Finite Temperature Excitations of a trapped Bose gas by Feynman-Kac path integral approach

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Abstract

We present results from a detailed Quantum Monte Carlo study of BEC applied to JILA experiment [Jin et al, Phys. Rev. Lett. 78, 764,1997][1]. This is the first Monte Carlo approach (based on Feynman-Kac path integral method) to the above problem where good qualitative agreement is found for both the lowest lying $m = 2$ and $m = 0$ mode. We found an upward shift of the experimental data for $m = 0$ mode at around $T = 0.7T_0$ ($T_0$ is defined as the predicted BEC transition temperature for a harmonically confined ideal gas) when the effect of noncondensate was considered.
1 Introduction

After the experimental realization of Bose Einstein Condensation in alkali vapors in 1995[2], and subsequent experiments pertinent to temperature dependence of frequencies and damping rate[1], there have been a lot of theoretical studies [3-9] to explain the experimental observations in connection with temperature dependent frequency shifts corresponding to different angular momenta, m=0 and m=2 modes in particular[2]. Results have been reported in which theoretical data agreed well with experimental values for m=0 mode showing an upward trend of frequencies with rise in temperature [4,9]. But in all cases the agreement is rather poor when it comes to m=2 mode. There is an agreement up to $T = 0.6T_0$, beyond which frequencies rise with increase in temperature deviating from the downward trend of experimental data. In this article, we would like to report a diffusion Monte Carlo study of the frequency shifts of m=2 and m=0 modes in a dilute gas of $Rb^{87}$. In our non mean field study, we see agreement with experimental study (Fig 3a of Ref 2) for $m = 2$ mode all the way to $T = 0.9T_0$ (Fig 6). When we consider the dynamics of the thermal cloud separately, the upward shift (Fig 7) at $T = 0.7T_0$ which is similar to JILA experiment is observed for $m = 0$ mode. This agrees with the results obtained from the revised gapless theory of Morgan[6,7].

The dynamical behavior of dilute alkali BECs at T=0 can be well described by Gross-Pitaevskii eqn(GPE)[10].

$$i\hbar \frac{\partial \phi(\vec{r}, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m_{Rb}} \frac{\Delta}{2} + V_{ext}(\vec{r}) + g|\phi(\vec{r}, t)|^2 \right] \phi(\vec{r}, t)$$

(1)

where $g = \frac{4\pi\hbar^2a}{m_{Rb}}$, 'a' is the scattering length and 'm_{Rb}' is the mass of Rb atom. But it seems to be inadequate at finite temperatures. The total density of the atoms is related to BEC density and normal component as follows: At T=0 the normal component is not equal to zero in the interacting case and is referred to as 'quantum depletion'. At finite temperature, thermal atoms also contribute to the normal component. Since mean field wavefunctions do not account for the normal component, it gives accurate energy spectrum if
depletion is small[11]. Near $T_0$, the quantum depletion becomes significant and mean field treatment breaks down.

The other mean field theories which have been used so far, are based on HF and HFB-Popov equations [12] and break down near $T_0$ as its effective single particle spectrum always displays a gap. In 1998, a self consistent gapless non-divergent theory[5] was developed and a closed set of coupled equations were solved numerically. In this analysis, only the dynamics of condensate was considered and downshift of data was observed for both $m = 0$ and $m = 2$ mode. Subsequently, with the more sophisticated theory of Morgan[6] an upward shift at $T = 0.6T_0$ was achieved[7,8] Analytic expressions[13] for temperature dependent frequencies were obtained for $m=0$ and $m=2$ by time dependent variational technique.

Eventhough Ref[7] has the best agreement with JILA data till date, solving coupled partial differential equations numerically is not an easy task. The chief purpose of this paper is to go beyond mean field theory with a comparatively simpler numerical procedure which would work at all temperatures. We propose to explore finite temperature aspect of BEC by quantum nonperturbative technique, namely Feynman- Kac (FK)[14-16] procedure. To be precise, we use Generalised Feynman-Kac (GFK) method[17] to make the rate of convergence faster. Since Quantum Monte Carlo methods are computationally expensive, we are simulating only 2000 interacting atoms at this moment. Increasing number of interacting atoms would change our results quantitatively, not qualitatively. This paper is organized as follows: In Sec 2, we discuss the path integral technique at zero and finite temperature as a many body technique, the Schroedinger formulation of Rb condensate and noncondensate, fundamental concepts of BEC and finite temperature excitations. In Sec 3, we discuss the numerical procedure. In Sec 4, we present all the numerical results pertinent to energies and frequencies at different temperature. Finally in Sec 5, we summarize our results.
2 Theory

To connect Feynman-Kac or Generalized Feynman Kac (GFK) to other many body techniques our numerical procedure (GFK)[18-19] has a straightforward implementation to Schroedinger’s wave mechanics. Since at low temperature the de Broglie wavelength of the atoms become appreciable, we do a full quantum treatment. 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. To calculate energy we approximate an exact solution (i.e., the GFK representation of it) to the Schroedinger’s equation, whereas most of the other numerical procedures approximate a solution to an approximate Schroedinger equation. From the equivalence of the imaginary time propagator and temperature dependent density matrix, finite temperature results can be obtained from the same zero temperature code by running it for finite time. So from all these aspects, Generalised Feynman-Kac method turns out to be a potentially good candidate as a sampling procedure for Bose gases at all temperatures. Next we consider the Feynman-Kac formalism and then show how it can be modified to get the Generalized Feynman-Kac version of it.
2.1 Path integral Theory at T=0

2.1.1 Feynman-Kac Path integretion

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

\[
\begin{align*}
    i \frac{\partial u(t, x)}{\partial t} &= (-\frac{\Delta}{2} + V)u(t, x) \\
    u(0, x) &= f(x)
\end{align*}
\]

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

\[
u(t, x) = E_x \exp\left[-\int_0^t V(X(s))ds\right]
\]

where \( X(t) \) is a Brownian motion trajectory and \( E_x \) 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 [20],

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

The above formalism is valid for any arbitrary dimension \( d \) (for a system of \( N \) particles in three dimensions \( d = 3N \)). Generalizations of the class of potential functions for which Eqns. 3 and 4 are valid are given by Simon[21] and include most physically interesting potentials, positive or negative, including, in particular, potentials with \( 1/x \) singularities. It can be argued that the functions determined by Eq(3) 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. Since the above energy formula gives the lowest energy corresponding to any symmetry, the same formula can be used to calculate ground and excited states of a quantum mechanical system. Although other interpretations are interesting, the simplest is that the Brownian motion distribution is just a useful mathematical construction which allows one to extract the physically relevant quantities, the ground and excited state energy of a quantum mechanical system. In
numerical implementation of Eq(4) 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 \([18]\) the vector in \( \mathbb{R}^{3N} \)

\[
W(l) \equiv W(t,n,l) = (w_1^1(t,n,l), w_2^1(t,n,l), w_3^1(t,n,l) \ldots \ldots w_1^N(t,n,l) w_2^N(t,n,l) w_3^N(t,n,l)
\]

where

\[
w_{ij}^l(t,n,l) = \sum_{k=1}^{l} \epsilon_{jk}^i \sqrt{\frac{\nu}{n}}
\]

with \( w_{ij}^l(0,n,l) = 0 \) for \( i = 1, 2, \ldots, N; j = 1, 2, 3 \) and \( l = 1, 2, \ldots, nt \). Here \( \epsilon \) is chosen independently and randomly with probability \( P \) for all \( i,j,k \) such that \( P(\epsilon_{jk}^i = 1) = P(\epsilon_{jk}^i = -1) = \frac{1}{2} \). It is known by an invariance principle\([22]\) that for every \( \nu \) and \( W(l) \) defined in Eq(5)

\[
\lim_{n \to \infty} P\left(\frac{1}{n} \sum_{l=1}^{nt} V(W(l))) \leq \nu \right)
\]

\[
= P\left(\int_0^t V(X(s))ds \leq \nu \right)
\]

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

\[
Z_m = \exp\left(-\left(-\frac{1}{n} \sum_{l=1}^{nt} V(W(l))\right) \right)
\]

and using the law of large numbers, \( (Z_1 + Z_2 + \ldots Z_{N_{rep}})/N_{rep} = Z(t) \) is an approximation to Eq(3)

\[
\mu \approx -\frac{1}{t} \log Z(t)
\]

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 infin-
ity 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 integration

To formulate the generalized Feynman-Kac method we first rewrite the
Hamiltonian as $H = H_0 + V_p$, where $H_0 = -\Delta/2 + \mu_T + \Delta \psi_T/2\psi_T$ and
$V_p = V - (\mu_T + \Delta \psi_T/2\psi_T)$. Here $\psi_T$ is a twice differentiable nonnegative
reference function and $H \psi_T = \mu_T \psi_T$. The expression for the energy can now
be written as

$$\mu = \mu_T - \lim_{t \to \infty} \frac{1}{t} \ln \left[ E_x \exp \left( - \int_0^t V_p(Y(s)) ds \right) \right]$$ \hspace{1cm} (11)

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} (12)

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 (11) converges rapidly.

2.2 Path integral theory at finite temperature

The temperature dependence comes from the realization that the imaginary
time propagator $k(2, 1)$ is identical to the temperature dependent density
matrix $\rho(2, 1)$ if $t \Rightarrow \beta = 1/T$ holds.

This becomes obvious when we consider the eqs[23]

$$-\frac{\partial k(2, 1)}{\partial t_2} = H_2 k(2, 1)$$ \hspace{1cm} (13)

and

$$-\frac{\partial \rho}{\partial \beta} = H_2 \rho(2, 1)$$ \hspace{1cm} (14)
and compare
\[ k(2, 1) = \sum_i \phi_i(x_2)\phi_i^*(x_1)e^{-(t_2-t_1)E_i} \] (15)

and
\[ \rho(2, 1) = \sum_i \phi_i(x_2)\phi_i^*(x_1)e^{-\beta E_i} \] (16)

For zero temperature FK, we had to extrapolate to \( t \Rightarrow \infty \). For finite run time \( t \) in the simulation, we have finite temperature results. In this section, we show how we change our formalism to go from zero to finite temperature. We begin with the definition of finite temperature. A particular temperature \( 'T' \) is said to be finite if \( \Delta E < kT \) holds. The temperature dependent density matrix can be written in the following form

\[ \rho(x, x', \beta) = \rho^{(0)}(x, x', \beta) \times <exp\left[-\int_0^\beta V_p[X(s)]ds\right]>_{DRW} \] (17)

The partition function can be recovered from the above as follows:

\[ \int \rho(x, \beta)dx = \int \rho^{(0)}(x, \beta)dx \times <exp[-\int_0^\beta V_p[X(s)]ds]>_{DRW} \] (18)

In the usual notation, the above equation reads as

\[ Z(x, \beta) = Z^0(x, \beta) \times <exp[-\int_0^\beta V_p[X(s)]ds]>_{DRW} \] (19)

At finite temperature thus free energy can be written as

\[ F = -lnZ(x, \beta)/\beta = -lnZ^0(x, \beta)/\beta - ln <exp[-\int_0^\beta V_p[X(s)]ds]>_{DRW}/\beta \] (20)
2.3 Schroedinger Formalism for Rb condensate at T=0

In the JILA experiment different frequency modes are labeled by their angular momentum projection on the trap axis. In cylindrical symmetry, $m = 2$ mode is an uncoupled one and there are two coupled oscillations for $m = 0$ mode [24]. As a matter of fact Stringari [25] showed that $m = 0$ mode is a coupled oscillation of a quadrupolar surface oscillation and a monopole. In the noninteracting case, these two modes are degenerate with $\omega/\omega_x = 2$.

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 harmonic oscillator potential. At low energy the stationary state for the condensate can be represented as

$$[-\Delta/2 + V_{\text{int}} + V_{\text{trap}}] \psi_0(\vec{r}) = \mu_c \psi_0(\vec{r})$$  \hspace{1cm} (21)

$$[-\Delta/2 + V_{\text{int}} + \frac{1}{2} \sum_{i=1}^{N} [x_i^2 + y_i^2 + \lambda_a z_i^2]] \psi_0(\vec{r}) = \mu_c \psi_0(\vec{r})$$  \hspace{1cm} (22)

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

$$V_{\text{int}} = V_{\text{Morse}} = \sum_{i,j} V(r_{ij}) = \sum_{i \neq j} D[e^{-\alpha(r-r_0)}(e^{-\alpha(r-r_0)} - 2)]$$  \hspace{1cm} (23)

In the above potential '$r_0$' is the location of the well minimum and 'α' is the width of the Morse potential. 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:

$$[-\frac{\partial}{\partial \rho}(\rho \frac{\partial}{\partial \rho}) - \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} - \frac{1}{2} \frac{\partial^2}{\partial z^2} + \frac{1}{2} \frac{\partial^2}{\partial \rho^2}(\rho^2 + \lambda_a^2 z^2)] \psi_0(\rho, z)$$

$$= \mu_c \psi_0(\rho, z)$$  \hspace{1cm} (24)
The energy '$\mu$' of the above equation can be calculated exactly which is

$$\mu_{n, n, m} = (2n_o + |m| + 1) + (n_z + 1/2)\lambda$$  \hfill (25)

In our guided random walk we use the noninteracting solution of Schroedinger equation as the trial function as follows [26]:

$$\psi_{n, n, m}(\vec{r}) \simeq \exp^{-\frac{z^2}{2}} H_{n_z}(z) \times e^{im\phi} \rho^m e^{-\rho^2/2} L_{n_o}^m(\rho^2)$$  \hfill (26)

### 2.4 The effect of noncondensate

In the case of noncondensate the system can be considered as a thermal gas. To calculate noncondensate energy and density we need to study the effect of noncondensate explicitly and consider the following stationary state for the thermal gas.

$$[-\Delta/2 + 2V_{int} + V_{trap}]\psi_j(\vec{r}) = \mu_{nc}\psi_j(\vec{r})$$  \hfill (27)

$$[-\Delta/2 + 2V_{int} + \frac{1}{2} \sum_{i=1}^{N} [x_i^2 + y_i^2 + \lambda z_i^2]\psi_j(\vec{r}) = \mu_{nc}\psi_j(\vec{r})$$  \hfill (28)

The basis wavefunction $\psi_j$ which describes the noncondensate should be chosen in such a way that it is orthogonal to $\psi_0$ as in Eq.(11) The most common way to achieve an orthogonal basis in Schroedinger prescription is to consider the dynamics of noncondensate in an effective potential[6,27] $V_{eff} = V_{trap} + 2V_{int}$. The factor 2 represents the exchange term between two atoms in two different states. The energy in the case of lowest lying modes then corresponds to $\mu = \mu_c + \mu_{nc}$. One can calculate the $\mu_{nc}$ using the same parameters as discussed in Sec 3.1.

### 2.5 Fundamentals of BEC

Even though the phase of Rb vapors at $T=0$ is certainly solid, Bose condensates are preferred in the gaseous 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\[28\] 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 square of the atomic density. It gets suppressed at low density. Magnetically trapped alkali vapors can be metastable depending on their densities and lifetimes. So by keeping the density low only two body collisions are allowed as a result which dilute gas approximation \[29\] still holds for condensates which tantamounts to saying $na^3 \ll 1$ (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 $a \ll r_{av}$ and zero point energy dominates (dilute limit). In the dense limit, for $a \approx r_{av}$ on the other hand the interatomic potential dominates. The gas phase is accomplished by reducing the material density through evaporative cooling.

\[11\]

2.6 Finite temperature Excitations:

Finite temperature excitation spectrum is obtained by using the path integral formalism used in Section 2.2. In our analysis, we first assume that the condensate oscillates in a static thermal cloud. There are no interactions between the condensate and the thermal cloud. The principal effect of finite temperature on the excitations is the depletion of condensate atoms. We want to calculate the collective excitations of Bose Einstein condensates corresponding to JILA Top experiment (m=2 and m=0 mode). Eventually for $m=0$ mode, we consider the effect of thermal cloud separately.

**Condensation fraction and Critical temperature:** In the noninteracting case for a harmonic type external force the theoretical prediction for condensation fraction is

\[ N_0/N = 1 - (T/T_0)^3 \]  \hspace{1cm} (29)

Critical temperature can be defined as

\[ T_c = \frac{0.94 \times \hbar \omega N^{1/3}}{k_B} \] \hspace{1cm} (30)
\[ \bar{\omega} = (\omega_p^2 \omega_z)^{1/3} \]  

From Eq.(29), we see that as temperature increases, condensation fraction decreases in the noninteracting case. Interaction lowers the condensation fraction for repulsive potentials. Some particles always leave the trap because of the repulsive nature of the potential and moreover, if temperature is increased further, more particles will fall out of the trap and get thermally distributed. This decrease in condensation fraction eventually would cause the shifts in the critical temperature. We would observe this in Section 4.2 (Fig. 4). Earlier this was done by W. Krauth[30] for a large number of atoms by path integral Monte Carlo method. In our analysis, we denote '\( T_0 \)' as transition temperature following Ref[2]
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 details of the potential in the case of pseudopotentials. We use Morse potential because it has a more realistic feature of having a repulsive core at $r_{ij} = 0$ than other model potentials. Secondly, using this realistic potential allows us to calculate the energy spectrum exactly as opposed to the case of $\delta$ function potential where it is calculated perturbatively[31]. In our case the interaction strength depends on two more additional parameters, $r_0$ and $\alpha$.

$$a = \frac{mD}{4\pi h^2} \int V(r)d^3r$$

(32)

It is worth mentioning over here that instead of actual scattering length we use the Born approximation to it. Since we are dealing with a case of low energy and low temperature it is quite legitimate to use the above expression as a trickery to calculate the strength of Morse interaction[32]. As a matter of fact in Ref[33] the author has justified using Eq.(32) for a $\delta$ function potential. So if it is justified to do it for $\delta$ function potential it is even more justified to do so for Morse potential which is finite and short-ranged.

The Morse potential for dimer of rubidium can be defined as

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

(33)

where $\alpha$ is the depth of the Morse potential. Using the above potential

$$D = \frac{4h^2 a \alpha^3}{me^{\alpha r_0}(e^{\alpha r_0} - 16)}$$

(34)

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

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

\[ = \mu |\psi(\vec{r}')| \] (35)

The above Hamiltonian can be rescaled by substituting \( \vec{r}' = s\vec{r} \) and \( \mu = \mu_0 U \) as

\[ \left[ -\frac{\hbar^2}{2ms^2} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j} \frac{4\hbar^2 a^3}{ms^3 e^{a\rho_0}(e^{a\rho_0} - 16)} \left[ e^{-a(r_{ij} - \rho_0)}(e^{-a(r_{ij} - \rho_0)} - 2) \right] \\
\quad + \frac{ms^2}{2} \left( \omega_x^2 \sum_{i=1}^{N} x_i'^2 + \omega_y^2 \sum_{i=1}^{N} y_i'^2 + \omega_z^2 \sum_{i=1}^{N} z_i'^2 \right) |\psi(\vec{r}')| \]

\[ = \mu_0 U |\psi(\vec{r}')| \] (36)

\[ \left[ \frac{1}{2} \sum_{i=1}^{N} \nabla_i^2 \right] \left[ -\frac{4a^3}{s e^{a\rho_0}(e^{a\rho_0} - 16)} \sum_{i<j} \left[ e^{-a(r_{ij} - \rho_0)}(e^{-a(r_{ij} - \rho_0)} - 2) \right] \\
\quad - \frac{m^2 \omega_x^2 s^4}{2\hbar^2} \sum_{i=1}^{N} \left( x_i'^2 + \frac{\omega_y^2}{\omega_x^2} y_i'^2 + \frac{\omega_z^2}{\omega_x^2} z_i'^2 \right) \right] |\psi(\vec{r}')| \]

\[ = -\mu_0 U |\psi(\vec{r}')| \] (37)

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

\[ \left[ \frac{1}{2} \sum_{i=1}^{N} \nabla_i^2 \right] \left[ -\frac{4a^3}{s e^{a\rho_0}(e^{a\rho_0} - 16)} \sum_{i<j} \left[ e^{-a(r_{ij} - \rho_0)}(e^{-a(r_{ij} - \rho_0)} - 2) \right] \\
\quad - \frac{m^2 \omega_x^2 s^4}{2\hbar^2} \sum_{i=1}^{N} \left( x_i'^2 + \frac{\omega_y^2}{\omega_x^2} y_i'^2 + \frac{\omega_z^2}{\omega_x^2} z_i'^2 \right) \right] |\psi(\vec{r}')| \]

\[ = -\mu_0 |\psi(\vec{r}')| \] (38)

With \( \omega_x = \omega_y = \frac{\omega_z}{\sqrt{3}} \), the above eqn becomes,

\[ \left[ \frac{1}{2} \sum_{i=1}^{N} \nabla_i^2 \right] \left[ -\frac{4a^3}{s e^{a\rho_0}(e^{a\rho_0} - 16)} \sum_{i<j} \left[ e^{-a(r_{ij} - \rho_0)}(e^{-a(r_{ij} - \rho_0)} - 2) \right] \\
\quad - \frac{m^2 \omega_x^2 s^4}{2\hbar^2} \sum_{i=1}^{N} \left( x_i'^2 + y_i'^2 + \lambda z_i'^2 \right) \right] |\psi(\vec{r}')| \\
\] \[ = -\mu_0 |\psi(\vec{r}')| \] (39)

14
\[
\frac{1}{2} \sum_{i=1}^{N} \nabla_i^2 - \gamma \sum_{i<j} [e^{-\alpha (r_{ij}-r_0)}(e^{-\alpha (r_{ij}-r_0)} - 2)] \\
- \frac{1}{2} \sum_{i=1}^{N} [x_i^2 + y_i^2 + \lambda z_i^2] \psi(\vec{r}) \\
= -\mu_0 \psi(\vec{r})
\] (40)

Now for \( \alpha = 0.29 \) and \( r_0 = 9.758 \) (both in oscillator units)[32]. We have checked that for these choice of parameters, Morse solution is extremely good. \( a = 52 \times 10^{-10} \) cm, \( s = 12 \times 10^{-7} \) cm, the interaction strength \( \gamma \) is given by

\[
\gamma = 4a\alpha^3 \frac{\alpha r_0}{se^{\alpha r_0}(e^{\alpha r_0} - 16)} = 2.64 \times 10^{-5}
\] (41)

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 \( \gamma = 2.64 \times 10^{-5} \), 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 outside the range of this limit, so the nonexistence of two-body bound states is ensured by choosing the above parameters.

Even though \( \gamma << 1 \), we solve the eigenvalue eqn nonperturbatively with Generalized Feynman-Kac procedure. Energies and frequencies at zero temperature are obtained by solving Eq. (4) and using Eq.(11). To calculate the analogous quantities at finite temperature we use Eq.(20). We can get the energy of both condensate and noncondensate using Eq.(4) Eq.(20 ) by generating a large number of paths and then averaging the results for all the paths. Since original Feynman-Kac method [14,15] is computationally inefficient we incorporate importance sampling in our random walk and use trial function of the form given in Eq.(26)

**Evaluation of temperature dependent mode frequencies**

Following the prescription in [4], we see that for a fixed 'N' relationship \( \mu(N_0, T) \simeq \mu(N,T=0)(\frac{N_0}{N})^{2/5} \) or equivalently \( N_0/N = [\frac{\mu(N_0, T)}{\mu(N,T=0)}]^{5/2} \) generates the condensation fraction \( N_0/N \) as a function of time. One can generate
this from experiments also. From the thermodynamical limit we get $N_0$ as a
function of time and run our zero temperature code with same number of $N_0$
as the dynamics of the finite temperature condensate are essentially the same
as those of a zero temperature condensate with the same value of $N_0$. This
is called method I. The other way to calculate energy is to run the code for
different simulation times corresponding to different temperatures as time is
defined as inverse temperature. This is identified as method II. $\mu(N_0, T)$ and
$\mu(N_0, T = 0)$ are calculated using $\mu = \frac{1}{N}(\mu_{\text{kin}} + \mu_{\text{ho}} + 2\mu_{\text{int}})$ and $\mu_{\text{kin}}$, $\mu_{\text{ho}}$
and $\mu_{\text{int}}$ are calculated as described in Ref[25]. Later in Fig.5 (our data) of
Section 4.2, we see the effects of interaction on the condensation fraction.
4 Results

4.1 Excitation spectra at $T=0$ for different symmetries

We chose $Rb^{87}$ as an example of a weakly interacting dilute Bose gas as in Ref[29]. We simulate 2000 Rb atoms interacting via the Morse potential. We choose $a = 52 \times 10^{-10} \text{cm}$, length scale $s$ of the problem as $12 \times 10^{-7} \text{cm}$. In the following table, we show the ground state energy of the particle. With repulsive interactions, the Energy/particle increases with the increase in number of particles in the trap [Fig. 1-2] whereas the energy gap between the different symmetry states decreases as evident from Fig. 3. However we see a different trend [Fig. 4] for $m = 0$ mode where the excitation frequencies increase with the increase in number of atoms. This agrees with the Hartree-Fock spectrum in the Fig 2 of Ref[33].

Table 1: Results for the ground state energy of 2000 $Rb^{87}$ atoms in a trap with $\omega_x = \omega_y = 1, \lambda = \omega_z = \sqrt{8}$ in the interacting case ; The table shows how energy varies with the number of particles in the Gross Pitaevski(GP) case [34] and GFK method.

| N   | E/N(GP)     | E/N(GFK)     |
|-----|-------------|--------------|
| 1   | 2.414       | 2.414 213    |
| 100 | 2.66        | 2.52230(5)   |
| 200 | 2.86        | 2.63141(1)   |
| 500 | 3.30        | 2.9588(4)    |
| 1000| 3.84        | 3.5047(4)    |
| 2000| 4.61        | 4.5962(3)    |
Figure 1: A plot for the Condensate Energy/Atom versus Number of atoms in trap for 2000 particles for the ground state; this work

Figure 2: A plot for the Condensate Energy/Particle versus Number of atoms in trap for 2000 particles for the \( m = 2 \) mode; this work
Table 2: frequency $\omega$ for lowest lying modes

| N   | mode of oscillation | energy  | $\omega$(this work) | $\omega$(JILA TOP) |
|-----|---------------------|---------|---------------------|-------------------|
| 2000| ground state        | 4.596(3)|                     |                   |
| 2000| $m = 2$            | 5.860(1)| 1.264(4)            | 1.4               |
| 2000| $m = 0$            | 7.295(3)| 2.699(6)            | 1.8               |

Figure 3: A plot of Excitation Frequency vs Number of Atoms for lowest lying $m = 2$ mode ;this work
Figure 4: A plot of Excitation Frequency vs Number of Atoms for lowest lying $m = 0$ mode; this work.

Figure 5: Frequencies for $m_0$; Ref 33.
4.2 Effects of temperature on condensation fraction

Density of condensate atoms decreases in the trap as temperature increases. This lowers the interaction energy of the condensate atoms resulting in a shift in the critical temperature. As a matter of fact in the interacting case, the critical temperature decreases. This is a very unique feature of trapped gas. In the

![Figure 6: Condensation fraction vs Reduced Temperature; this work. The middle curve corresponds to the 2000 interacting atoms (GFK summation data; our work) and the outer one corresponds to the noninteracting case. The innermost curve also corresponds interacting atoms [Ref 37]. The number of condensed particles decreases with the interaction.](image-url)
4.3 Effects of temperature on the frequency shifts; comparison with other experiments and theories

Next we give an account of how our path integral simulations compare with other theoretical and experimental data. Fig 3a in Ref[2] represents JILA TOP data where one observes a large temperature dependent frequency shift for both \( m=0 \) and \( m=2 \) modes. For \( m=2 \) mode, starting from Stringari limit it decreases all the way up to \( 0.9 T_0 \) whereas for \( m=0 \) mode it shows a rising trend with rise in temperature. Our path integral data for \( m=2 \) mode in Fig[6] shows similar decreasing trend as JILA TOP data in Fig 3a of Ref[2] and best theoretical data in Fig 1 of Ref[7] all the way up to \( 0.9 T_0 \) whereas data generated by Hartree-Fock-Bogoliubov[HFB] method in Fig 1 of Ref[4] agree with JILA TOP only up to \( 0.7 T_0 \). Finally our data Fig[7] for temperature variation of \( m=0 \) mode agrees with JILA data in Fig[3a] of Ref[2] and Morgan data in Fig 1 of Ref[7] when the effect of thermal cloud is considered.

Figure 7: Effects of temperature on \( m = 2 \) mode; this work
Figure 8: Effects of temperature on $m = 0$ mode from GFK considering non-condensate dynamics [this work], shows resemblance with JILA [2] and Morgan et al [7]

4.4 Discussions

We are solving the full Hamiltonian with some realistic potential and thereby trying to solve the many body problem fully quantum mechanically and non-perturbatively. So for both $m = 0$ and $m = 2$ modes, our calculations adopting Feynman Kac path integral technique represent the collective behavior of the Bose gas. Our work [Fig. 6] agrees with JILA experiment [2] for $m=2$ mode. The other theoretical work shows the reverse trend [Fig 1 of Ref 4]. We found that considering the dynamics of condensates alone and the effect of finite temperature as static thermal cloud, we do not achieve the upward shifts of frequencies as shown by JILA data for $m=0$ mode. In fact, we agree with Ref [5] that as $m=0$ happens to be a coupled mode, we need to consider the dynamics of thermal cloud to obtain a satisfactory agreement with the experimental data. Eventually We consider the dynamics of thermal cloud and get the upward shift of data [Fig 7] as observed in JILA [2] and Ref [7,8].

At T=0 for $m = 2$, we observe that as N increases the energies grow, but the splitting between the ground and excited state decreases - an essential feature of Bose Condensation. But in the similar case for $m = 0$ mode we observe that both the energies and the gap between the ground and
higher excited states increase with increase in number of atoms. This agrees with Hartree-Fock spectrum of Ref[33] where the author had to improve these results by using random phase approximation to get an agreement with the experimental results. For \( m = 2 \) mode the Stringari limit turns out to be 1.264(4) as opposed to the experimental value of 1.4. On the other hand \( m = 0 \) mode the Stringari limit is 2.699(6) as opposed to the experimental value of 1.8. So for the coupled \( m = 0 \) mode, our path integral method does not work better than Hartree-Fock theory and thereby does not yield a correct value of Stringari limit. The reason that the quantitative agreement between the Stringari limit predicted by us particularly for \( m = 0 \) mode and the experiments is not good, might be the use of Gaussian wave functions as the trial functions. In general, the frequencies of collective modes do not have direct correspondence to harmonic oscillator states because they do not include correlations. It is legitimate to use harmonic oscillator solutions as trial functions for \( m = 2 \) mode as JILA experiment does not correspond to the Thomas Fermi limit[35]. But for \( m = 0 \) mode we need to include correlations in the wave function as \( m = 0 \) is a coupled mode.
5 Conclusions:

We have used GFK to bring out the many body effects between the cold Rb atoms. Numerical work with bare Feynman-Kac procedure employing modern computers was reported[15] for the first time for few electron systems after forty years of the original work[14] and seemed to be really useful for calculating atomic ground states[19]. A fairly good success in atomic physics motivated us to apply it to Condensed matter Physics.

Gross-Pitaevskii (GP) technique[33] does not include correlations in the solutions explicitly and calculates energy at the variational level. These energies are upper bounds to the actual energies of the system. We have been successful in achieving a lower value for Rb ground state than that obtained by GP. This correct trend in our calculated energies for different symmetry states enables one to calculate the frequencies more accurately by Feynman Kac path integral method. As a result, Diffusion Monte Carlo codes based on nonperturbative quantum approach can handle temperature very accurately and we do not see any breakdown near $T_c$. For the first time we have calculated finite temperature properties beyond mean field approximation by Quantum Monte Carlo technique. The only other non mean field calculations at $T = 0$ worth mentioning in this context is the work done by Blume et al[36]. We have calculated spectrum of Rb gas by considering realistic potentials like Morse potential etc. instead of conventional pseudopotentials for the first time.

We have been able to calculate the lowest lying excitation frequencies for $m = 0$ and $m = 2$ modes by Feynman-Kac path integral technique in a very simple way. We have found an alternative to Gross-Pitaevskii technique and other mean field calculations which works at all the temperature. Simulating 2000 atoms with the path integral method we have been able to capture some of the signatures of Bose condensation like decrease of excitation frequencies with number of atoms, lowering of condensation fraction in the interacting case etc. In our non mean field study, we see agreement with experimental study all the way to $T = 0.9 T_c$ [Fig. 6]. This is because of the fact that we have been able to solve the related many body theory very
accurately with the nonperturbative and quantum mechanical approach. At this point our results agree with the experimental results only qualitatively as we are restricting ourselves to the choice of Gaussian trial functions. To improve our results quantitatively we need to use correlated trial functions. This would be a nontrivial extension of the present work and will be reported elsewhere. The simplicity in our method is appealing as it is extremely easy to implement and our fortran code at this point consists of about 270 lines. In fact mere ability to add, subtract and toss a coin enables one to solve many body theory with our path integral technique.

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 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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