

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 around T_c (is defined as the predicted BEC transition temperature for a harmonically confined ideal gas when the effect of noncondensate was considered.

I. 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 $m=2$ 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 $m=0$ 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 7). When we consider the dynamics of the thermal cloud separately, the upward shift (Fig 8) 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 well described by Gross-Pitaevski eqn(GPE)[10].

$$i\hbar \frac{\partial \phi(\vec{r}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m_{Rb}} \Delta + V_{ext}(\vec{r}) + g |\phi(\vec{r}, t)|^2 \right] \phi(\vec{r}, t) \quad (1)$$

$$g = \frac{4\pi\hbar^2 a}{m_{Rb}}$$

where '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 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 the 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 theory 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 these 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 $m=2$ mode by variational Monte carlo technique.

Even though 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 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 Generalized 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. The paper is organized as follows: In Sec 1 we have the introduction. In Sec 2, we discuss the path integral technique at zero and finite temperatures as a many body technique, the Schroedinger formulation of Rb condensate and non-condensate, 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.

II. THEORY

To connect Feynman-Kac(FK) or Generalized Feynman Kac(GFK) to other many body techniques our numerical procedure[18,19] has straight-forward implementation to Schroedinger's wave mechanics. Since at low temperature the de-Broglie wavelength of the atoms becomes 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 wavefunction keep points in the chosen nodal region, provide an upper bound for the lowest energy of that symmetry. The nodal region with the lowest energy serves as a least upper bound. If the nodal region has exact nodal structure of the true wave-function the random walk is exact in the limit scale, time for walk and the number of walkers 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 of an approximate Schroedinger equation. From the equivalence of 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 of these aspects, Generalized 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 integration

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

$$i \frac{dU(x, t)}{dt} = \left(\frac{\Delta}{2} - V(x) \right) U(x, t), \quad (2)$$

with $x \in \mathbb{R}^d$, $d = 3N$ and $U(x, 0) = 1$. The Feynman-Kac solution to this equation is

$$U(x, t) = E \exp \left[-\int_0^t V(x(s)) ds \right], \quad (3)$$

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[20].

$$\mu = \lim_{t \rightarrow \infty} \frac{1}{t} \ln E \exp \left[-\int_0^t V(x(s)) ds \right] \quad (4)$$

The formalism is valid for any arbitrary dimensions 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 the 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 gives the lowest energy corresponding to any symmetry, the same formula can be used to calculate the 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 the excited state energy of a quantum mechanical system. In numerical implementation of the 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 integer n and l define [16] the vector in \mathbb{R}^{3N} .

$$W(l) \equiv W(t, n, l) = (w_1^1(t, n, l), w_2^1(t, n, l), w_3^1(t, n, l), \dots, w_1^N(t, n, l), w_2^N(t, n, l), w_3^N(t, n, l)) \quad (5)$$

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

where
 (6)

with $w_j^i(t, n, l) = 0$ for $i = 1, 2, \dots, N; j = 1, 2, 3$ and $l = 1, 2, \dots, nt$. Here ϵ 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 [17] that for every v and $W(l)$ defined above.

$$\lim_{n \rightarrow \infty} P \left(\frac{1}{n} \sum_{l=1}^{nt} V(W(l)) \leq v \right) \leq v$$

$$= P \left(\int_0^t V(X(s)) ds \leq v \right) \quad (7)$$

Consequently for large n ,

$$P \left[\exp \left(-\frac{1}{n} \int_0^t V(X(s)) ds \right) \leq v \right] \quad (8)$$

$$\approx P \left[\exp \left(-\frac{1}{n} \sum_{l=1}^{nt} V(W(l)) \right) \leq v \right]$$

By generating N_{resp} independent replications $Z_1, Z_2, \dots, Z_{N_{resp}}$ of

$$Z_m = \exp \left(-\frac{1}{n} \sum_{l=1}^{nt} V(W(l)) \right) \quad (9)$$

And using the law of large numbers,
 $(Z_1 + Z_2 + \dots + Z_{N_{resp}}) / N_{resp} = Z(t)$

is an approximation to

$$Eq(2) \quad \mu \approx -\frac{1}{t} \log Z(t) \quad (10)$$

Here $W^m(t)$, $m = 1, 2, \dots, N_{resp}$ denotes the m^{th} realization of $W(t)$ out of N_{resp} independently run simulations. In the limit of large t and N_{resp} this approximation approaches an equality and forms the basis of a computational scheme for the solution of a many particle system with a prescribed symmetry. In dimension 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 $H_0 = -\Delta/2 + \mu_T + \Delta\psi_T/2\psi_T$ and $V_p = V - (\mu_T + \Delta\psi_T/2\psi_T)$. Here ψ_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

$$\mu = \mu_T - \lim_{t \rightarrow \infty} \frac{1}{t} \ln E \exp \left[-\int_0^t V(x(s)) ds \right] \tag{11}$$

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

$$dY(t) = \frac{\Delta\psi_T(Y(t))}{\psi_T(Y(t))} dt + dX(t) \tag{12}$$

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 (10) 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 eqns[23]

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

$$-\frac{\partial \rho(2,1)}{\partial \beta} = H_2 \rho(2,1)$$

and
 (14)

$$k(2,1) = \sum_i \varphi_i(x_2) \varphi_i^*(x_1) e^{-(t_2-t_1)E_i} \tag{15}$$

$$\rho(2,1) = \sum_i \varphi_i(x_2) \varphi_i^*(x_1) e^{-\beta E_i} \tag{16}$$

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 $\Delta E < kT$ holds. The temperature dependent density matrix can be written in the following form

$$\rho(x, x', \beta) = \rho^{(0)}(x, x', \beta) \left\langle \exp \left[-\int_0^\beta v_p[X(s)] ds \right] \right\rangle_{DRW} \tag{17}$$

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

$$Z(x, x', \beta) = \rho^{(0)}(x, x', \beta) \left\langle \exp \left[-\int_0^\beta v_p[X(s)] ds \right] \right\rangle_{DRW} \tag{18}$$

In the usual notation, the above equation reads as

$$Z(x, \beta) = Z^0(x, \beta) \left\langle \exp \left[-\int_0^\beta v_p[X(s)] ds \right] \right\rangle_{DRW} \tag{19}$$

At finite temperature thus the free energy can be written as

$$F = -\ln Z(x, \beta) / \beta = -\ln Z^0(x, \beta) / \beta - \ln \left\langle \exp \left[-\int_0^\beta v_p[X(s)] ds \right] \right\rangle_{DRW} / \beta \tag{20}$$

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 oscillation for $m=0$ mode. As a matter of fact Stringari[25] showed that $m=0$ mode is a coupled oscillation of a quadrupolar surface oscillation and monopole. In the non-interacting 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.

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

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

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

Where $\frac{1}{2} \sum_{i=1}^N [x_i^2 + y_i^2 + \lambda_a z_i^2]$ is the anisotropic potential with

$$\lambda_a = \frac{\omega_z}{\omega_x}$$

anisotropy factor

Now

$$V_{\text{int}} = V_{\text{Morse}} = \sum_{i,j} V(\mathbf{r}_{ij}) = \sum_{i<j} D[e^{-\alpha(r-r_0)}(e^{-\alpha(r-r_0)} - 2)] \quad (23)$$

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 :

$$\left[-\frac{1}{2\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial}{\partial \rho} \right) - \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} - \frac{1}{2} \frac{\partial^2}{\partial z^2} + \frac{1}{2} (\rho^2 + \lambda_a^2 z^2) \right] \psi(\rho, z) = \mu \psi(\rho, z) \quad (24)$$

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

$$\mu_{n_\rho, n_z, m} = (2n_\rho + |m| + 1) + (n_z + 1/2)\lambda_a \quad (25)$$

In our guided random walk we use the solution of the Schroedinger equation in the noninteracting case as the trial

$$\psi_{n_\rho, n_z, m}(\vec{r}) \cong e^{-\frac{z^2}{2}} H_{n_z}(z) x e^{im\phi} \rho^m e^{-\rho^2/2} L_{n_\rho}^m(\rho^2) \quad (26)$$

function[26]:
 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 Schrödinger equation for harmonic oscillator in d-dimension as the trial function as follows: ¹⁶

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.

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

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

The basis wavefunction ψ_j which describes the noncondensate should be chosen in such a way that it is

orthogonal to ψ_0 . The most common way to achieve an orthogonal basis in Schroedinger prescription is to consider the dynamics of noncondensate in an effective potential

$$V_{\text{eff}} = V_{\text{trap}} + 2V_{\text{int}}$$

The factor 2 represents the exchange term between two atoms on two different states. The energy in the case of lowest lying modes then corresponds to

$\mu = \mu_c + \mu_{\text{nc}}$. One can calculate the μ_{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 solid phase 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, η , the ratio of zero point energy and molecular binding energy lies between 10^{-5} and 10^{-3} . According to the theory of corresponding states¹⁷ since for the T=0 state of alkali metals, η 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 keeping the density low only two body collisions are allowed as a result of which dilute gas approximation¹¹ 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.¹¹ The gas phase is accomplished by reducing the material density through evaporative cooling.

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. There 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 modes). 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

$$N_0 / N = 1 - (T/T_0)^3 \quad (29)$$

Critical temperature can be defined as

$$T_c = \frac{0.94x\hbar\bar{\omega}N^{1/3}}{k_B} \tag{30}$$

$$\bar{\omega} = (\omega_\rho^2\omega_z)^{1/3} \tag{31}$$

From equation (29) we see that as temperature increases, condensation fraction decreases in the non-interacting case. Interaction lowers the condensation fraction for repulsive potentials. Some particles always leave the trap because of the repulsive nature of the particles and moreover, if temperature is increased further, more particles will fall out of the trap and get thermally distributed. The decrease in condensation fraction eventually would cause the shifts the critical temperature. We observe this in sec 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[1]

III. 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 parameter of this problem, the scattering wavelength ‘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. Socondly, using this realistic potential allows us to calculate the energy spectrum exactly as opposed to the case of δ function potential where it is calculated perturbatively[31]. In our case the interaction strength depends on two more additional parameters, r_0 and α

$$a = \frac{mD}{4\pi\hbar^2} \int V(r)d^3r \tag{32}$$

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 δ function potential. So if it is justified to do it for δ 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

$$\sum_{i,j} V(r_{ij}) = \sum_{i<j} D[e^{-\alpha(r-r_0)}(e^{-\alpha(r-r_0)} - 2)] \tag{33}$$

where α is the depth of the Morse potential. Using the above potential

$$D = \frac{4\hbar^2 a\alpha^3}{me^{\alpha r_0}(e^{\alpha r_0} - 16)} \tag{34}$$

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

$$[-\hbar^2/2m \sum_{i=1}^N \nabla_i'^2 + \sum_{i,j} V(r'_{ij}) + \frac{m}{2}(\omega_x^2 \sum_{i=1}^N x_i'^2 + \omega_y^2 \sum_{i=1}^N y_i'^2 + \omega_z^2 \sum_{i=1}^N z_i'^2)]\psi(\vec{r}') = \mu\psi(\vec{r}') \tag{35}$$

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

$$[-\frac{\hbar^2}{2ms^2} \sum_{i=1}^N \nabla_i^2 + \sum_{i<j} \frac{4\hbar^2 a\alpha^3}{ms^3 e^{\alpha r_0}(e^{\alpha r_0} - 16)} [e^{-\alpha(r-r_0)}(e^{-\alpha(r-r_0)} - 2)] \frac{ms^2}{2} (\omega_x^2 \sum_{i=1}^N x_i^2 + \omega_y^2 \sum_{i=1}^N y_i^2 + \omega_z^2 \sum_{i=1}^N z_i^2)]\psi(\vec{r}) = \mu_0 U\psi(\vec{r}) \tag{36}$$

dividing the above equation by $-\frac{\hbar^2}{ms^2}$ throughout we get

$$[\frac{1}{2} \sum_{i=1}^N \nabla_i^2 - \sum_{i<j} \frac{4a\alpha^3}{se^{\alpha r_0}(e^{\alpha r_0} - 16)} \sum_{i<j} [e^{-\alpha(r-r_0)}(e^{-\alpha(r-r_0)} - 2)] - \frac{m^2\omega_x^2 s^4}{2\hbar^2} (\sum_{i=1}^N x_i^2 + \frac{\omega_y^2}{\omega_x^2} \sum_{i=1}^N y_i^2 + \frac{\omega_z^2}{\omega_x^2} \sum_{i=1}^N z_i^2)]\psi(\vec{r}) = -\mu_0 \frac{Ums^2}{\hbar^2} \psi(\vec{r}) \tag{37}$$

Now let $\frac{m^2\omega_x^2 s^4}{2\hbar^2} = 1 \Rightarrow s^2 = \frac{\hbar}{m\omega_x}$ is the natural unit of

length. Let $\frac{Ums^2}{\hbar^2} = 1 \Rightarrow U = \frac{\hbar^2}{ms^2} = \hbar\omega_x$ is the natural unit of energy. Then in the dimensionless form the above equation can be written as

$$[\frac{1}{2} \sum_{i=1}^N \nabla_i^2 - \sum_{i<j} \frac{4a\alpha^3}{se^{\alpha r_0}(e^{\alpha r_0} - 16)} \sum_{i<j} [e^{-\alpha(r-r_0)}(e^{-\alpha(r-r_0)} - 2)] - \frac{1}{2} \sum_{i=1}^N (x_i^2 + \frac{\omega_y^2}{\omega_x^2} y_i^2 + \frac{\omega_z^2}{\omega_x^2} z_i^2)]\psi(\vec{r}) = -\mu_0\psi(\vec{r}) \tag{38}$$

With $\omega_x = \omega_y = \frac{\omega_z}{\sqrt{\lambda}}$, the above equation becomes,

$$\left[\frac{1}{2} \sum_{i=1}^N \nabla_i^2 - \sum_{i<j} \frac{4a\alpha^3}{se^{\alpha r_{ij}} (e^{\alpha r_{ij}} - 16)} \sum_{i<j} [e^{-\alpha(r-r_0)} (e^{-\alpha(r-r_0)} - 2)] \right. \\ \left. - \frac{1}{2} \sum_{i=1}^N (x_i^2 + y_i^2 + \lambda z_i^2) \right] \psi(\vec{r}) = -\mu_0 \psi(\vec{r}) \quad (39)$$

or equivalently

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

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

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

For mean field calculation the value of interaction strength was taken to be 4.33×10^{-3} . For this problem we are interested in the limit $\gamma \ll 1$. The case $\gamma \gg 1$ is usually known as the Thomas Fermi limit. $\gamma = 2.64 \times 10^{-5}$, the eigenvalue equation reduces to minimally coupled 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 dimmers is outside the range of this limit, so the nonexistence of two-body bound states is ensured by choosing the above parameters.

Even though $\gamma \ll 1$, we solve the eigenvalue Eq(4) 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) and Eq(20) by generating a large number of paths and 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 $\mu(N_0, T) \cong \mu(N, T = 0) \left(\frac{N_0}{N} \right)^{2/5}$ or

equivalently $\frac{N_0}{N} = \left[\frac{\mu(N_0, T)}{\mu(N, T = 0)} \right]^{5/2}$

generates the condensation fraction $\frac{N_0}{N}$ as a function of time. One can generate this from experiment also. From the thermodynamic 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 is essentially the same as those of a zero temperature condensate with the same value of N_0 . The other way to calculate energy is to run the code for different simulation time 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

$$\mu = \frac{1}{N} (\mu_{kin} + \mu_{ho} + 2\mu_{int}) \quad \text{and} \quad \mu_{kin}, \mu_{ho} \text{ and } \mu_{int} \text{ are}$$

calculated as described in Ref[25]. Later in fig 5 (our data) of Section 4.2, we see that the effect of interaction on the condensation fraction.

IV. 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 atoms interacting via the Morse potential. We choose $a = 52 \times 10^{-10}$ cm and $s = 12 \times 10^{-7}$ cm. In the following table we show the ground state energy of the particles. With repulsive interaction, the Energy/Particle increases with 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 particles. This agrees with the Hartree-Fock spectrum in the Fig 2 of Ref[33].

Table I Results for the ground state energy of 2000 Rb^{87} atoms in a trap with $\omega_x = \omega_y = 1$, and $\lambda = \omega_z = \sqrt{8}$ 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	2.63 141(1)
500	3.30	2.9588(4)
1000	3.84	3.5047(4)
2000	4.61	4.5962(3)

Table 2: Frequency ω for the lowest lying modes

N	Mode of oscillation	energy	ω (this work)	ω (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

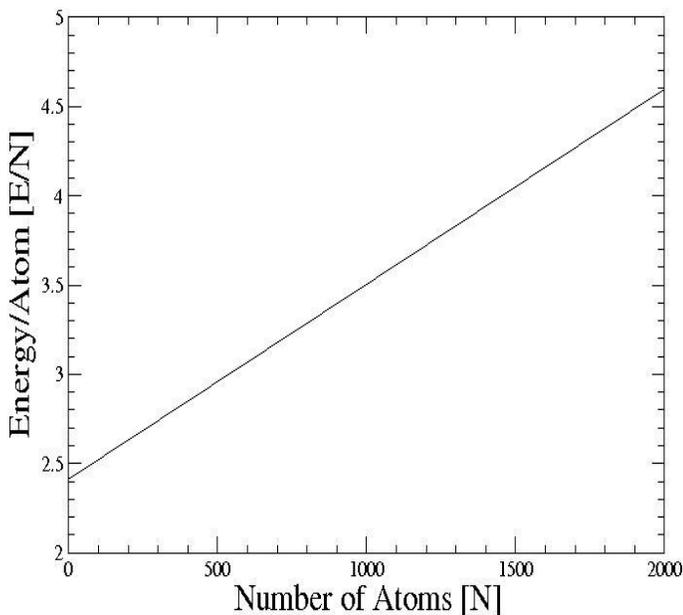


Figure 1 A plot for the Condensate Energy/Atom versus Number of atoms in trap for 2000 particles for the ground state; this work

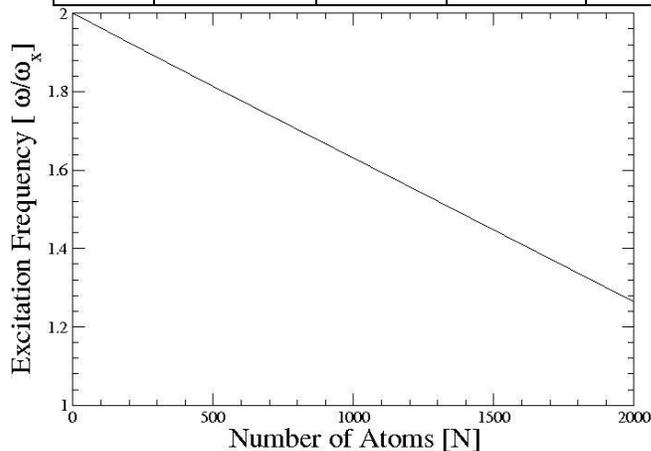


Fig 3. A plot of Excitation Frequency vs Number of Atoms for lowest lying m=2 mode; this work

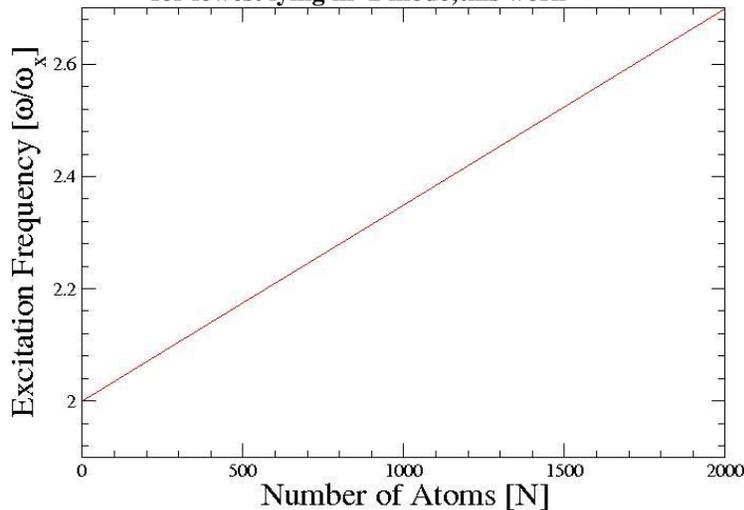


Figure 4: A plot of Excitation Frequency vs Number of atoms for lowest lying m=0 mode; this work

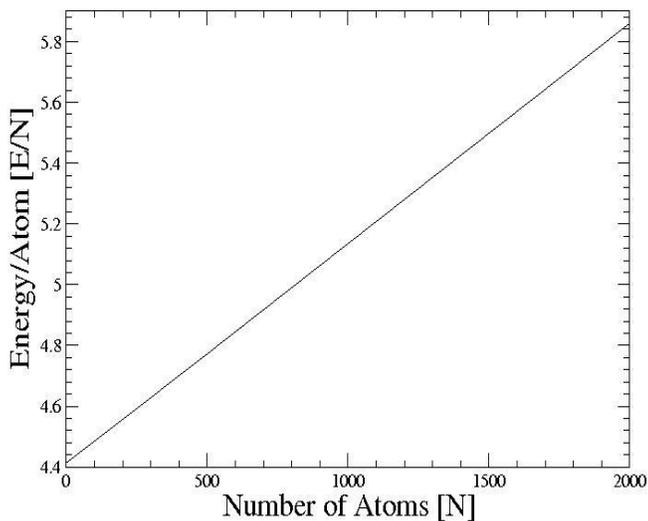


Fig 2 A plot for the Condensate Energy/Particle versus Number of atoms in trap for 2000 particles for the m=2 mode; this work

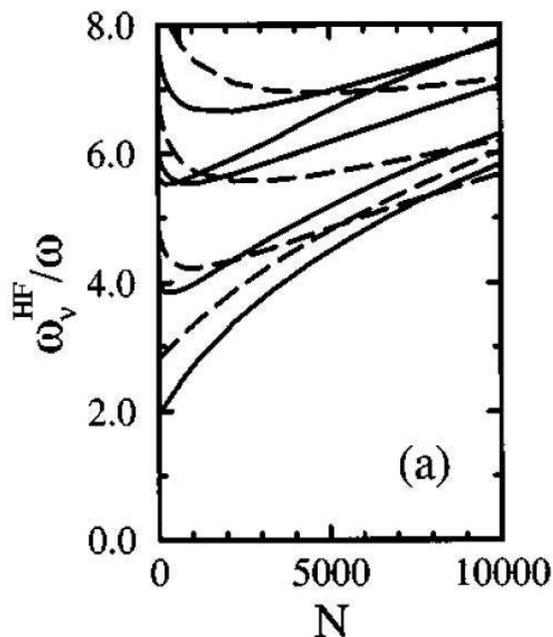


Figure 5: Frequencies for m=0

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 the trapped gas.

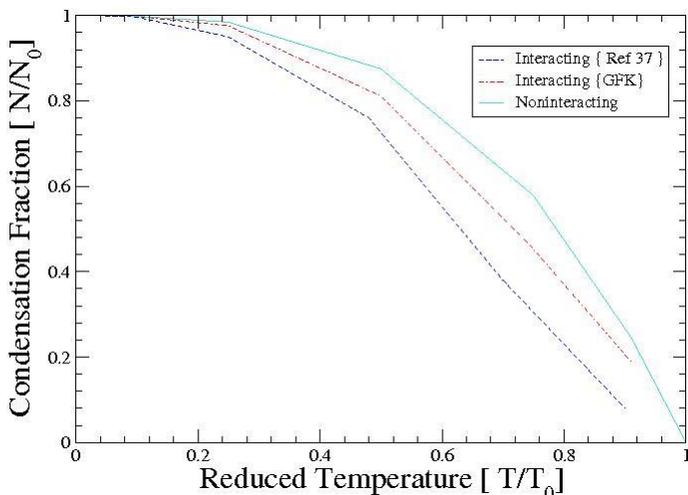


Figure 6. Condensation fraction vs Reduced temperature; this work . The middle curve corresponds to the 2000 interacting atoms (GFK simulation data; our work) and the outer one corresponds to the interacting case. The innermost curve also corresponds interacting atoms[Ref 37] . The number of condensed particles decreases with the interaction.

4.3 Effects of temperature on the frequency shifts; comparison with other experiments and theories.

Since 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 wher 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 $0.9T_0$ 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 up to $0.9T_0$ whereas data generated by by Hartree-Fock-Bogoliubov[HFV] method in Fig[1] of Ref[4] agree with JILA TOP only up to $0.7T_0$. Finally our data Fig[7] for temperature of $m=0$ mode agrees with JILA data in Fig[3a] of Ref[2] nad Morgan data in fig 1 of Ref[7] when the effect of thermal cloud is considered.

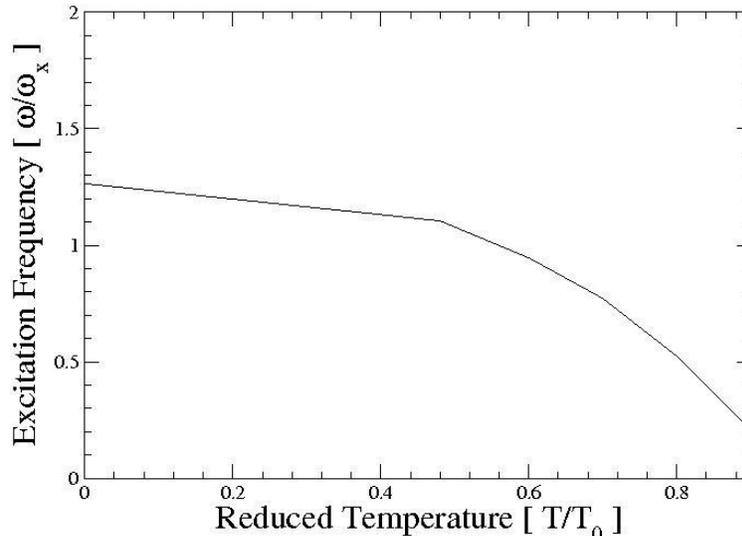


Fig 7 Effects of temperature on m=2; this work

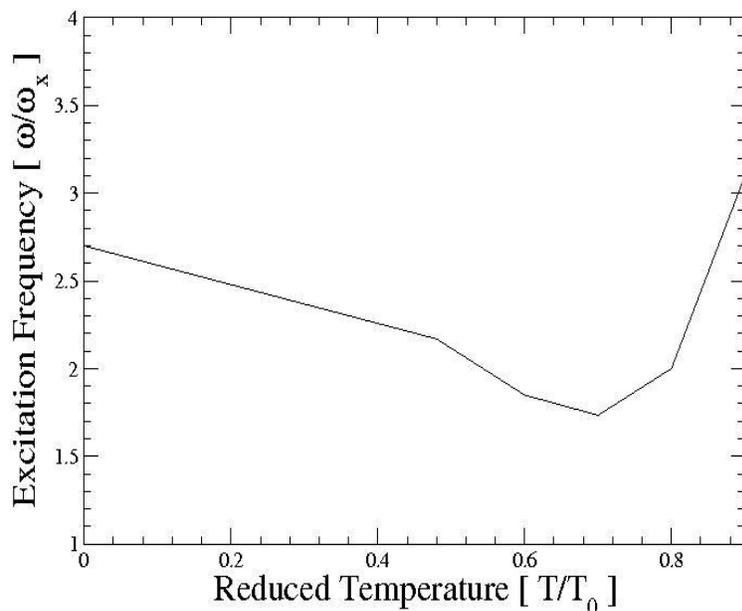


Figure 8: Effects of temperature on m=2 mode; this work

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 7] 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 the 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 8] 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 increases 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 Stringari limit turns out to be 1.264(4) as opposed to the experimental value of 1.4. on the other hand for $m=0$ mode the Stringari limit is 2.699(6) as opposed to 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 the Gaussian wave functions as the trial functions. In general, the frequencies of the 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 trial functions as $m=0$ is a coupled mode.

V. 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 40 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.

Cross-Pitaevski(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 of 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-Pitaevski technique and other mean-field calculations which work 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 $T = 0.9T_c$ [Fig 7]. 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. This would be a nontrivial extension of the present work and will be reported elsewhere. The simplicity in our code 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 in progress. We are continuing on this problem and hope that this technique will inspire others to do similar calculations.

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