Chapter 2

Methodology

2.1 Correlated potential harmonic expansion method : CPHEM

As explained earlier that GP equation ignores interatomic correlations and it is non-linear in nature. So to go beyond the mean-field approach and tackle really large number of particles we will utilize a correlated potential harmonic expansion method (CPHEM). This method basically is a truncated subset of HHEM method which regards only two-body correlation and ignores all higher-body correlations. It can handle realistic interatomic interaction like van der Waals interaction, Calegero-Sutherland and Lennard-Jones potential etc. Here we will discuss the methodology in detail :

2.1.1 Potential hamonic basis calculation

Consider a system of N = (A + 1) identical spinless bosons, each of mass m, confined in a spherically symmetric harmonic oscillator potential of frequency ω . The N-body Schrödinger equation for the trapped atoms can be written as

$$\left[-\frac{\hbar^2}{2m}\sum_{i=1}^N \nabla_i^2 + \sum_{i=1}^N \frac{1}{2}m\omega^2 r_i^2 + \sum_{i,j>i}^N V(\vec{r_i} - \vec{r_j}) - E\right]\psi(\vec{r_1}, ..., \vec{r_N}) = 0,$$
(2.1)

where second term is the external harmonic oscillator potential, where $\vec{r_i}$ is the position vector of *i*-th particle from the centre of mass (CM). Third term $V(\vec{r_i} - \vec{r_j})$

is the two-body interacting potential. Now we introduce A number of Jacobi vectors as

$$\vec{\zeta}_i = \sqrt{\frac{2i}{i+1}} \left(\vec{r}_{i+1} - \frac{1}{i} \sum_{j=1}^i \vec{r}_j \right), \quad (i = 1, ..., A).$$
(2.2)

The *i*-th Jacobi vector is proportional to the vector separation of the (i + 1)-th particle from the CM of the fist *i*-th particle. The CM vector is given by

$$\vec{R} = \frac{1}{N} \Big(\sum_{i=1}^{N} \vec{r_i} \Big).$$
(2.3)

The constants in front of the Jacobi vector is chosen in such a way that they satisfy the the following

$$\frac{1}{2}\sum_{i=1}^{N}\nabla^{2}_{\vec{r}_{i}} = \sum_{j=1}^{N-1}\nabla^{2}_{\vec{\zeta}_{j}} + \frac{1}{2N}\nabla^{2}_{\vec{R}}.$$
(2.4)

By using these Jacobi vectors we can separate out the N-body Schrödinger equation in centre of mass motion and relative motion. The Schrödinger equation for the relative motion is

$$\left[-\frac{\hbar^2}{m}\sum_{i=1}^{A}\nabla_{\vec{\zeta}_i}^2 + V_{trap} + \sum_{i,j>i}^{A}V(\vec{\zeta}_i - \vec{\zeta}_A) - E_R\right]\psi(\vec{\zeta}_1, ..., \vec{\zeta}_A) = 0,$$
(2.5)

where E_R is the energy of the relative motion and

$$V_{trap} = \sum_{i=1}^{A} \frac{1}{2} m \omega^2 \zeta_i^2.$$
 (2.6)

The evolution of the system can be traced by following the motion of a single point in 3A-dimensional hyperspace. The hyperspherical variables are used to define the corresponding polar coordinates of this point. The hyperspherical coordinates are constituted by the hyperradius r and (3N - 4) = (3A - 1) hyperangles. Out of these, 2A hyperangles $(\varphi_j, \vartheta_j, j = 1, 2, ..., A)$ are just spherical polar angles of A Jacobi vectors $(\vec{\zeta_1}, ..., \vec{\zeta_A})$ and (A - 1) angles $(\phi_2, \phi_3, ..., \phi_A)$ defines the relative length of the Jacobi vectors through

$$\zeta_{A} = r\cos\phi_{A}$$

$$\zeta_{A-1} = r\sin\phi_{A}\cos\phi_{A-1}$$

$$\zeta_{A-2} = r\sin\phi_{A}\sin\phi_{A-1}\cos\phi_{A-2}$$

$$\zeta_{A-3} = r\sin\phi_{A}\sin\phi_{A-1}\sin\phi_{A-2}\cos\phi_{A-3}$$

$$\vdots$$

$$\vdots$$

$$\zeta_{2} = r\sin\phi_{A}\sin\phi_{A-1}.....\sin\phi_{3}\cos\phi_{2}$$

$$\zeta_{1} = r\sin\phi_{A}\sin\phi_{A-1}.....\sin\phi_{3}\sin\phi_{2}\cos\phi_{1}$$
(2.7)

The hyperradius can be defined in terms of Jacobi vectors as

$$r = \left[\sum_{i=1}^{A} \zeta_i^2\right]^{\frac{1}{2}} = \left[\frac{2}{A+1} \sum_{i,j>i}^{A+1} r_{ij}^2\right]^{\frac{1}{2}},$$
(2.8)

where r_{ij} is the relative distance between the ij-pair of particles and r determines the global size of the system. We express the 3A-dimensional Laplace operator in terms of these 3A hyperspherical coordinates as

$$\sum_{i=1}^{A} \nabla_{3A}^2 \equiv \sum_{i=1}^{A} \nabla_{\vec{\zeta}_i}^2 = \frac{\partial^2}{\partial r^2} + \frac{3A-1}{r} \frac{\partial}{\partial r} - \frac{\mathcal{L}^2(\Omega_A)}{r^2}, \qquad (2.9)$$

 $\mathcal{L}^2(\Omega_A)$ is the grand orbital operator in 3A-dimensional space which is obtained from a recurrence formula [29] and has the form

$$\mathcal{L}^{2}(\Omega_{A}) = 4(1-z^{2})\frac{\partial^{2}}{\partial z^{2}} + 6[2-A(1+z)]\frac{\partial}{\partial z} + 2\frac{l^{2}(\omega_{ij})}{1+z} + 2\frac{\mathcal{L}^{2}(\Omega_{A-1})}{1-z}, \qquad (2.10)$$

where $z = \cos 2\phi$, $\omega_{ij} = (\vartheta, \varphi)$ and $\mathcal{L}^2(\Omega_{A-1})$ is the grand orbital operator in 3(A-1)-dimensional space. The general grand orbital operator, $\mathcal{L}^2(\Omega_A)$ of Eq. (2.10) is defined through,

$$\mathcal{L}_{i}^{2}(\Omega_{i}) = \frac{\partial^{2}}{\partial \phi_{i}^{2}} + [3(i-2)\cot\phi_{i} + 2(\cot\phi_{i} - \tan\phi_{i})]\frac{\partial}{\partial\phi_{i}} + \frac{l^{2}(\omega_{i})}{\cos^{2}\phi_{i}} + \frac{\mathcal{L}_{i-1}^{2}(\Omega_{i-1})}{\sin^{2}\phi_{i}}$$

$$(2.11)$$

$$\mathcal{L}_{i}^{2}(\Omega_{i}) = 4(1 - z_{i}^{2})\frac{\partial^{2}}{\partial z_{i}^{2}} + 6[2 - i(1 + z_{i})]\frac{\partial}{\partial z_{i}} + 2\frac{l^{2}(\omega_{i})}{1 + z_{i}} + 2\frac{\mathcal{L}_{i-1}^{2}(\Omega_{i-1})}{1 - z_{i}}, \quad (i = 2, 3, ..., A),$$
(2.12)

where $z_i = \cos 2\phi_i$, ω_i represents the set of two polar angles of Jacobi vector $\vec{\zeta}_i$. Note that $\mathcal{L}_1^2(\Omega_1) = l^2(\omega_1)$ and $\mathcal{L}_A^2(\Omega_A) = \mathcal{L}^2(\Omega_A)$. The eigenfunction of $\mathcal{L}^2(\Omega_A)$ is called the hyperspherical harmonics (HH) and is given (without angular momentum coupling) by [30]

$$Y_{[\mathcal{L}]}(\Omega_A) = Y_{l_1m_1}(\omega_1) \prod_{j=2}^{A} Y_{l_jm_j}(\omega_j)^{(j)} P_{\mathcal{L}_j}^{l_j,\mathcal{L}_{j-1}}(\phi_j)$$
(2.13)

where

$${}^{(j)}P_{\mathcal{L}_{j}}^{l_{j},\mathcal{L}_{j-1}} = \left\{ \frac{2\nu_{j}\Gamma(\nu_{j}-n_{j})\Gamma(n_{j}+1)}{\Gamma(\nu_{j}-n_{j}-l_{j}-1/2)\Gamma(n_{j}+l_{j}+3/2)} \right\}^{\frac{1}{2}} \times (\cos\phi_{j})^{l_{j}}(\sin\phi_{j})^{\mathcal{L}_{j-1}}P_{n_{j}}^{\nu_{j-1},l_{j}+1/2}(\cos2\phi_{j})$$

$$(2.14)$$

$$(j=2,3....A),$$

with

$$\nu_{j} = \nu_{j-1} + 2n_{j} + l_{j} + 3/2$$

= $\mathcal{L}_{j} + \frac{3j}{2} - 1$
= $\mathcal{L}_{j-1} + 2n_{j} + l_{j} + \frac{3j}{2} - 1 \ (j = 2, 3, ..., A)$
(2.15)

In Eq. (2.14) $P_n^{\alpha,\beta}(x)$ is a Jacobi polynomial. In Eq. (2.13) $[\mathcal{L}]$ represents the set of quantum numbers

$$\{(l_1, m_1), (l_2, m_2), \dots, (l_N, m_A), n_2, n_3, \dots, n_A\}$$

for a fixed value of grand orbital quantum number $\mathcal{L} = \mathcal{L}_A$. The quantum number \mathcal{L}_i is defined as

$$\mathcal{L}_i = \mathcal{L}_{i-1} + 2n_i + l_i, \qquad (2.16)$$

with $\mathcal{L}_1 = l_1$. Hence

$$\mathcal{L} \equiv \mathcal{L}_A = l_1 + \sum_{j=2}^A 2n_j + l_j.$$
(2.17)

If we expand the full wavefunction in the complete set of hyperspherical harmonics (HH) basis then tremendous numerical complexity arises. Exact numerical treatment becomes unmanageable for systems containg more than three particles. Here we are dealing with weakly interacting Bose-Einstein condensate as the density (n)is very low the system is very dilute in nature, the average interparticle distance is much larger than the range of interatomic interactions (a_s) . The phase space density $na_s^3 << 1$ so the three-body collisions are negligible. Thus, for the description of weakly interacting condensate, one can safely ignore the effect of three-body and higher-body correlations as three and higher body interaction are irrelevant so molecule formation is forbidden. It facilitates us to decompose the many-body wave function ψ into a subset of HHEM, which includes the two-body correlations only. The full many-body wave function ψ is then decomposed in two-body Faddeev components (ϕ_{ij}) which is a function of only r_{ij} and r. This decomposition reduces the numerical complexity a lot by truncating the active degrees of freedom to only four for any number of bosons. Since, only two-body correlation is relevant so the total wave function can be written in terms of Faddeev component for the interacting pair of bosons as

$$\psi = \sum_{i,j>i}^{N} \phi_{ij}(\vec{r}_{ij}, r).$$
(2.18)

 ϕ_{ij} is symmetric under the parity operation (P_{ij}) and satisfies Faddeev equation

$$[T + V_{trap} - E_R]\phi_{ij} = -V(\vec{r}_{ij})\sum_{k,l>k}^N \phi_{kl}, \qquad (2.19)$$

where $T = -\frac{\hbar^2}{m} \sum_{i=1}^{A} \nabla_{\xi_i^2}^2$ is the total kinetic energy. Summing both sides over all (ij) pairs, we get back the *N*-body Schrödinger equation. Thus, the total angular momentum and orbital quantum number of the whole system arise only for the interacting pair. The Faddeev component can be expanded in proper potential harmonic (PH) basis as

$$\phi_{ij}(\vec{r}_{ij},r) = r^{-\frac{(3A-1)}{2}} \sum_{K} \mathcal{P}^{lm}_{2K+l}(\Omega^{ij}_A) u^l_K(r), \qquad (2.20)$$

where Ω_A^{ij} is the full set of hyperangles in the 3A dimensional space for the (ij)-th interacting pair. An analytical expression for the PH basis, $\mathcal{P}_{2K+l}^{lm}(\Omega_A^{ij})$, in 3A

dimensional space can be found in Ref. [32] given as

$$P_{2K+l}^{lm}(\Omega_A^{ij}) = Y_{lm}(\omega_{ij}')^{(A)} P_{2K+l}^{l,0}(\phi) Y_0(D-3), \qquad (2.21)$$

D = 3A = 3(N-1) and $Y_0(D-3)$ is the zero-th order hyperspherical harmonics (HH). In the (3A - 1) dimensional space, HH basis is constituted by $(\vec{\zeta_1}, ..., \vec{\zeta_A})$ Jacobi vectors. $Y_{lm}(\omega'_{ij})$ is the spherical harmonics for the interacting pair of particles and $\omega' = (\varphi, \vartheta)$, where φ and ϑ are the polar angles of r_{ij} . So the hyperradius for the (A - 2) particles can be written as

$$\rho_{ij} = \left[\sum_{i=1}^{A-1} \zeta_i^2\right]^{1/2},\tag{2.22}$$

so that

$$r^2 = r_{ij}^2 + \rho_{ij}^2. (2.23)$$

The hyperangle ϕ is introduced as $r_{ij} = r \cos \phi$ and $\rho_{ij} = r \sin \phi$. Besides r, ϕ, φ and ϑ there are (3A - 4) remaining variables. These are constituted by 2(A - 1)polar angles associated with (A - 1) Jacobi vectors $(\vec{\zeta_1}, ..., \vec{\zeta_{A-1}})$ and (A - 2) angles defining their relative lengths and collectively denoted by $\Omega_{(A-1)}^{ij}$ called hyperangles in the 3(A - 1)-dimensional space. The corresponding form of Laplace operator is given in the reference [31]. The set of (3A - 1) quantum numbers of HH is now reduced to only 3 as for the (A - 1) noninteracting pair

$$l_1 = l_2 = \dots = l_{A-1} = 0$$

$$m_1 = m_2 = \dots = m_{A-1} = 0$$

$$n_1 = n_2 = \dots = n_{A-1} = 0$$
(2.24)

and for the interacting pair $l_A = l$, $m_A = m$ and $n_A = K$. Thus, the 3Adimensional Schrödinger equation reduces effectively to a four-dimensional equation with the relevant set of quantum numbers: hyperradius r, orbital angular momentum quantum number l, azimuthal quantum number m, and grand orbital quantum number (2K + l) for any N. Substitution of Eq. 2.20 into the Schrödinger equation we finally get a coupled differential equation as

$$\begin{bmatrix} -\frac{\hbar^2}{m}\frac{d^2}{dr^2} + \frac{\hbar^2}{mr^2} \{\mathcal{L}(\mathcal{L}+1) + 4K(K+\alpha+\beta+1)\} \\ + V_{trap}(r) - E_R \end{bmatrix} U_{Kl}(r) \\ + \sum_{K'} f_{Kl} V_{KK'}(r) f_{K'l} U_{K'l}(r) = 0, \qquad (2.25)$$

where $U_{Kl}(r) = f_{Kl} u_K^l(r)$, $\mathcal{L} = l + \frac{3N-6}{2}$, $\alpha = \frac{3N-8}{2}$, $\beta = l + \frac{1}{2}$, l being the orbital angular momentum of the system contributed by the interacting pair and and K is called the grand orbital quantum number. f_{Kl} is a constant and represents the overlap of the PH for interacting pair of particles with the sum of PHs corresponding to all pairs [29] and given by

$$f_{Kl}^{2} = \sum_{k,l>k} \langle P_{2K+l}^{lm}(\Omega_{A}^{ij}) \mid P_{2K+l}^{lm}(\Omega_{A}^{kl}) \rangle.$$
(2.26)

The analytic form of f_{Kl}^2 is given by

$$f_{Kl}^{2} = 1 + \left[2(A-1)(-\frac{1}{2})^{l}P_{K}^{\alpha\beta}(-\frac{1}{2}) + \frac{(A-1)(A-2)}{2}P_{K}^{\alpha\beta}(-1)\delta_{l,0}\right]/P_{K}^{\alpha\beta}(1)$$
(2.27)

Details prescription of the methodology was discussed in our earlier works [33, 34, 35, 36, 38, 39]. Resulting potential matrix element $V_{KK'}(r)$ is given by

$$V_{KK'}(r) = \int \mathcal{P}_{2K+l}^{lm'}(\Omega_A^{ij}) V(r_{ij}) \mathcal{P}_{2K'+l}^{lm}(\Omega_A^{ij}) d\Omega_A^{ij}.$$
 (2.28)

2.1.2 Inclusion of short-range correlation function

In the experimentally achieved BEC, the range of interatomic interaction is generally smaller than the average interparticle separation. This is required to prevent atom loss due to three-body collisions and formation of molecules. In GP theory, the effective interaction is determined by a single parameter - the s-wave scattering length (a_s) . The sign of a_s determines nature of the interaction: a positive (negative) value of a_s represents the repulsive (attractive) interaction. By considering zero range contact δ interaction, the GP theory neglects the shape of the potential. But for large number of bosons the effect of the range and shape of the potential is an important issue [34, 35]. Inclusion of a finite-range realistic two-body interaction is required. Note that a realistic interatomic interaction is always attractive at larger separations, and has a strong short-range repulsion which avoids the molecule formation. So, in our simulation a realistic interatomic interaction viz, van der Waals potential has been considered to reflect the detailed structure of the two-body potential which has a attractive long-range tail and short-range repulsive core. The van der Waals interaction has two parameters : a hard core of radius r_c and C_6 . By solving the zero-energy two-body Schrödinger equation

$$-\frac{\hbar^2}{m}\frac{1}{r_{ij}^2}\frac{d}{dr_{ij}}\left(r_{ij}^2\frac{d\eta(r_{ij})}{dr_{ij}}\right) + V(r_{ij})\eta(r_{ij}) = 0, \qquad (2.29)$$

one can get a_s . The asymptotic form of the short-range correlation function, $\eta(r_{ij})$, is in general accepted as $c_1r_{ij} + c_2$ and the corresponding s-wave scattering length is $a_s = -\frac{c_2}{c_1}$. For fixed C_6 value, we adjust the hard core radius r_c , such that a_s has the desired value. This $\eta(r_{ij})$ is further used in the Eq. 2.20 to get the new basis as

$$\phi_{ij}(\vec{r}_{ij},r) = r^{-\frac{(3A-1)}{2}} \sum_{K} \mathcal{P}^{lm}_{2K+l}(\Omega^{ij}_A) u^l_K(r) \eta(r_{ij}).$$
(2.30)

and we call it correlated PH (CPH) basis.

Thus, $\eta(r_{ij})$ correctly reproduces the correct short-range separation of the interacting pair and offers fast convergence in the PH basis. Instead of using Eq. 2.28, the potential matrix is further calculated by using the equation

$$V_{KK'}(r) = (h_K^{\alpha\beta} h_{K'}^{\alpha\beta})^{-\frac{1}{2}} \int_{-1}^{+1} \left\{ P_K^{\alpha\beta}(z) V\left(r\sqrt{\frac{1+z}{2}}\right) \right\} P_{K'}^{\alpha\beta}(z) \eta\left(r\sqrt{\frac{1+z}{2}}\right) W_l(z) dz, \qquad (2.31)$$

where $z = \cos(2\phi)$, $h_K^{\alpha\beta}$ and $W_l(z)$ are respectively the norm and the weight function of the Jacobi polynomial $P_K^{\alpha\beta}(z)$ [84]. By substituting this interaction potential term along with the CPHEM basis in the Eq. 2.25 we can solve the final coupled differential equation by our numerical method.

It is to be noted that the inclusion of the short-range correlation function in the PH basis makes it non-orthogonal. Standard procedure can be adopted to handle this kind of non-orthogonal basis. However, in our simulation we have checked that $\eta(r_{ij})$ differs from a constant value near the narrow interval about the origin. As the BEC length scale a_{ho} is very large in comparison with the interatomic separation so the overlap matrix becomes a constant matrix. For the relevant values of the global size of the system $r \sim \sqrt{3N}a_{ho}$ the effect of the constant matrix is taken into consideration by a suitable asymptotic constant value.

2.1.3 Choice of system parameters

We had chosen the interaction potential to be the van der Waals potential, with a short-range repulsive hard core of radius r_c and a long attractive tail, given as

$$V(r_{ij}) = \infty \quad \text{for } r_{ij} < r_c$$

= $-\frac{C_6}{r_{ij}^6} \quad \text{for } r_{ij} \ge r_c.$ (2.32)

For the experimental BEC, the range of the two-body interaction is much smaller than the average interparticle separation. The interatomic interaction for such dilute BEC can be represented by a single parameter - s-wave scattering length (a_s) . We take characteristic oscillator length $a_{ho} = \sqrt{\frac{\hbar}{m\omega}}$ as the unit of length scale. Energies are expressed in the unit of oscillator energy $(\hbar\omega)$. In a spherically symmetric trap of frequency $\omega = 2\pi \times 77.78$ Hz, the scattering length a_s is 100 Bohr = 0.00433 o.u for ⁸⁷*Rb* atoms - it corresponds to the JILA trap experiment. In our numerical simulation, we calculate a_s from the asymptotic behaviour of the two-body wave function calculated from the zero energy solution of the twobody Schrödinger equation [37]. The value of a_s changes from negative to positive passing through an infinite discontinuity as r_c decreases [37]. At each discontinuity one extra node in the two-body wave function appears that corresponds to one extra two-body bound state. For ${}^{87}Rb$ atoms the value of $C_6 = 6.4598 \times 10^{-11}$ o.u. For ${}^{87}Rb$ atoms in JILA trap we chose $r_c = 1.121 \times 10^{-3}$ o.u which corresponds to one-node in the two-body wave function and results $a_s = 0.00433$ o.u = 100 Bohr. Whereas for ⁷Li condensate in RICE trap $a_s = -27.3$ Bohr $= -45.7 \times 10^{-5}$ o.u. The magnetic trap was a roughly symmetric harmonic oscillator with frequencies $\nu_x = 150.6$ Hz, $\nu_y = 152.6$ Hz and $\nu_z = 131.5$ Hz. We use an isotropic harmonic oscillator with frequency $\nu = (\nu_x \nu_y \nu_z)^{\frac{1}{3}} = 144.6$ Hz. For ⁷Li the value of $C_6 =$ 1.71487×10^{-12} o.u [85]. For ⁷Li atoms in RICE trap, we fix $r_c = 5.3378 \times 10^{-4}$ o.u which corresponds to zero-node in the two-body wave function and results $a_s = -45.7 \times 10^{-5}$ o.u. Attractive BEC is not stable under the increment in the particle number. If we increase the number of trapped bosons the central density of the condensate increases eventually the system collapses because the kinetic energy is unable to balance the interaction energy. The corresponding critical number of atoms for collapse for ^{7}Li condensate is $N_{cr} = 1400$ [4, 38, 39].

2.1.4 Calculation of many-body effective potential

With this choice of parameters and taking the two-body interaction as van der Waals interaction, we solve the coupled differential equation by hyperspherical adiabatic approximation (HAA) [86, 87] where the hyperspherical motion is adiabatically decoupled from the hyperangular motion. The potential matrix together with the hypercentrifugal repulsion is diagonalized for a fixed value of r. The lowest eigenvalue, called the lowest eigenpotential $\omega_0(r)$ is further used in the hyperradial differential equation,

$$\left[-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + \omega_0(r) - E_R\right]\zeta_0(r) = 0.$$
(2.33)

 $\omega_0(r)$ provides the many-body effective potential in the hyperradial space in which the condensate moves as a single quantum entity. We obtain E_R and the hyperradial wave function $\zeta_0(r)$ in the extreme adiabatic approximation (EAA) [86, 87] by solving Eq. 2.33 by Runge-Kutta method subject to appropriate boundary conditions. The center of mass energy is 1.5 $\hbar\omega$ which is further added to energy eigenvalue to calculate the total energy. In this effective potential, the hyperradial excitations for l = 0 are calculated. Similarly, for l > 0, hyperradial excitations in the eigenpotential $\omega_l(r)$ are obtained for different values of l. However, for l > 0, as the numerical computation becomes very slow, we made some approximations. From our numerical analysis, we checked that the main contribution to the potential matrix comes from the diagonal hypercentrifugal term and we disregard the off-diagonal matrix element for l > 0. Thus, the effective potential $\omega_l(r)$ in the hyperradial space for l > 0 is obtained by adding the hypercentrifugal term corresponding to a particular value of l with the potential matrix element for l = 0. This approximation has been numerically tested for the calculation of thermodynamic properties of interacting bosons in JILA trap [3].

In an earlier work, calculation the ground state energy and low-lying collective excitations with CPHEM method are compared with the experimental results [39]. The results are also compared with the mean-field results and hydrodynamic model, the beyond mean-field effect, finite sized effect and the effect of interatomic correlation have been extensively discussed. Thus, the present methodology not only offers the beyond mean-field physics but a self-sufficient many-body technique which can tackle few hundred to a quite large number of particles in the trap by a single code [34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44]. In our present problem we calculate a large number of energy levels E_{nl} , where *n* runs from 0 to 300 and *l* runs from 0 to 200. Of course, the upper cut-off in *n* and *l* are finally determined by the convergence in the chemical potential.

2.2 Multiconfigurational time-dependent Hartree method for boson: MCTDHB

We consider the time-dependent many-body Schrödinger equation (TDSE),

$$i\partial_t |\Psi\rangle = \hat{H}|\Psi\rangle.$$
 (2.34)

Here, $|\Psi\rangle$ is the many-body state and the *N*-particle Hamiltonian \hat{H} in dimensionless units [88] reads,

$$H = \sum_{i=1}^{N} \left(-\frac{1}{2} \frac{\partial^2}{\partial x_i^2} + V(x_i) \right) + \sum_{i < j} W(x_i - x_j), \qquad (2.35)$$

where we set the trapping potential either to be the external harmonic trap as $V(x_i) = \frac{1}{2}x_i^2$ or optical lattice potential as $V(x_i) = V_{OL}\sin^2(kx_i)$ with V_{OL} as the depth of the potential. $W(x_i - x_j)$ is the two-body interaction potential. All quantities are dimensionless and expressed in harmonic oscillator units. For contact interaction, the interaction potential takes the form

$$W(x_i - x_j) = \lambda \delta(x_i - x_j), \qquad (2.36)$$

where λ is the interaction strength, for the contact interaction, determined by the scattering length a_s and the transverse confinement frequencies [90]. For longranged dipolar interaction

$$W(x_i - x_j) = \frac{g_d}{|x_i - x_j|^3 + \alpha_0},$$
(2.37)

where g_d is the dipolar interaction strength and α_0 is a short-range cut-off to avoid the divergence at $x_i = x_j$. We choose the cut-off parameter $\alpha_0 = 0.05$ such a way that the effective interaction $V_{eff} = \int_{-10.0}^{10.0} \frac{1}{x^3 + \alpha_0} dx = \int_{-10.0}^{10.0} \delta(x) dx = 1.0$. For the present study, we restrict to few interacting bosons for all our calculations and consider repulsive interactions, $\lambda > 0$ and $g_d > 0$, exclusively. To investigate the stationary properties of the system, we propagate the wave function in imaginary time using the MCTDHX software [69, 70, 71, 72] to solve the MCTDHB equations of motion [53, 54, 55, 56, 57]; thereby the system relaxes to the ground state.

The computation of the exact many-body wave function is a difficult problem. To handle the time-dependent Schrödinger equation, Eq. (2.34), we expand the many-body wave function $|\Psi\rangle$ of N interacting bosons in a complete set of timedependent permanents $|\vec{n};t\rangle = |n_1, ..., n_M;t\rangle$ with at most M single particle states or orbitals. The MCTDHB ansatz for the many-body wave function is thus

$$|\Psi(t)\rangle = \sum_{\vec{n}} C_{\vec{n}}(t) |\vec{n};t\rangle.$$
(2.38)

Here, the permanents $|\vec{n};t\rangle$ are symmetrized bosonic many-body states that are also referred to as "configurations". The sum in Eq. (2.38) runs on all configurations \vec{n} of N particles in M orbitals. The number of permanents and coefficients $C_{\vec{n}}(t)$ is $N_{conf} = \begin{pmatrix} N+M-1\\ N \end{pmatrix}$. In the second quantized representation, the permanents are given as

$$|\bar{n};t\rangle = |n_1,...n_M;t\rangle = \prod_{i=1}^M \left(\frac{\left(\hat{b}_i^{\dagger}(t)\right)^{n_i}}{\sqrt{n_i!}}\right)|vac\rangle.$$
(2.39)

Here $\hat{b}_k^{\dagger}(t)$ is the bosonic creation operator which creates a boson in the timedependent single particle state $\phi_k(\vec{r},t)$. Note that the expansion coefficients $\{C_{\vec{n}}(t); \sum_i n_i = N\}$ and the orbitals $\{\phi_i(x,t)\}_{i=1}^M$ that build up the permanents are explicitly time-dependent and variationally optimized quantities [89]. In MCT-DHB, $\vec{n} = (n_1, n_2, ..., n_M)$ represent the occupations of the orbitals in a single configuration and $n_1 + n_2 + ... + n_M = N$, M is the number of single particle functions that make up the permanents. Note that in the limit of $M \to \infty$, the set of permanents $\{|\vec{n};t\rangle\}$ span the whole Hilbert space and the expansion is exact. However, for practical calculation, we limit the size of the Hilbert space ensuring convergence in the measured quantities like the energy, one- and two-body density matrix with respect to the number of single particle states M. A set of coupled equations of motion for, both, the time-dependent expansion coefficients $C_{\vec{n}}(t)$ and the time-dependent orbitals $\phi_k(\vec{r}, t)$ are obtained by requiring the stationarity of the action of the time-dependent Schrödinger equation [53, 54] under variations of $C_{\vec{n}}(t)$ and $\phi_k(\vec{r}, t)$. MCTDHB is thus fundamentally different from exact diagonalization, i.e., an ansatz built with *time-independent* orbitals. The set of coupled equations are solved simultaneously for the ground state using imaginary time propagation [69, 70, 71, 72].