Condensate characteristics of bosons in a tilted optical lattice

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Abstract. In this work we study the properties of interacting bosons in a tilted triple well optical lattice potential. A tilted optical lattice is possible to create in an experiment with charged bosons in presence of an electric field. The ground state energy, occupation densities in each well and first order correlation function of occupation densities as a function of the tilt parameter for \( N = 90 \) bosons using recently developed Multiconfigurational time-dependent Hartree method for bosons (MCTDHB) are studied. The ground state energy falls off with the tilt parameter for a given value of the barrier height and interparticle interaction. Also the tilt parameter is observed to restrict the fragmentation of the occupation densities in each well and thus promote condensation. Further the correlation between the bosons in different wells enhances with the tilt parameter and at large values the bosons in the first and the third wells are correlated apart from the correlation among the bosons in the same well, while the occupancy in the middle one seems to be uncorrelated with the other two. Such correlation between different wells is not observed in absence of the tilt effect for the same barrier height of the potential and interparticle interaction strength.

1. Introduction
In recent years, the successful experimental realization of Bose-Einstein condensates with the help of optical lattices provided a suitable paradigm to study different exotic quantum phenomena of cold atoms[1]. The Gross-Pitaevskii mean-field theory is one of the efficient tool to study the static and dynamic properties of Bose-Einstein condensates. Though this theory is an excellent tool for explaining weakly correlated bosonic systems, it has some limitations. As this theory deals with only one time-dependent single-particle state (orbital) to explain Bose-Einstein condensates, it can not explain phenomena like fragmentation of condensates or Mott-insulator phase transition which require more than one single-particle state.

In recent years, an essentially exact, numerically efficient and multi-orbital many-body theory is developed which is known as multi-configuration time-dependent Hartree approach (MCTDH). Very recently, a bosonic version of MCTDH, called Multiconfigurational time-dependent Hartree method for bosons (MCTDHB)[2, 3, 4] is developed. It describes the static and dynamical properties of fragmented condensates. So MCTDHB is the generalization of the (one-orbital) Gross-Pitaevskii mean field theory.

In this work, we wish to study a system of weakly correlated bosons in an optical lattice potential and specifically a triple well. S.Sachdev et. al[5] have studied a system of ultracold charged bosonic atoms in an optical lattice potential and in presence of a gradient (produced
possibility by an applied electric field). Motivated by this paper, we study the static properties of a system of bosonic atoms in a tilted triple optical potential well using MCTDHB.

2. Formalism

Alon et al.[3] provided the complete derivation of the MCTHDB equations and also the details of the numerical implementation of MCTDHB. The use of time-adaptive optimized basis states is the main idea of this method. This method is a fully variational approach and there is no restriction for the number of orbitals, geometry, dimensionality, and interparticle interactions of the time-dependent many-boson problem. In this section we discuss in brief about this method.

The starting point of MCTDHB approach is the time-dependent variational principle (TDVP)[6]. The variational principle is based on the action,

\[ S = \langle \psi | H - i \frac{\partial}{\partial t} | \psi \rangle \]

Then the principle of least action (namely, \( \delta S(\psi(t), \psi^*(t)) = 0 \)) is employed to determine the equations of motion. Here the Hamiltonian of Eq.(1) reads as,

\[ \hat{H}(r_1, r_2, ..., r_N) = \sum_{j=1}^{N} \hat{h}(r_j) + \sum_{k>j=1}^{N} \hat{W}(r_j - r_k) \]

where \( r_j \) is the position of the \( j^{th} \) boson. The first term \( \hat{h} \) is the one-body Hamiltonian and is given as \( \hat{h}(r) = \hat{T}(r) + \hat{V}(r) \), where \( \hat{T}(r) \) is kinetic energy and \( \hat{V}(r) \) is the external potential (that is, \( V_{\text{trap}}(x) \) here). The second term \( \hat{W}(r_j - r_k) = \lambda_0 \delta(r_j - r_k) \) is the two-body interaction term. It is approximated as a \( \delta \)-function to incorporate the hardcore feature of bosons in the interparticle interaction term. The ground state energy is given by[7, 8],

\[ E = N \left\{ \int \psi^* \hat{h} \psi d\vec{r} + \frac{\lambda_0(N-1)}{2} \int |\psi|^4 d\vec{r} \right\} \]

where we have written the coefficient of the interaction term as, \( \lambda = \lambda_0(N-1) \), where \( \lambda \) is the interaction parameter and \( \lambda_0 \) is the interaction strength. A particular value of \( \lambda \), namely \( \lambda = 2 \) is chosen here, so that fragmentation of the condensate can be noted for a given barrier height and tilting parameter. This issue is elaborated later.

In second quantized notations, the bosonic field operator which annihilates a particle at position \( r \), corresponding to a set of \( M \) orthonormal, time-dependent functions (orbitals) \( \{ \phi_k(r, t) \} \) is given as,

\[ |\Psi(r)\rangle = \sum_{k=1}^{M} \hat{a}_k \phi_k(r, t) \]

Here the bosonic annihilation and creation operators obey their usual commutation relations at any given time. The time-dependent permanents with the help of the bosonic creation operators, \( \hat{a}_k^\dagger \) can be written as,

\[ |\vec{n}; t\rangle = \frac{[a_1^\dagger(t)]^{n_1}[a_2^\dagger(t)]^{n_2}...[a_M^\dagger(t)]^{n_M}}{\sqrt{n_1!n_2!n_3!...n_M!}} |0\rangle \]
where \( \vec{n} = (n_1, n_2, n_3, ... n_M) \) are the occupations of the orbitals preserving the total number of particles as \( n_1 + n_2 + ... + n_M = N \).

The ansatz made for many-boson wave function is,

\[
|\Psi(t)\rangle = \sum_{\vec{n}} C_{\vec{n}}(t)|\vec{n};t\rangle
\]

(6)

the summation in Eq.(6) runs over all possible configurations, that means \( N \) bosons are distributed over \( M \) accessible orbitals. The time-dependent many particle Schrödinger equation which governs the time evolution of \( N \) correlated bosons is given as \( (\hbar = 1) \),

\[
\hat{H}\Psi = i\frac{\partial \Psi}{\partial t}
\]

(7)

Now the main objective is to find out the exact solution of the many-boson time-dependent Schrödinger equation[3, 4], that is, to determine the time evolution of the expansion coefficients \( \{C_{\vec{n}}(t)\} \) and the orbitals \( \{\phi_k(r,t)\} \). Now we employ the Lagrangian formalism of the time-dependent variational principle[6] to evaluate the time evolution of \( \{C_{\vec{n}}(t)\} \) and \( \{\phi_k(r,t)\} \) which in turn gives the MCTDHB equations of motion. The different steps of our approach are:

(i) Variation with respect to the expansion coefficients \( C_{\vec{n}}(t) \):

Here the variation of the functional action with respect to the coefficients is considered and the equation of motion for expansion coefficients is obtained as[3, 4],

\[
H(t)C(t) = i\frac{\partial C(t)}{\partial t}
\]

(8)

This equation of motion is a first-order differential equation and the matrix \( H(t) \) is time-dependent as it is evaluated in the time-dependent permanents \( |\vec{n};t\rangle \) and \( |\vec{n}';t\rangle \).

(ii) Variation with respect to the orbitals \( \{\phi_k(r,t)\} \):

Considering variation with respect to the orbitals, the equation of motion for orbitals is obtained as[3, 4],

\[
i|\dot{\phi}_j\rangle = \hat{P}[\hat{h}|\phi_j\rangle + \sum_{k,s,q,l=1}^{M} \rho_{jk}^{-1} \rho_{ksql} \hat{W}_{sl}|\phi_q\rangle]
\]

(9)

where

\[
\hat{P} = 1 - \sum_{j'=1}^{M} |\phi_{j'}\rangle \langle \phi_{j'}|
\]

(10)

here \( \rho_{jk} \) is the one body reduced density matrix (RDM) and \( \rho_{ksql} \) is the two body reduced density matrix (RDM).

2.1. RDM and Natural occupations

The \( p^{th} \) order reduced density matrix (RDM) is defined as[4],

\[
\hat{\rho}^{(p)} = \frac{N!}{(N-p)!} Tr_{N-p}[|\Psi(t)\rangle \langle \Psi(t)|]
\]

(11)
Here $Tr_{N-p}[]$ is the partial trace runs over $(N - p)$ particles and diagonal $\rho^{(p)}$ corresponds to $p$-particle probability distribution at time $t$. The $p^{th}$ order RDM, $\rho^{(p)}$ expanded in its eigenfunctions is given as,

$$\rho^{(p)}(r_1, ..., r_p| r_1', ..., r_p'; t) = \sum_i n_i^{(p)}(t) \alpha_i^{(p)}(r_1, ..., r_p; t) \alpha_i^{*(p)}(r_1', ..., r_p'; t)$$ (12)

where $n_i^{(p)}(t)$ is the $i^{th}$ eigenvalue of the $p^{th}$ order RDM and $\alpha_i^{(p)}$ is the eigenfunction in real space. For $p = 1$, $\alpha_i^{(1)}$ is known as natural orbitals and $n_i^{(1)}(t)$ is known as natural occupations.

The $p^{th}$ order correlation function of an $N$ boson system at a time $t$ is given as,

$$g^{(p)}(r_1', ..., r_p', r_1, ..., r_p; t) = \frac{\rho^{(p)}(r_1, ..., r_p| r_1', ..., r_p'; t)}{\prod_{i=1}^{p} \rho^{(1)}(r_i| r_i'; t) \rho^{(1)}(r_i'| r_i; t)}$$ (13)

The diagonal $g^{(p)}(r_1', ..., r_p', r_1, ..., r_p; t)$ of the $p^{th}$ order correlation function in the real space is a measure of the $p^{th}$ order coherence.

Eqs.(12) and (13) are the working formulae for obtaining the occupation densities and first-order correlation function that will yield the coherence properties of bosons in a tilted triple well respectively.

3. Physical Observables and Results

We consider a representative system of $N = 90$ bosons in a tilted triple well potential of the form as follows (Fig.(1)),

$$V_{trap}(x) = -\alpha x + V_0(\sin(2x))^4$$ (14)

This trapping potential has sufficiently large barrier height, that is, $V_0 = 250$ in our case and it is maintained for the entire proceedings. Here $\alpha$ is the tilting parameter. The tilting term $\alpha x$ is similar to ‘potential energy’ of a charged particle in an electric field. In our case $\alpha$ ranges from 0 to 5. A brief justification of using such values for $\alpha$ is included later. As mentioned earlier, we have chosen $\lambda = 2$, such that the fragmentation of the condensate is observed in absence of the tilting effect $\alpha = 0$ for a barrier height, $V_0 = 250$. Non zero values of $\alpha$ are benchmarked with respect to this. Further, we have considered three basis states ($M = 3$). Our main aim is to study the static properties of weakly correlated bosons in a tilted triple well. For this purpose we have used an open source version of the MCTDHB algorithm[3].
3.1. Bose-Einstein Condensation and Fragmentation

In order to make the terminologies that have been used in this paper clear, we define a few relevant quantities such as condensation and fragmentation of the condensates. Bose-Einstein condensation can be defined with the help of natural orbital occupation numbers \(n^{(1)}_i\)[4, 9]. An identical bosonic system is said to be in a condensed state if the largest eigenvalue of the first-order RDM is of the order of the number of particles in the system, that is[4, 9],

\[
n^{(1)}_1 = \mathcal{O}(N)
\]  

(15)

So a bosonic state with \(N\)-bosons is said to be maximally coherent when \(n^{(1)}_1 = N\) and \(|g^{(1)}| = 1\). Bosonic states with largest natural occupation number close to \(N\) are known as depleted condensates. When two natural orbital occupation number is of the order of the total number of particles, that is, \(n^{(1)}_1, n^{(1)}_2 = \mathcal{O}(N)\), then one get a two-fold fragmentation of the condensate. Again for, \(n^{(1)}_1, n^{(1)}_2, n^{(1)}_3 = \mathcal{O}(N)\) a three-fold fragmented condensate emerges and so on.

3.2. Ground state energy and occupation density

We study the ground energy per particle, \(E/N\) and occupation density, \(n^{(1)}_i/N\) as function of the tilting parameter, \(\alpha\) for constant values of interparticle interaction, \(\lambda_0\) and barrier height, \(V_0\). From Fig.2(a), it is observed that \(E/N\) decreases with \(\alpha\). The decrease is slow for smaller values of \(\alpha\). From \(\alpha \simeq 0.8\) onward, a rapid fall of \(E/N\) is observed.

Fig.2(b) shows the behavior of the occupation density, \(n^{(1)}_i/N\) of natural orbitals of the many body wave function as a function of tilting parameter. Without tilting (that is with \(\alpha = 0\)) there is a three-fold fragmentation of the condensate. With the inclusion of the tilting angle, the three-fold fragmented state disappears. There is a gradual decrease in the occupation density of the first natural orbital, \(n^{(1)}_1/N\) and correspondingly a gradual increase in the occupation density of the third natural orbital, \(n^{(1)}_3/N\) till \(\alpha \simeq 0.8\). Whereas the occupation density of the second natural orbital, \(n^{(1)}_2/N\) remains constant till \(\alpha \simeq 0.8\). However, beyond \(\alpha \simeq 0.8\), a rapid change in the occupation density is observed. For higher values of \(\alpha\) \((\alpha = 5)\), the third natural orbital becomes fully condensed and correspondingly the occupation densities in the second and first natural orbitals become negligibly small. So ‘tilting’ leads to a transition from a fragmented to a condensed state for the bosons.
3.3. Coherence Properties

To get a deeper understanding about the properties of the condensate, the modulus squared of the normalized first-order correlation function $|g^{(1)}(x'_1, x_1)|^2$ at different tilting parameter is studied. Fig.3(a) shows $|g^{(1)}(x'_1, x_1)|^2$ for $\alpha = 0$. It is observed that there is no coherence between the wells and bosons reside in individual wells. Similar scenario is observed till $\alpha = 0.8$. For $\alpha > 0.8$, we observe correlation between the bosons of the third and first well and vice-versa apart from the correlation of bosons in the same well (Fig.3(b)). But for this value of $\alpha$, there is no correlation between the bosons of the middle well with the other two wells. Of course, there is correlation among the bosons in the same well. With further increase of the tilting angle $\alpha$, this observed coherence between different wells is destroyed gradually (Fig.3(c)). For higher values of $\alpha$ ($\alpha = 5$), the observed coherence between different wells totally destroyed and the third well becomes fully populated.

4. Conclusions

We have studied the static properties such as the ground state energy and occupation density of the natural orbitals of a system of 90 bosons in presence of a tilted triple well potential using MCTDHB approach. In presence of a tilting potential, the ground state energy per particle decreases starting with a very high value and it falls off rapidly for higher values of $\alpha$ corresponding to a fixed barrier height and interparticle interaction. Further, a transition from fragmented to condensate state is observed with increase in tilting angle.

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