Calculation of T_c of ^{87}Rb BEC using High-order Effective Actions

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OVERVIEW

We apply the $N=1$ approximation [1] for the efficient calculation of the condensation temperature of a rotating ^{87}Rb Bose-Einstein condensate (BEC) in an anharmonic trap, realized in a recent experiment [2]. First, we briefly introduce the used approximation and discuss its advantages. Then we focus on the theoretical description of the experiment and on the numerical calculation of the condensation temperature. At the end, we compare our results with previous semiclassical calculations [3].

N=1 APPROXIMATION

We present a universal approach for a treatment of general many-body non-relativistic systems starting from the time-dependent Schrödinger equation [4,5]

$$i\hbar\frac{\partial A(\vec{a},\vec{b};t)}{\partial t}=\left(-\sum_{i=1}^{N_a}\frac{\hbar^2}{2M}\Delta_i+V(\vec{a})\right)A(\vec{a},\vec{b};t)\,,$$

where the potential V contains all external fields and interactions. Inspired by the path-integral formalism, its solution in the imaginary time can be written as

$$A(\vec{a},\vec{b};t)=\underbrace{\left(\frac{M}{2\pi\hbar t}\right)^{N_a d/2}\exp\left(-\frac{M\vec{\delta}^2}{2\hbar t}-\frac{t}{\hbar}V(\vec{x})\right)}_{\text{Standard mid-point path-integral expression}}\underbrace{\exp\left(-\sum_{m=2}^{\infty}\sigma^{(m)}(\vec{x},\vec{\delta},t)\right)}_{\text{Corrections }\sigma^m\propto t^m},$$

where $\vec{x}=\frac{1}{2}(\vec{a}+\vec{b})$, $\vec{\delta}=\vec{b}-\vec{a}$, and all vectors are $N_a\times d$ dimensional.

By keeping all corrections up to level $m=p$ in the sum on the right-hand side of the last equation we construct $A^{(p)}(\vec{a},\vec{b};t)$ converging to the continuum as

$$A(\vec{a},\vec{b};t)=A^{(p)}(\vec{a},\vec{b};t)+O(t^p).$$

The exponent of $A^{(p)}(\vec{a},\vec{b};t)$ (mid-point exponent + corrections up to level p) is usually called effective action of level p. In terms of the path-integral formalism, we are de facto calculating transition amplitudes without the time-slicing procedure, i.e. we use $N=1$ time slices. Therefore we refer to this method as $N=1$ approximation [1].

General properties of transition amplitudes imply:

$$\sigma^{(m)}(\vec{x},\vec{\delta},t)=\sum_{k=0}^{m}t^{m-k}\vec{\delta}_{i_1}\ldots\vec{\delta}_{i_{2k}}c^{i_1,\ldots,i_{2k}}_{m,k}(\vec{x}).$$

Now the Schrödinger equation for the amplitude can be rewritten in the form of recursive relations for the coefficients $c^{i_1,\ldots,i_{2k}}_{m,k}(\vec{x})$. Such relations are most easily solved in an automated way using symbolic software package *Mathematica* in conjunction with the *MathTensor* module. For general many-body theory, we have obtained closed-form expressions up to level $p=10$. All the details of the method can be found in Refs. [4-6], and we present here the solution up to level $p=4$.

EXAMPLE: p=4 ACTION

$$\begin{aligned}
\sigma^{(2)} &= \frac{t^2}{12}\partial^2 V+\frac{t\delta_i\delta_j}{24}\partial^2_{ij}V\\
\sigma^{(3)} &= -\frac{t^3}{24}\partial_i V\partial_i V+\frac{t^3}{240}\partial^4 V+\frac{t^2\delta_i\delta_j}{480}\partial^2_{ij}\partial^2 V+\frac{t\delta_i\delta_j\delta_k\delta_l}{1920}\partial^4_{ijkl}V\\
\sigma^{(4)} &= \frac{t^4}{6720}\partial^6 V-\frac{t^4}{120}\partial_i V\partial_i\partial^2 V-\frac{t^4}{360}\partial^2_{ij}V\partial^2_{ij}V-\frac{t^3\delta_i\delta_j}{480}\partial_k V\partial^3_{kij}V\\
&\quad+\frac{t^3\delta_i\delta_j}{13440}\partial^2_{ij}\partial^4 V-\frac{t^3\delta_i\delta_j}{1440}\partial^2_{ik}V\partial^2_{kj}V+\frac{t^2\delta_i\delta_j\delta_k\delta_l}{53760}\partial^4_{ijkl}\partial^2 V\\
&\quad+\frac{t\delta_i\delta_j\delta_k\delta_l\delta_m\delta_n}{322560}\partial^6_{ijklmn}V
\end{aligned}$$

ENERGY SPECTRA

In the path-integral formalism we usually extract low-lying energy levels of the system from the $t\to\infty$ limit according to: $E_0=\lim_{t\to\infty}[-\log Z(t)/t]$.

Instead, we want to use finite t information, i.e. closed-form analytic expressions $A^{(p)}(\vec{a},\vec{b};t)$ to obtain energy spectra. One way to do this is to solve the eigenproblem of the space-discretized matrix $A^{(p)}(\vec{a},\vec{b};t)$ whose eigenvalues tend to $\exp(-tE_n)$ and eigenfunctions to $\psi_n(\vec{x})$ [7]. The space discretization is characterized by the size of the space grid Δ. The main benefit of this procedure follows from the fact that the discretization error here is given by:

$$\Delta E_0\sim\exp\left(-\frac{2\pi^2 t}{\Delta^2}\right),$$

which allows the optimization of parameters while keeping the error fixed. Using effective actions systematically improves this method (Fig. 1).

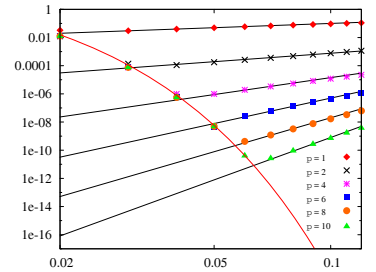

Fig. 1: Deviations from the exact ground-state energy $|E_0^{(p)}-E_0|$ ($E_0=1.47714975357799(4)$) vs. t for different levels p of effective actions for V_{BEC}, with parameters $\omega_\perp=\Omega$, $k=4$, $L=3$, $\Delta=0.2$. The error is $\propto t^p$. The red curve is the discretization error ΔE_0.

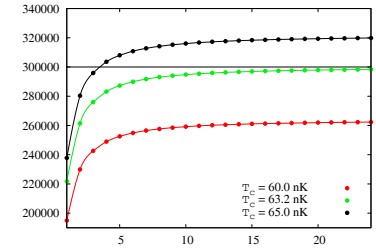

Fig. 2: Values $S(m)=\sum_{m'=1}^{m}N_{m'}$ vs. m for the experimental setup, $\Omega=\omega_\perp$, $E_0=\hbar(0.11626691511\,\omega_\perp+\omega_z/2)$, $T_c\approx 63.2$nK . In the numerical calculations $p=18$ effective actions were used. The horizontal line shows the number of bosons in the experiment, $N_a=3\times10^5$.

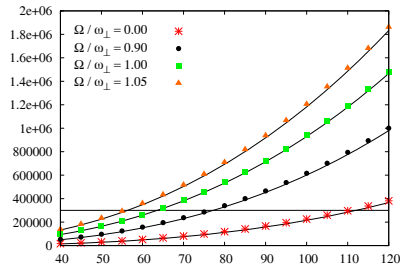

Fig. 3: Plot of N_a vs. T[nK] for different rotation frequencies. In all cases $k=k_{exp}$. In the numerical calculations $p=18$ effective actions were used. The horizontal line shows the number of bosons in the experiment $N_a=3\times10^5$. From the graph we read off the condensation temperature $T_c\approx 63.2$nK for the experimental setup, $\Omega=\omega_\perp$. Solid lines give semiclassical results from Ref. [3].

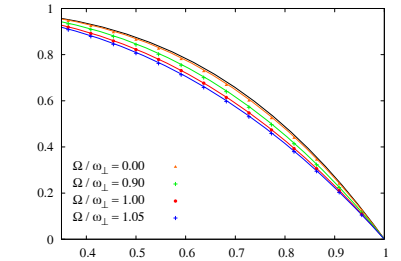

Fig. 4: Plot of N_0/N_a vs. T/T_c for different rotation frequencies. In all cases $k=k_{exp}$. In the numerical calculations $p=18$ effective actions were used. We use $T_c=110$nK in all cases, with the appropriate number of particles. Solid lines represent semiclassical values from Ref. [3].

FAST ROTATING BEC

Fast rotation of a BEC is a challenging subject from both experimental and theoretical point of view. Theoretically, it is expected that in the rapidly rotating setup the system will enter interesting modes, some of them closely related to the quantum Hall physics [8]. Experimentally, it is a delicate matter to achieve fast rotation and to keep the spatial confinement of atoms. In the recent experiment [2], this problem was overcome by introducing an additional anharmonic part into the common harmonic trapping potential for the ensemble of $N_a=3\times10^5$ ^{87}Rb atoms:

$$V_{BEC}=\tfrac{M}{2}(\omega_\perp^2-\Omega^2)r_\perp^2+\tfrac{M}{2}\omega_z^2z^2+\tfrac{k}{4}r_\perp^4,$$
$$\omega_\perp=2\pi\times64.8\text{ Hz},\omega_z=2\pi\times11.0\text{ Hz},k_{exp}=2.6\times10^{-11}\text{ Jm}^{-4}.$$

This type of setup has allowed fast rotating frequencies $\Omega\sim\omega_\perp$. Following the analysis of this system as a rotating ideal Bose gas [3], we apply the presented general approach to the calculation of the condensation temperature T_c of the BEC in the fast-rotating anharmonic trap.

NUMERICAL CALCULATION

Within the grand-canonical ensemble the partition function of non-interacting bosons is given by

$$\mathcal{Z}=\sum_\nu\exp(-\beta(E_\nu-\mu N_\nu))=\prod_k\frac{1}{1-e^{-\beta(E_k-\mu)}},$$

where $\beta=1/k_BT$ is the inverse temperature, μ is the chemical potential, and k counts single-particle eigenstates.

The free energy can now be calculated as:

$$\begin{aligned}\mathcal{F} &= -\frac{1}{\beta}\log\mathcal{Z}=\frac{1}{\beta}\sum_k\log\left(1-e^{-\beta(E_k-\mu)}\right)=\\ &= -\frac{1}{\beta}\sum_{m=1}^{\infty}\frac{e^{m\beta\mu}}{m}\sum_k e^{-m\beta E_k}=-\frac{1}{\beta}\sum_{m=1}^{\infty}\frac{e^{m\beta\mu}}{m}\mathcal{Z}_1(m\beta),\end{aligned}$$

where $\mathcal{Z}_1(m\beta)$ is a single-particle partition function. Condensation temperature is defined by imposing that there are no particles in the ground state,

$$N_0=0,\ \mu=E_0,$$

while the average particle number is equal to the number of atoms in the experiment. In that case, the condensation temperature can be determined from the relation:

$$N_a=-\frac{\partial\mathcal{F}}{\partial\mu}=\sum_{m=1}^{\infty}\underbrace{(e^{m\beta E_0}\mathcal{Z}_1(m\beta)-1)}_{N_m}.$$

To this end we proceed as follows. For a range of rotation frequencies, we calculate a single-particle partition function as:

$$\mathcal{Z}_1(m\beta)=\frac{1}{2\sinh(m\beta\omega_z/2)}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dxdy\,A^{(p)}(x,y,x,y;m\beta),$$

and a single-particle ground-state energy E_0 as previously explained. Then we perform the summation and search for the value of β_c such that the defining relation holds. The numerical results are presented on Figs. 2, 3 and 4.

The obtained results are in good agreement with the semiclassical calculations [3]. In all the considered cases, the numerically calculated condensation temperature is slightly lower from the corresponding semiclassical value, in accordance with the known fact that the finite-size corrections always reduce the condensation temperature of bosons in harmonic traps [9,10].

SUMMARY

- We have successfully applied $N=1$ approximation to the calculation of the condensation temperature of a BEC in a fast rotating anharmonic trap.
- The presented approach is ideally suited for the treatment of dilute Bose gases.
- We plan to extend this method to interacting Bose and Fermi systems.

ACKNOWLEDGEMENTS

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