Dipole and monopole modes in the Bose-Hubbard model in a trap

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Abstract

The lowest-lying collective modes of a trapped Bose gas in an optical lattice are studied in
the Bose-Hubbard model. An exact diagonalization of the Hamiltonian is performed in a one-
dimensional five-particle system in order to find the lowest few eigenstates. Dipole and breathing
character of the eigenstates is confirmed in the limit where the tunneling dominates the dynamics,
but under Mott-like conditions the excitations do not correspond to oscillatory modes.
I. INTRODUCTION

Exciting collective modes is a useful and popular tool for probing the many-body physics of trapped atomic gases. Following the first creation of a trapped condensate in 1995 \[1\], modes in these systems have been subject to extensive theoretical and experimental study \[2\]. The fundamental zero-temperature theory was laid down about half a century ago \[3\], and was readily adapted to the case of trapped condensates \[4\]. In three dimensions, oscillatory modes are naturally classified according to their multipolarity, and can be selectively excited by deforming the magnetic trap, or applying laser pulses that repel or attract the atoms in selected regions of space \[5, 6\].

The picture is complicated considerably if one adds an optical lattice, consisting of one or several standing laser waves that act as a spatially periodic potential on the atoms. In the limit of a weak optical potential, the mode frequencies are simply given by those of the trapped Bose-Einstein condensed cloud in the absence of an optical lattice, but renormalized by the effective mass acquired by the bosons in the periodic potential \[7, 8\]. Away from this limit, however, the presence of an optical lattice offers quite different physics, and a new phase appears, namely the Mott insulator, when the interactions are strong \[9, 10\]. In addition, when an external trapping potential is present, there exist parameter regimes where spatially separated regions of Mott-insulating and superfluid behavior coexist \[11, 12\]. The behavior of the trapped gas and the nature of its collective modes are expected to become quite different in these regimes compared to the quite well understood case of a trapped cloud with no optical lattice present \[13\].

In order to be able to address both the strongly and weakly interacting case and the crossover between these, we shall study the Bose-Hubbard model in the exactly solvable case of few bosons and in one dimension. The method shall be exact diagonalization in a truncated basis. This way we hope to gain qualitative knowledge of the spectrum that applies also to larger systems and higher dimensions. The paper is organized as follows. The Hamiltonian and the numerical method are explained in Sec. II. The nature of the ground state and the low-lying excitations in a shallow trap is investigated in Sec. III and the case of a tight trap in Sec. IV. Concluding remarks are given in Sec. V.
The starting point is the Bose-Hubbard Hamiltonian \[ H = \sum_r \frac{U}{2} a_r^\dagger a_r^\dagger a_r a_r - \frac{J}{2} a_r^\dagger (a_{r+1} + a_{r-1}) + \frac{\omega^2 r^2}{2} a_r^\dagger a_r. \] (1)

The first term in this Hamiltonian describes the interactions which are effectively repulsive if \( U > 0 \) (which is the case in this paper), the second, so-called tunneling or hopping term is associated with the kinetic energy, and the last term describes the external trapping potential. The index \( r \) denotes the spatial position and takes on integer values. Such a one-dimensional Hubbard model describes a system with a tight trap in the directions perpendicular to the lattice so that the other degrees of freedom are frozen out, thus resembling a coupled chain of quantum dots. Higher dimensions will make the picture more complicated, but the main qualitative features observed in the present paper are expected to carry over to higher dimensions.

The Hamiltonian contains three physical parameters. The tunneling strength \( J \) can be written
\[
J = \frac{\hbar^2}{m^* \delta r^2},
\]
where \( \delta r \) is the spacing between wells and \( m^* \) is the effective mass acquired by the atoms due to the periodic potential [8]. The interaction strength \( U \) is related to trap parameters through the relation
\[
U = \frac{4\pi \hbar^2 a}{m} \int d^3 r |\Psi_{TB}(r)|^4,
\]
where \( a \) is the \( s \)-wave scattering length and \( \Psi_{TB} \) is the ground-state wave function in one potential well in the tight-binding approximation. The effective trap frequency \( \omega \) is defined in terms of the bare particle mass \( m \) and trap frequency \( \Omega \) as
\[
\omega = \sqrt{m \Omega \delta r}.
\]

Let us at this point rescale the Hamiltonian and work in units of \( J \); formally we set \( J = 1 \) and retain \( U \) and \( \omega \) as the two parameters of the system. In addition to the parameters already discussed, the number of atoms \( N \) or alternatively the chemical potential is a parameter of the system; we shall fix \( N = 5 \) in this study. Furthermore, for a few-particle system the even/odd parity of the number of sites \( L \) may also play a decisive role; such effects vanish in
the limit of large systems. For definiteness only odd $L$ will be considered, but some attention will be paid to parity effects where appropriate.

In a number-conserving formalism, the natural basis is the set of real-space Fock states that are also eigenstates of the interaction and trap energies:

$$| \ldots n_{r-1}n_r n_{r+1} \ldots \rangle = \ldots (a_{r-1}^\dagger)^{n_{r-1}}(a_r^\dagger)^{n_r}(a_{r+1}^\dagger)^{n_{r+1}} \ldots |0\rangle.$$ \hspace{1cm} (5)

The trapping potential implies a finite system size: it turns out that between one and 25 sites is needed to accommodate a system of five particles for the trap parameters considered here. The size of the basis for a system of size $L$ with $N$ particles is $(N+L-1)!/[N!(L-1)!]$; for $N = 5$, $L = 25$ the number of states is 118755. Clearly, the computations can be made much more efficient if the basis is truncated so that the many improbable Fock states do not contribute: it is immediately obvious that states such as $|N000 \ldots 0\rangle$, where all the particles are concentrated at one endpoint of the lattice, make only a very small contribution to the dynamics.

There is, therefore, much to be gained if the basis is truncated. The following scheme turns out to be practical for both strong and weak coupling, although it was designed for dealing with Mott-insulator-like conditions where the interactions are strong. Start with a single Fock state labeled $|1'\rangle$, for instance the state with all the particles at the same site, $|1'\rangle = |\ldots 00N00 \ldots \rangle$. Now enumerate all the states, $|2'\rangle, \ldots, |n_1'\rangle$, that can be constructed from $|1'\rangle$ by one application of the tunneling term in the Hamiltonian (1), and construct the Hamiltonian matrix elements in the process. Operate again with the tunneling Hamiltonian on the states $|2'\rangle, \ldots, |n_1'\rangle$ to form new states $|n_1' + 1\rangle, \ldots, |n_2'\rangle$, taking care not to double-count states; iterate this step $p$ times so that a basis is formed that consists of $n_p'$ states. Within this basis, the Hamiltonian is now diagonalized and the ground state is found. Among the $n_p'$ Fock states in the preliminary basis, choose the one that has the largest overlap with the ground-state eigenvector and label it $|1''\rangle$. Now discard all the other Fock states that were just constructed, and instead iterate the whole scheme again to construct a new basis $|1''\rangle, \ldots, |n_p''\rangle$; do the iteration a few (say, $M = 3$ or 4) times. The basis thus constructed, $|1^{(M)}\rangle, \ldots, |n_p^{(M)}\rangle$, will contain all the Fock states that have significant overlap with the ground state for the given physical parameters; in a sense, by constructing this basis tunneling effects to $p$th order have been incorporated. Convergence with respect to $p$ and $M$ is readily checked, so that the diagonalization can for all practical purposes be
considered exact.

The diagonalization is performed with ARPACK, which uses an Arnoldi algorithm.

III. MODES IN SHALLOW TRAPS

The competition between the tunneling, interaction and trap energies gives rise to a rich phase diagram (cf. [9, 12]). Consider first the shallow trap. Figure 1 displays the ground-state density distribution for values of $U$ ranging from weak to strong interactions, with $\omega = 0.3$. The quantum fluctuations of the number of particles in the central well are displayed in Fig. 2. It is seen that we are in the fluctuation-dominated, superfluid regime. The very slight suppression of fluctuations in the centermost well is in fact a signal that we are in the vicinity of the Mott insulating regime; if the trapping strength is increased, this suppression becomes stronger, as shall be discussed in Sec. IV. For the present trapping strength, $\omega = 0.3$, the effect is barely noticeable even for $U = 100$.

In this shallow trap, the competition between the tunneling and interaction is decisive in the interior of the system, while the trap still determines the size and the behavior close to the boundary. The density is spread out over many sites, and therefore the system resembles a trapped, Bose-condensed cloud in the absence of a lattice. It is in this “trapped BEC” regime that the experiments of Ref. [7] were conducted. While five particles are too few to be considered truly in the trapped BEC regime, the results reported here still give a hint of that limit, as is seen in Fig. 1. In a trapped condensate in the absence of an optical lattice, the density distribution is Gaussian for weak coupling, but flattens out and takes on the shape of an inverted parabola for stronger coupling [2]. The density profiles shown in Fig. 1 can of course not be expected to exactly follow this behavior, because of the discreteness, but the dependence on coupling is similar.

The mode frequencies, i.e. the excitation energies relative to the ground state, for the lowest four excited states are displayed in Fig. 3. When the coupling becomes weak, the mode frequencies approach integer multiples of the trap frequency with the expected degeneracies in a harmonic trap. Restoring dimensions, with the aid of Eqs. (2, 4), we find in fact [7, 8]

$$E_n = q\sqrt{\frac{m}{m^*}}\hbar\Omega,$$

with $q$ integer. Clearly the integer level spacing is approximate, as is the degeneracy,
FIG. 1: Ground-state density profile for different values of on-site interaction $U$ in a shallow trap with $\omega = 0.3$.

because in the $N = 5$ case discreteness is still manifest. The anticipated dipole and monopole (breathing) oscillations are visualized in Fig. 4 where the density evolution in time of a superposition of the ground state and each excited state is shown together with the mean position and width of the cloud.

In a trapped BEC, as the coupling grows stronger the frequency of the dipole mode stays constant while that of the monopole mode decreases $[2]$: in the Thomas-Fermi limit in one
FIG. 2: Quantum fluctuations in the ground-state density, \( \langle \delta n \rangle = \langle n^2 \rangle - \langle n \rangle^2 \), for different values of \( U \) in the shallow trap, with \( \omega = 0.3 \).

dimension it is down to \( E_2 = \sqrt{3} \omega \approx 1.73 \omega \). In the present system, one cannot hope to see this limit, but there is indeed a drop of the second excitation frequency while the lowest one initially stays constant. As the coupling strength approaches and exceeds unity, however, the discreteness of the system becomes manifest in a \( U \)-dependence, although weak, of the dipole frequency. The dipole and monopole character of the first and second excited state, respectively, are unchanged, as is exemplified in Fig. 3.
FIG. 3: Lowest excitation frequencies in units of the trap frequency $\omega$ in a shallow trap with $\omega = 0.3$. Full lines represent the results for the three lowest excited states obtained by exact diagonalization. Dashed line is the outcome of the Bogoliubov approximation.

In the limit of weak interactions, one expects the Bogoliubov approximation to be valid. This approximation can for an inhomogeneous system be effected by linearizing the Gross-Pitaevskii equation around its ground-state solution \[2\]. The latter equation is obtained by replacing the field operators in the Hamiltonian, Eq. (1), by their expectation values, $a_r \rightarrow z_r = \langle a_r \rangle$, resulting in the discrete difference equation

$$U|z_r|^2 z_r = \frac{J}{2}(z_{r+1} + z_{r-1}) + \frac{\omega^2}{2}r^2 z_r.$$

In fact, solving the full Gross-Pitaevskii equation also for the excited states turned out to be easier than diagonalizing the linearized Bogoliubov equations, and therefore the former
FIG. 4: Time dependence of the density profile for a system with $U = 0.1$ and $\omega = 0.3$ (weak trapping and weak interactions). The different sets of bars show the density at successive time instances for a system prepared in a superposition of the ground state and an excited state (left panel, first excited state; right panel, second excited state) with the amplitudes 0.92 and 0.4, respectively. The curves in the lower two panels show the variation of the center-of-mass position and mean squared radius with time, showing the dipole and breathing character, respectively, of the oscillations. To enhance visibility, the curve for the mean squared radius has been shifted down by an amount equal to its time average, defining the plotted quantity as

$$\langle \delta r^2 \rangle = \langle \psi(t)|r^2|\psi(t)\rangle - \bar{r}^2$$

where $\bar{r}^2$ is the time average.

The method was chosen. The result thus obtained for the first excited state is included in Fig. 3, and it can be seen that the Bogoliubov approximation fails appreciably even for weak interactions. The reason is that the derivation of the Gross-Pitaevskii equation assumes...
that the number of atoms in the ground state, $N_0$, greatly exceeds the quantum fluctuations around it, which, however, are of order unity; for the case of five particles this condition is certainly not met.\cite{14}

IV. Modes in Tight Traps

Let us now turn to the case of a tight trap. Figure 5 displays the ground-state density distribution for values of $U$ ranging from weak to strong interactions, in a trap with frequency $\omega = 4.0$. The physics is here determined by the balance between interactions and trap and the tunneling has little effect. The phase diagram has much more structure in this limit compared to the shallow-trap case.

For weak interactions ($U \lesssim 0.1$), all the particles simply gather in the central well (or
FIG. 6: Ground-state density in the case of a tight trap, $\omega = 4.0$.

the two central wells, if $L$ were even). With increasing $U$ the density distribution flattens, and for strong enough interactions the ground state resembles a Mott insulating state, with one particle in each of the centermost wells. (If the even/odd parity of the number of wells and the number of particles do not match, the edge sites will be partially filled.) Figure [4]
verifies that in this state the quantum fluctuations are minimal, which warrants the use of the term Mott state. The transition to the Mott state in this five-particle system is in fact quite sharp. Also in the limit of small $U$, the quantum fluctuations become small, but they only vanish completely in the limit $\omega \rightarrow \infty$ and the transition is not sharp.

FIG. 7: Quantum fluctuations in the ground-state density in a tight trap, $\omega = 4.0$. 
Between the two extremes, the shape of the atom cloud is determined by a balance between interactions and trap potential. It is quite easy to estimate the crossover values of $U$ where the system changes between different types of ground state (we avoid speaking of phases for this finite system). If the effective size of the system is $R$ sites, the interaction energy $E_i$ and trap energy $V$ scale as

$$E_i \sim \frac{N^2 U}{R}, \quad V \sim \omega^2 R^2. \quad (8)$$

Balancing these yields $R^3 \sim N^2 U/\omega^2$ or

$$U = \frac{\omega^2 R^3}{N^2}. \quad (9)$$

The Mott state, where $R = N$, thus sets in above $U = \omega^2 N$; inserting the present parameters we get $U = 80$. When the particles gather in the centermost well, $R$ is equal to 1; this happens when $U = \omega^2/N^2 \approx 0.5$ or smaller. This back-of-the-napkin argument is in almost quantitative agreement with the exact numerical findings.

The lowest few mode frequencies as functions of $U$ when $\omega = 4.0$ are displayed in Fig. 8. (Observe that, in order to emphasize physical interpretation, the frequencies were in Fig. 3 given in units of the trap frequency $\omega$, but here it is given in units of the tunneling $J$). The dependence on coupling seen in Figs. 6-7 is seen to have clear consequences also for the mode frequencies. In the central-well limit, $U \lesssim 1$, the frequencies are easily interpreted since the trap determines all the physics, and all the eigenstates of the Hamiltonian are pure Fock states or superpositions of degenerate Fock states. The lowest two modes are superpositions of the two possible states that result when one particle is removed from the central site and put in one of the two neighboring ones, $|\ldots 00410\ldots\rangle$ and $|\ldots 01400\ldots\rangle$. The limiting value of the excitation frequency is equal to $\omega^2/2 = 8$, the excess energy of one particle being moved to a neighboring site. The energy of the degenerate third and fourth excited states is twice this, since they have two particles in an off-center well. One may expect that among the two lowest excitations, the superposition with a minus sign corresponds to a dipole mode and the plus sign corresponds to a breathing mode. Indeed, this is confirmed in Fig. 9 where the time evolutions of the modes are visualized, but note the small amplitude of the oscillations. The time dependence is merely due to the small deviations from perfect confinement that are still left in the moderately strong trap with frequency $\omega = 4.0$; it can easily be realized that no current can flow in a system whose eigenstates are pure Fock states.
in configuration space. To see this, consider preparing an initial state as a superposition of two eigenstates of the system, $|\psi\rangle = \alpha|A\rangle + \beta|B\rangle$, and study its time evolution,

$$|\psi(t)\rangle = e^{-iE_A t} \left( \alpha|A\rangle + e^{-i\omega_{AB} t} \beta|B\rangle \right),$$

where $\omega_{AB} = E_B - E_A$. Now expand the time evolution in Fock states $|f\rangle$, and obtain for the density at the position $r$,

$$\langle \psi(t)|a_r^\dagger a_r|\psi(t)\rangle = \sum_f |\alpha\langle f|A\rangle + e^{-i\omega_{AB} t} \beta\langle f|B\rangle|^2 \langle f|a_r^\dagger a_r|f\rangle,$$

and we see immediately that if $|A\rangle$ and $|B\rangle$ have no Fock state components in common, there can be no time dependence. This fact lies behind the insulating nature of the Mott state, but as we have seen, it also prohibits the dynamics in the limit of a very strong trap.

FIG. 8: Lowest few excitation frequencies in a tight trap, $\omega = 4.0$. Dashed lines represent the Bogoliubov approximation.
As the coupling gets stronger, the degeneracy is lifted and an intricate pattern of level crossings follows; however, the dipole/monopole character of the two lowest modes is retained until $U$ approaches the value of approximately 50, where a mixing of the dipole and monopole modes starts to be visible, as seen in Fig. 10. When $U \gtrsim 100$, we are in the Mott state and the mixing is complete so that the four lowest-lying modes are degenerate with an energy equal to $5\omega^2/2$; this is the energy difference between the second and third well from the center as each excited state corresponds just to a displacement of a particle from the center. In fact, each of the two lowest excited states has very high overlap (the overlap is 0.98 when $U = 100$) with one of the pure Fock states $|\ldots011111000\ldots\rangle$ and $|\ldots000111110\ldots\rangle$, i. e., the ground-state configuration displaced from the center by one lattice site. The third and fourth excited states are separated from the first two by an exceedingly small energy gap.
FIG. 10: Same as Fig. 4 but here the trapping frequency is $\omega = 4.0$ and the coupling is $U = 40$. (about 0.005 in units of $J$), and are mainly superpositions of the state $|\ldots 010111100 \ldots \rangle$ and its mirror reflection. As seen in Fig. 11, excitation of one of these modes does not result in oscillation; this is again a consequence of the fact that the eigenstates are pure Fock states in the spatial representation. Indeed, this is a Mott insulating state and excitation does not result in particle flow.

Returning to the mode frequency plot in Fig. 8, the frequencies have also been calculated in the Bogoliubov approximation and are included as dashed lines. Somewhat surprisingly, the Bogoliubov approximation performs better in the strong-trapping regime than in the weak-trapping regime, although one would naively expect the accuracy to be worse when tunneling is suppressed: the quantum fluctuations in local density are small. The apparent paradox is resolved by noting that in this limit the system is in fact a Bose-Einstein condensate: all particles occupy the same state, namely the one confined to the central well.
V. CONCLUSIONS

The mode frequencies of a trapped boson system in an optical lattice have been studied with attention to the dependencies on trap strength and interactions. In the weakly-trapped limit, it is shown that the mode frequencies have the usual character of dipole oscillations for the lowest-lying mode and breathing oscillations for the next-lowest, and the frequencies are, despite the low number of particles and the discreteness, seen to approximately approach the result for a harmonically trapped gas when the interactions vanish. Discreteness effects set in when the interaction energy is comparable to the tunneling. For sufficiently strong trapping, the number fluctuations are quenched, and the dynamics therefore absent, in two limits: when the interactions are strong, even the five-particle system displays a quite sharp transition to a Mott insulating state. When on the other hand the trapping potential
dominates completely, all the particles are trapped in the central well and the amplitude of any oscillation goes to zero. It turns out that the Bogoliubov approximation is capable of approximating the mode frequencies better for strong trapping than for weak trapping: in the weak-trapping case the number of particles is too small for the Bogoliubov approximation to work, but a strong trap quenches the fluctuations around the Bose-Einstein condensed ground state.

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It is important here to make a distinction between quantum fluctuations in different quantities. In a Bose-Einstein condensed state, the occupation of the lowest single-particle state is macroscopic, and the quantum fluctuations around this solution are small (hence it is in field theory called a classical solution). On the other hand, the quantum fluctuations in the occupation of each site are big in this regime, unlike in the Mott state.