mean variance (y axis) is dimensionless.

resonance for lower order processes is of the order of $1/J$, i.e., the tunneling time. The response from higher-order processes continues to increase in magnitude for longer times: for the second-order process at $2\,U$, the resonance is established from times of the order of $2/J$. For higher-order processes, the response takes significantly longer to develop fully.

It is important to note that the qualitative features are still present for noncommensurate filling. As shown in Fig. 4, noncommensurate filling results in a more prominent continuous spectrum, as might be expected in a system with defects. However, we still see distinct Mott insulator peaks, albeit with somewhat greater widths.

We now turn to the dependence of excitations on the number of lattice sites for a range of four to eight lattice sites. For more than five lattice sites and $U/J\geqslant 20$, the changes in the results as a function of lattice size become modest (see Fig.

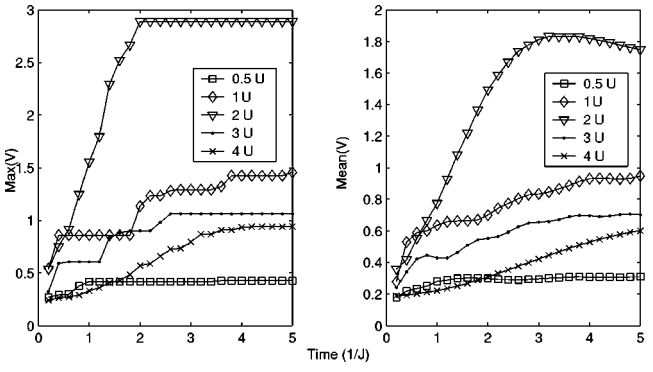

FIG. 6. Plot of the number variance as a function of perturbation time for the five most important peaks ($0.5U$, $1\,U$, $2\,U$, $3\,U$, and $4\,U$) for four lattice sites, $U=20$, $J=1$, and $n_{\text{av.occ.}}=3$. The left plot shows the maximum value of the number variance, the right plot shows the number variance averaged over time. The maximum and mean variance (y axis) are dimensionless.

5). Even for the smaller configurations, i.e., four and five sites, the important features look qualitatively the same. This leads us to be reasonably confident of the relevance of the principal features of our calculations for the larger systems studied in laboratories.

IV. CONCLUSION

We have presented a range of simulations of atoms in an optical lattice in the region of a quantum phase transition. We have shown that the change in atom number variance is a good indicator of excitations produced by tilting the lattice potential. Moreover, we have seen that the main features of the excitation spectrum are weakly dependent on the size of the lattice and confirm the origin of resonances seen in recent experiments [4,7]. In addition, we observe higher-order effects in the response that fit very well into the picture of excitations at multiples of the energy gap U in an infinite lattice. We find that the time dependence of the response varies with the complexity of the underlying process: while the simplest nearest-neighbor hopping sets in at about a tunneling time, the higher-order processes take much longer. Our results also indicate that noncommensurate filling does not obscure the Mott insulator peaks in the response of the lattice. This implies that the change in atom number variance could be a useful probe even in nonideal systems, such as lattices with defects.

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