Feynman-Kac path integral approach
for the energy spectrum of many
boson systems

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Abstract

We study the ground and excited states of weakly interacting Bose
gases (with positive and negative scattering lengths) in connection
with Bose Einstein condensation to test the validity of using the mean
field theory and Born approximation. They behave as new quantum
fluids (a gas in the weak limit and a liquid in the dense limit and we
study their many body physics in the dilute limit within the realistic
potential model (Morse type) by Feynman-Kac path integral tech-
nique. Within numerical limitations, this method is exact in principle
and turns out to be a better alternative to GP as all the ground and
excited states properties can be calculated in a much simpler way.
1 Introduction

With the experimental realization of Bose Einstein Condensation in alkali gases[1], the study of many boson systems has become an area of active research interest. Previous numerical procedures are based on mean field theory like Gross Pitaevski [2] etc. They seem to work well for ground state properties but turn out to be approximate as they fail to include correlations in the many body theory. Investigations of effects beyond mean field theory is an important task and makes the many boson systems interesting even from the many body perspective[3]. Moreover earlier calculations with δ function potential do not solve the many body problem exactly but only within a perturbation theory as in a system of Bose gas with δ function potential, particles do not collide [4]. As a result, speculations ( particularly excitation frequencies etc ) based on these methods differ drastically for different experimental modes. So an alternative to GP was necessary which can describe the effect of interaction in a more reliable way and predict the excitation frequencies and other properties more accurately. Even though Monte Carlo techniques are slow, computationally expensive and faces sign problem for fermionic systems, these are the only numerical techniques available for these kind of many body systems, which are exact and can include correlations in a reliable way. We also test the validity of Born approximation at low energy and temperature.

We propose to apply a quantum Monte Carlo technique based on Feynman-Kac formalism[5-7] of Quantum Mechanics which forms the basis for a simple and accurate way to calculate ground and excited state properties. To be precise, we apply Generalized Feynman Kac ( GFK) method [8-10] for attractive and repulsive potentials for many boson system of alkali gases ( Rb and Li respectively ). In our model the atoms in the dilute gas interact through Morse potential instead of conventional pseudopotential. Since at low temperature the de Broglie wavelength of the atoms become appreciable, we do full quantum treatment. To connect GFK to other many body techniques our numerical procedure ( GFK ) has a straightforward implementation to Schroedinger’s wave mechanics. GFK is essentially a path
integral technique with trial functions for which operations of the group of the wave function keep points in the chosen nodal region, provide an upper bound for the lowest state energy of that symmetry. The nodal region with the lowest energy serves as a least upper bound. If the nodal region has exact nodal structures of the true wave function the random walk is exact in the limit scale, time for walk, and number of walks get arbitrarily large. $Rb^{87}$ and $Li^{7}$ both having odd number of electrons and odd number of nuclei obey Bose statistics. So we do not need to worry about sign problem for these calculations. Our method gives more accurate values for the ground and excited state energies as to calculate energy we approximate an exact solution (i.e., the GFK representation of it) to the Schrödinger’s equation, whereas most of the other numerical procedures approximate a solution to an approximate Schrödinger equation. Since we work with the bosonic system our results are exact within the numerical limitations. There are other Monte Carlo calculations which are worth mentioning in this context are ground state calculation by Diffusion Monte Carlo method [11] and path integral Monte Carlo (with temperature dependence) [12]. This paper is organized as follows. In Sec 2, we present the general formalism of Feynman-Kac and Generalized Feynman-Kac method and then describe it for the ground and excited state of trapped Bosons. In Sec 3, we describe the numerical procedure. In Sec 4 we present results for positive ($Rb^{87}$) and negative ($Li^{7}$) scattering lengths. Finally in Sec 5 we summarize our achievements.

2 Theory

2.1 Path integral Theory at $T=0$

2.1.1 Feynman-Kac Path integration

For the Hamiltonian $H = -\Delta/2 + V(x)$ consider the initial value problem

$$i\frac{\partial u}{\partial t} = (-\frac{\Delta}{2} + V)u(x, t)$$

$$u(0, x) = f(x)$$

(1)
with $x \in \mathbb{R}^d$ and $u(0, x) = 1$. The solution of the above equation can be written in Feynman-Kac representation as

$$u(t, x) = E_x \exp\{-\int_0^t V(X(s))ds\}$$

(2)

where $X(t)$ is a Brownian motion trajectory and $E$ is the average value of the exponential term with respect to these trajectories. The lowest energy eigenvalue for a given symmetry can be obtained from the large deviation principle of Donsker and Varadhan [13],

$$\lambda = -\lim_{t \to \infty} \frac{1}{t} \ln E_x \exp\{-\int_0^t V(X(s))ds\}$$

(3)

Generalizations of the class of potential functions for which Eqs. 2 and 3 are valid are given by Simon[14] and include most physically interesting potentials, positive or negative, including, in particular, potentials with $1/x$ singularities. It also means that the functions determined by Eq(2) will be the one with lowest energy of all possible functions independent of symmetry. Restrictions on allowed Brownian motions must be imposed to get a solution of the desired symmetry if it is not the lowest energy solution for a given Hamiltonian. Although other interpretations are interesting, the simplest is that the Brownian motion distribution is just a useful mathematical construction which allows one to extract a physically relevant quantity, the ground and excited state energy of a quantum mechanical system. In numerical implementation of Eq(3) the 3N dimensional Brownian motion is replaced by 3N independent, properly scaled one dimensional random walks as follows. For a given time $t$ and integers $n$ and $l$ define [6] the vector in $\mathbb{R}^{3N}$

$$W(l) \equiv W(t, n, l) = (w_1^1(t, n, l), w_2^1(t, n, l), w_3^1(t, n, l),..., w_1^N(t, n, l)w_2^N(t, n, l)w_3^N(t, n, l))$$

(4)

where

$$w_j^i(t, n, l) = \sum_{k=1}^{l} \frac{\epsilon_{jk}^i}{\sqrt{n}}$$

(5)

with $w_j^i(0, n, l) = 0$ for $i = 1, 2, ..., N; j = 1, 2, 3$ and $l = 1, 2, ..., nt$. Here $\epsilon$ is chosen independently and randomly with probability $P$ for all $i, j, k$ such
that $P(\epsilon^i_{jk} = 1)=P(\epsilon^i_{jk} = -1)=\frac{1}{2}$. It is known by an invariance principle[15] that for every $\nu$ and $W(l)$ defined in Eq(4)

$$\lim_{n \to \infty} P\left(\frac{1}{n} \sum_{l=1}^{nt} V(W(l)) \leq \nu\right) = P\left(\int_0^t V(X(s))ds \leq \nu\right)$$

Consequently for large $n$,

$$P[\exp(-\int_0^t V(X(s))ds) \leq \nu] \approx P[\exp(-\frac{1}{n} \sum_{l=1}^{nt} V(W(l))) \leq \nu]$$

By generating $N_{rep}$ independent replications $Z_1, Z_2, \ldots, Z_{N_{rep}}$ of

$$Z_m = \exp(-\frac{1}{n} \sum_{l=1}^{nt} V(W(l)))$$

and using the law of large numbers, $(Z_1 + Z_2 + \ldots Z_{N_{rep}})/N_{rep} = Z(t)$ is an approximation to Eq(2)

$$\lambda \approx -\frac{1}{t} \log Z(t)$$

Here $W^m(l), m = 1, 2, N_{rep}$ denotes the $m^{th}$ realization of $W(l)$ out of $N_{rep}$ independently run simulations. In the limit of large $t$ and $N_{rep}$ this approximation approaches an equality, and forms the basis of a computational scheme for the lowest energy of a many particle system with a prescribed symmetry.

In dimensions higher than 2, the trajectory $X(t)$ escapes to infinity with probability 1. As a result, the important regions of the potential are sampled less and less frequently and the above equation converges slowly. Now to speed up the convergence we use Generalized Feynman-Kac (GFK) method.

### 2.1.2 Generalized Feynman Kac path integretion

To formulate the (GFK) method, we first rewrite the Hamiltonian as $H = H_0 + V_p$, where $H_0 = -\Delta/2 + \lambda_T + \Delta \psi_T/2\psi_T$ and $V_p = V - (\lambda_T + \Delta \psi_T/2\psi_T)$. 

5
Here $\psi_T$ is a twice differentiable nonnegative reference function and $H\psi_T = \lambda_T\psi_T$. The expression for the energy can now be written as

$$\lambda = \lambda_T - \lim_{t \to \infty} \frac{1}{t} \ln E \exp \{-\int_0^t V_\psi(Y(s))ds\}$$  \hspace{1cm} (10)

where $Y(t)$ is the diffusion process which solves the stochastic differential equation

$$dY(t) = \frac{\Delta \psi_T(Y(t))}{\psi_T(Y(t))} dt + dX(t)$$  \hspace{1cm} (11)

The presence of both drift and diffusion terms in this expression enables the trajectory $Y(t)$ to be highly localized. As a result, the important regions of the potential are frequently sampled and Eq (3) converges rapidly.

### 2.2 Schroedinger Formalism for Rb and Li condensate

Case 1: A system of few Rb atoms interacting through a model potential in an isotropic trap.

$$[-\Delta/2 + V_{int} + \frac{1}{2} \sum_{i=1}^{N} [x_i^2 + y_i^2 + z_i^2]]\psi(\vec{r}) = E\psi(\vec{r})$$  \hspace{1cm} (12)

The atoms here interact through a model potential $Dsech^2(r/r_0)$

Case 2: Systems of Rb and Li atoms interacting through Morse potential trapped inside an anisotropic trap. We choose to work in the cylindrical coordinates as the original experiment had an axial symmetry, cylindrical coordinates are the natural choices for this problem. We consider a cloud of N atoms interacting through repulsive potential placed in a three dimensional anharmonic oscillator potential. At low energy the motion of condensate can be represented as

$$[-\Delta/2 + V_{int} + \frac{1}{2} \sum_{i=1}^{N} [x_i^2 + y_i^2 + \lambda z_i^2]]\psi(\vec{r}) = E\psi(\vec{r})$$  \hspace{1cm} (13)

where $\frac{1}{2} \sum_{i=1}^{N} [x_i^2 + y_i^2 + \lambda z_i^2]\psi(\vec{r})$ is the anisotropic potential with anisotropy factor $\lambda = \frac{\omega_z}{\omega_x}$. Now

$$V_{int} = V_{Morse} = \sum_{i,j} V(r_{ij}) = \sum_{i<j} D[e^{-\alpha(r-r_0)}(e^{-\alpha(r-r_0) - 2}]$$  \hspace{1cm} (14)
The above Hamiltonian is not separable in spherical polar coordinates because of the anisotropy. In cylindrical coordinates the noninteracting part behaves as a system of noninteracting harmonic oscillators and can be written as follows:

\[
\begin{align*}
&\left[- \frac{1}{2\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) - \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} - \frac{1}{2} \frac{\partial^2}{\partial z^2} \\
&+ \frac{1}{2} (\rho^2 + \lambda^2 z^2) \right] \psi(\rho, z) \\
&= E \psi(\rho, z)
\end{align*}
\] (15)

The energy 'E' of the above equation can be calculated exactly which is

\[
E_{n_\rho n_z m} = (2n_\rho + |m| + 1) + (n_z + 1/2)\lambda
\] (16)

Since we are dealing with many Boson systems having very small number of particles, (In JILA experiment the number of particles is of the order of 2000 and does not correspond to Thomas-Fermi limit). So it is quite legitimate to use Gaussian trial functions for modes which are not coupled. In our guided random walk we use the solution of Schröedinger equation for harmonic oscillator in d-dimension as the trial function as follows [16]:

\[
\psi_{n_\rho n_z m}(\mathbf{r}) \simeq \exp \left( -\frac{z^2}{2} L_{n_\rho}^{(m)}(\rho^2) \right) \]
(17)

2.3 Fundamentals of BEC

Even though the phase of Rb vapors at T=0 is certainly solid, Bose condensates are preferred in the gasous form over the liquids and solids because at those higher densities interactions are complicated and hard to deal with on an elementary level. They are kept metastable by maintaining a very low density. For alkali metals, \( \eta \), the ratio of zero point energy and molecular binding energy lies between \( 10^{-5} \) and \( 10^{-3} \). According to the theory of corresponding states[17] since for the T=0 state of alkali metals, \( \eta \) exceeds a critical value 0.46, the molecular binding energy dominates over the zero point motion and they condense to solid phase. But again the life time of a gas is limited by three body recombination rate which is proportional to the
sqaure of the atomic density. It gets suppressed at low density. Magnetically trapped alkali vapors can be metastable depending on their densities and lifetimes. So keeping the density low only two body collisions are allowed as a result of which dilute gas approximation [11] still holds for condensates which tantamounts to saying \( na^3 << 1 \) (\( a \) is the scattering length of s wave). Now defining \( n = N/V = r_{av}^{-3} \) as a mean distance between the atoms ( definition valid for any temperature ), the dilute gas condition reads as \( a << r_{av} \) and zero point energy dominates (dilute limit). In the dense limit, for \( a \approx r_{av} \) on the other hand the interatomic potential dominates [11]. The gas phase is accomplished by reducing the material density through evaporative cooling.

### 3 Numerical procedure

#### 3.1 Dilute limit

In the dilute limit and at very low energy only binary collisions are possible and no three body recombination is allowed. In such two body scattering at low energy first order Born approximation is applicable and the interaction strength 'D' can be related to the single tunable parameter of this problem, the s-wave scattering length 'a' through the relation given below. This single parameter can specify the interaction completely without the detail of the potential in the case of pseudopotentials. We study a system of Rb particles interacting through following two repulsive potentials.

A. Model potential \( V(r) = Dsech^2(r/r_0) \)

B. Morse potential for dimer of rubidium

\[
\sum_{i,j} V(r_{ij}) = \sum_{i<j} D[e^{-\alpha(r-r_0)}(e^{-\alpha(r-r_0)} - 2)]
\]

with more realistic feature of having repulsive core at \( r_{ij} = 0 \) than other model potentials. In our case, the interaction strength depends on two more additional parameters, \( r_0 \) and \( \alpha \).

\[
a = \frac{mD}{4\pi\hbar^2} \int V(r) d^3r
\]
Case I. For potential 'A', the above yields \( D = \frac{12a\hbar^2}{m\pi^2r_0^4} \). The Hamiltonian for a system of Rb gas in an isotropic trap interacting through a potential \( V(r) \) can be written as

\[
\left\{-\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i,j} V(r'_{ij}) \right\} \\
+ \sum_{i=1}^{N} \left( \frac{m}{2} \omega_i^2 (x_i'^2 + y_i'^2 + z_i'^2) \right) \psi(\vec{r}') \\
= E\psi(\vec{r}')
\] (20)

The above Hamiltonian can be rescaled by substituting \( \vec{r}' = s\vec{r} \) and \( E = E_0U \) and the interaction strength in the dimensionless form can be written as

\[
\gamma_1 = \frac{12a}{sr_0^3\pi^2} = 3.05 \times 10^{-3}
\] (21)

with \( r_0 = 1.2 \).

Case II. Again for potential 'B' the Born approximation yields

\[
D = \frac{4\hbar^2a\alpha^3}{me_{\alpha\pi r_0}(e^{\alpha r_0} - 16)}
\] (22)

The Hamiltonian for Rb gas with an asymmetric trapping potential and Morse type mutual interaction can be written as

\[
\left\{-\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i,j} \right\} \\
+ \sum_{i,j} \left( \frac{m}{2} \omega_x^2 \sum_{i=1}^{N} x_i'^2 + \omega_y^2 \sum_{i=1}^{N} y_i'^2 + \omega_z^2 \sum_{i=1}^{N} z_i'^2 \right) \psi(\vec{r}') \\
= E\psi(\vec{r}')
\] (23)

The above Hamiltonian can be rescaled by substituting \( \vec{r}' = s\vec{r} \) and \( E = E_0U \) as

\[
\left\{-\frac{\hbar^2}{2ms^2} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i,j} \frac{4\hbar^2a\alpha^3}{ms^3e_{\alpha\pi r_0}(e^{\alpha r_0} - 16)} \left[ e^{-\alpha(r_{ij} - r_0)}(e^{-\alpha(r_{ij} - r_0)} - 2) \right] \right\} \\
+ \sum_{i,j} \left( \frac{ms^2}{2} \omega_x^2 \sum_{i=1}^{N} x_i'^2 + \omega_y^2 \sum_{i=1}^{N} y_i'^2 + \omega_z^2 \sum_{i=1}^{N} z_i'^2 \right) \psi(\vec{r}) \\
= E_0U\psi(\vec{r})
\] (24)

\[
\left[ \frac{1}{2} \sum_{i=1}^{N} \nabla_i^2 - \frac{a\alpha^3}{se_{\alpha\pi r_0}(e^{\alpha r_0} - 16)} \sum_{i,j} \left[ e^{-\alpha(r_{ij} - r_0)}(e^{-\alpha(r_{ij} - r_0)} - 2) \right] \right]
\]
\[- \frac{m^2 \omega_x^2 s^4}{2\hbar^2} \sum_{i=1}^{N} (x_i^2 + \frac{\omega_y^2}{\omega_x^2} y_i^2 + \frac{\omega_z^2}{\omega_x^2} z_i^2)] \psi(\vec{r}) = -E_0 \frac{U ms^2}{\hbar^2} \psi(\vec{r}) \] (25)

Let \( \frac{m^2 \omega_x^2 s^4}{\hbar^2} = 1 \Rightarrow \) is the natural unit of length. Let \( \frac{U ms^2}{\hbar^2} = 1 \Rightarrow U = \frac{\hbar^2}{m s^2} = \hbar \omega_x \) is the natural unit of energy. Then the standard form of the equation becomes

\[
\left[ \frac{1}{2} \sum_{i=1}^{N} \nabla_i^2 - \frac{4 a\alpha^3}{s e^{\alpha r_0} (e^{\alpha r_0} - 16)} \sum_{i<j} [e^{-\alpha(r_{ij} - r_0)} (e^{-\alpha(r_{ij} - r_0)} - 2)] \sum_{i<j} \right] \psi(\vec{r}) \\
- \frac{1}{2} \sum_{i=1}^{N} (x_i^2 + \frac{\omega_y^2}{\omega_x^2} y_i^2 + \frac{\omega_z^2}{\omega_x^2} z_i^2)] \psi(\vec{r}) \\
= -E_0 \psi(\vec{r}) \] (26)

With \( \omega_x = \omega_y = \frac{\omega_x}{\sqrt{\lambda}} \), the above eqn becomes,

\[
\left[ \frac{1}{2} \sum_{i=1}^{N} \nabla_i^2 - \frac{4 a\alpha^3}{s e^{\alpha r_0} (e^{\alpha r_0} - 16)} \sum_{i<j} [e^{-\alpha(r_{ij} - r_0)} (e^{-\alpha(r_{ij} - r_0)} - 2)] \sum_{i<j} \right] \psi(\vec{r}) \\
- \frac{1}{2} \sum_{i=1}^{N} [x_i^2 + y_i^2 + \lambda z_i^2] \psi(\vec{r}) \\
= -E_0 \psi(\vec{r}) \] (27)

\[
\left[ \frac{1}{2} \sum_{i=1}^{N} \nabla_i^2 - \gamma \sum_{i<j} [e^{-\alpha(r_{ij} - r_0)} (e^{-\alpha(r_{ij} - r_0)} - 2)] \sum_{i<j} \right] \psi(\vec{r}) \\
- \frac{1}{2} \sum_{i=1}^{N} [x_i^2 + y_i^2 + \lambda z_i^2] \psi(\vec{r}) \\
= -E_0 \psi(\vec{r}) \] (28)

Now for \( \alpha = .35 \) and \( r_0 = 11.65 \) (both in oscillator units)[4,18], the Morse potential become almost noninteracting and the results become substantially lower than GP. We find a better agreement with GP by choosing \( \alpha = .29 \) and \( r_0 = 9.67 \). We have checked that for these choice of parameters, Morse solution is extremely good. \( a = 52 \times 10^{-10}, s = .12 \times 10^{-5}, \) the interaction strength \( \gamma \) is given by

\[
\gamma_2 = 4 \frac{a\alpha^3}{s e^{\alpha r_0} (e^{\alpha r_0} - 16)} = 4.9 \times 10^{-5} \] (29)
For mean field calculation the value of interaction strength was taken to be $4.33 \times 10^{-3}$. For this problem we are interested in the limit $\gamma << 1$. The case $\gamma >> 1$ is usually known as the Thomas Fermi limit. For $\gamma = 4.9 \times 10^{-5}$, the eigenvalue equation reduces to a minimally perturbed system of $d$ dimensional anisotropic oscillator where $d = 3N$ and $N$ is the number of particles. The whole concept of bound states of Morse dimers is very outside the range of this limit, so the nonexistence of two-body bound states is ensured by choosing the above parameters.

Case III. Using the same Morse potential with $\alpha = 0.4$ and $r_0 = 6.8$, one can generate attractive interaction for $Li^7$ as well. In this case the interaction strength turns out to be

$$\gamma_3 = 4 \frac{a\alpha^3}{e^{\alpha r_0}(e^{\alpha r_0} - 16)} = -9.345 \times 10^{-6}$$

Even though $\gamma << 1$, we solve the eigenvalue eqn nonperturbatively with Generalized Feynman-Kac procedure. Energies at zero temperature are obtained for ground and excited states by solving Eq.(1) and using Eq.(3). Since original Feynman-Kac method [5-6] is computationally inefficient we incorporate importance sampling in our random walk and use trial function of the form given in Eq.(17)
4 Results

Case 1. A system of Rb atoms in an isotropic trapping and interacting through a model potential
\( Dsech^2(r/r_0) \).

Table 1: In column 2, ground state energies for 3-20 particles in an isotropic trap with potential 'a' in units of \( \hbar \omega \bot \) for \( a = 0.00305a_h \). Columns 3-5 represent the same energies by Blume and Green(BG)[19], GP and modified GP respectively.

| N  | \( E_{GFK} \)   | \( E_{BG} \)   | \( E_{GP} \)   | \( E_{GP,mod} \) |
|----|----------------|----------------|----------------|-----------------|
| 3  | 4.50925(3)     | 4.51037(2)     | 4.51032        | 4.51032         |
| 5  | 7.53086(5)     | 7.53439(6)     | 7.53432        | 7.53434         |
| 10 | 15.13867(3)    | 15.1539(2)     | 15.1534        | 15.1535         |
| 20 | 30.58460(4)    | 30.639(1)      | 30.638         | 30.639          |

4.1 Positive scattering length: Rb

As the potential does not sustain any many body bound state (which is ensured by suitably choosing the value of the parameters \( \alpha \) and \( r_0 \)) and the scattering length is positive the system behaves as a gas or as a metastable state which can be long-lived at very low densities[3]. In the table below, we explicitly show the expectation values of trap potential, interatomic potential and kinetic energy as three components of total energy for different number of particles and it is observed that virial theorem is satisfied in each case[20].

\[
2E_{kin} - 2E_{HO} + 3E_{pot} = 0
\]  \( (31) \)

From Fig 1, 2 and 3, we see that energy/particle rises with increase in number of atoms in the trap for different symmetry states. From Fig 4, 5 and 6, we see that in the case of Rb, increase in number of particles in the trap lowers the central density. From the ground state data, the aspect ratio of
velocity distribution i.e., \( \sqrt{\frac{\langle p_x^2 \rangle}{\langle p_z^2 \rangle}} \) is calculated and its values are given in the last column of Table 2. The value of aspect ratio in the noninteracting limit corresponds to \( \sqrt{\lambda} \) and with increase in number of particles this value increases and in the Thomas Fermi limit it should correspond to \( \lambda \). From our data, we verify this trend of aspect ratio (Fig 7).

Table 2: Results for ground state of Rb with \( \lambda = \sqrt{8} \). Chemical potential and energy are in units of \( \hbar \omega_\perp \) and length is in units of \( a_\perp \). Numbers in the brackets correspond to the reference [20].

| N   | \( \mu \)      | E/N | E/N_{kin} | E/N_{ho} | E/N_{pot} | \( \sqrt{\langle x^2 \rangle / \langle z^2 \rangle} \) |
|-----|-----------------|-----|-----------|-----------|-----------|---------------------------------|
| 1   | 2.414213        | 2.414213 | 1.207409 | 1.206803 | 0.0       | 1.679563 (1.68333)               |
| 10  | 2.448952        | 2.431595(5) | 1.202488 | 1.211725 | 0.017369 | 1.684900 (1.68333)               |
| 40  | 2.564350        | 2.489287(1) | 1.196455 | 1.217758 | 0.075068 | 1.68732 (1.68333)               |
| 70  | 2.678893        | 2.546602(6) | 1.188591 | 1.225621 | 0.132339 | 1.688079 (1.68333)               |
| 100 | 2.792482        | 2.603549(3) | 1.180656 | 1.233556 | 0.189134 | 1.688960 (1.79545)               |
|     | (2.88)          | (2.66)      |           |           |           | (1.79545)                        |
| 200 | 3.149535        | 2.790757(7) | 1.061734 | 1.35247  | 0.367660 | 1.690056 (1.88888)               |
|     | (3.21)          | (2.86)      |           |           |           | (1.88888)                        |
Figure 1: A plot for the Condensate Energy/Particle versus Number of atoms in trap for 200 particles for the ground state: $n_z = n_\rho = m = 0$; this work

Table 3: Results for excited states of Rb gas with $\lambda = \sqrt{8}$

| N  | $E/N_{n_z=n_\rho=0,m=1}$ | $E/N_{n_z=n_\rho=0,m=2}$ | $E/N_{n_z=n_\rho=0,m=3}$ |
|----|--------------------------|--------------------------|--------------------------|
| 10 | 3.428526(1)              | 4.424937(2)              | 5.422566 (1)             |
| 40 | 3.474993(3)              | 4.462418(3)              | 5.445864(4)              |
| 70 | 3.520849(5)              | 4.500300 (4)             | 5.472183(6)              |
| 100| 3.566892(4)              | 4.537793 (6)             | 5.494076(7)              |
| 200| 3.718571(8)              | 4.662026(7)              | 5.590799(8)              |
Figure 2: A plot for the Condensate Energy/Particle versus Number of atoms in trap for 200 particles for the 1st excited state: $n_z = n_\rho = 0, m = 1$; this work.

Figure 3: A plot for the Condensate Energy/Particle versus Number of atoms in trap for 200 particles for the 2nd excited state: $n_z = n_\rho = 0, m = 2$; this work.
Figure 4: Ground state wave function of Rb along the x axis for $N = 10$ [this work]

Figure 5: Ground state wave function of Rb along the x axis for $N = 40$ [this work]
Figure 6: Ground state wave function of Rb along the x axis for $N = 100$ [this work]

Figure 7: Aspect ratio in $Rb^87$ as a function of $N$. The horizontal line corresponds to a number close to $\sqrt{\lambda}$ [this work]
4.2 Negative scattering length: Li

In this section we report the calculations for Li. Since Li has negative scattering length, in Li gas the atoms interact with each other with attractive force and when this force becomes larger than molar binding energies the gas collapses. But it is observed that if the number of particles in the gas is not too high, then zero point energy still can exceed this attractive force and still there can be a metastable state. Since we are dealing with only 200 atoms this does not pose any threat to our work. As Morse potential can be used both for positive and negative scattering lengths[21], we use Morse potential for Li gas too and choose $\alpha = 0.4$ and $r_0 = 6.8$ to produce an attractive type of interaction between Li atoms. In this case anisotropy factor is $\lambda = 0.72$ and scattering length is $-27a_0$. From Fig 8, 9 and 10, it is evident that increase in number of particles sharply increases the central density with contrast to Rb gas with positive scattering length where it decreases with increase in number of particles. In Fig 11, we plot aspect ratio of Li gas as a function of number of particles in the gas.
Table 4: Results for ground state of Li, $\lambda = \sqrt{8}$ Chemical potential and energy are in units of $\hbar \omega_{\perp}$ and length is in units of $a_{\perp}$. Numbers in the brackets correspond to the reference [22].

| N   | $\mu$     | E/N   | $E/N_{\text{kin}}$ | $E/N_{\text{ho}}$ | $E/N_{\text{pot}}$ | $\sqrt{<x^2>/<z^2>}$ |
|-----|-----------|-------|--------------------|--------------------|--------------------|---------------------|
| 1   | 1.360000  | 1.360000 | 0.680273          | 0.679726           | 0.00000            | 0.847555            |
|     |           | 1.360000 |                   |                    |                    | (0.84873)           |
| 10  | 1.354930  | 1.357467(1) | 0.680486         | 0.6795132          | -0.002534          | 0.848088            |
| 40  | 1.338018  | 1.349014(3) | 0.681689         | 0.678310           | -0.010990          | 0.848529            |
| 70  | 1.32108   | 1.340545(5) | 0.682509         | 0.677490           | -0.019458          | 0.848998            |
| 100 | 1.304113  | 1.332061(6) | 0.683446         | 0.676553           | -0.027943          | 0.849123            |
|     | (1.327)   | (1.344) |                    |                    |                    | (0.850728)          |
| 200 | 1.247306  | 1.303674(7) | 0.687241         | 0.672758           | -0.056346          | 0.849731            |
|     | (1.291)   | (1.326) |                    |                    |                    | (0.854858)          |

Figure 8: Ground state wave function of Li along the x axis for N = 10 [this work]
Figure 9: Ground state wave function of Li along the x axis for $N = 40$ [this work]

Figure 10: Ground state wave function of Li along the x axis for $N = 100$ [this work]
Figure 11: Aspect ratio in $li^7$ as a function of $N$.

5 Conclusions:

Numerical work with bare Feynman-Kac procedure employing modern computers was reported[6] for the first time for few electron systems after forty years of original work[5] and seemed to be real useful for calculating atomic ground and excited states[7]. Tremendous success[9] in atomic physics motivated us to apply it to condensed matter physics. We have performed our calculations only with 200 particles. Nonetheless we have been able to demonstrate some of the 'Holy Grails’ of Bose Condensation, namely we have been able to calculate energy, chemical potential, aspect ratio etc which reasonably agree with existing results achieved through other methods. The reason for this is that even with small number of particles we have solved many boson systems nonperturbatively and fully quantum mechanically. Within the numerical limitations our many body technique is exact as solve the full Hamiltonian with realistic potentials. We have calculated spectrum of Rb and Li gas by considering realistic potentials like Morse potential, instead of conventional pseudopotentials for the first time, thus allowing one to do the calculation exactly as opposed to the case of $\delta$ function potential where it is
calculated perturbatively.

We have been successful in achieving a lower value for Rb in both isotropic and anisotropic cases and Li ground state than that obtained by Gross-Pitaevski technique[2]. As a matter of fact in all three cases our results stay lower than those coming from GP. For the isotropic case (Case 1 with a system of 3-20 Rb atoms) this does not contradict results of Lieb and Yngvason (LY) [23] which states that energies obtained from GP equation provide an lower bound to the actual ground state of a Bose gas with non-negative, finite range, spherical two-body potential. This is due to the fact that mean field theory inherent in GP equation does not apply for system with small number of particles[11]. In the case of anisotropic case, LY theorem does not apply as the interacting two body potential is non spherical in nature. Only general principle that applies here is the energies coming from the GP technique used in ref[1] are variational estimates (results in this case are obtained by minimizing the energy functional corresponding to the Hamiltonian with mean field interaction instead of having some correlations explicitly.) and provide an upper bound for the diffusion Monte Carlo or similar exact calculations. This is again in conformity with Dyson’s upper bound [24] for low density Bose gas. We also found that Born approximation is valid at low energy and low temperature. Using this approximation we could produce results in all three cases which favorably compare to those given in the literature. However it is crucial to choose the parameters used in the potential correctly as these parameters control the strength of the interaction directly. There are no hard and fast rules for how weak the interaction should be as it was pointed out in the noble lecture[25]. ” It is far more dilute and weakly interacting than liquid helium super fluids, for example, but far more strongly intercating than the nonintercating light in a laser beam”.

We have found an alternative to Gross-Pitaevski technique and other mean field calculations. The method is extremely easy to implement compared to mean field techniques and our fortran code at this point consists of about 270 lines. The simplicity in our many body theory is appealing as the mere ability to add, subtract and toss a coin enables one to solve the many
body problem. We employ an algorithm which is essentially parallel in nature so that eventually we can parallelize our code and calculate thermodynamic properties of bigger systems (of the order of 2000 atoms) taking advantage of new computer architectures. This work is in progress. We are continuing on this problem and hope that this technique will inspire others to do similar calculations.
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