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Relative Shift Approximation on a trapped interacting Bose gas near transition temperature

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Abstract

By using a mean-field approach we calculate the shift of critical temperature of interacting Bose gas in an anisotropic harmonic trap, which is due to the shift of eigen-energy. In this physical picture, we show the interacting with repulsive forces increase of the energy gap in uniform Bose gas but decrease in trapped Bose gas. Estimating the energy shift the first order in the scattering length related to density of thermal and condensate state, carefully take care the Bose distribution function we find this two density is same order and both affect the T_c . The analytic result for density and eigen-energy for the shift of the critical temperature is derived.

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I. INTRODUCTION

The Bose-Einstein Condensation (BEC) is one of the most striking consequences of quantum statistics [1]. Since the observation of BEC in 1995 [2], it has drawn renewed attention of theorists. The number of condensate atoms in the experiments ranged from hundreds to millions. This number is not truly macroscopic. As a consequence, the thermodynamic limit has never been reached exactly. Hence, strictly speaking, BEC of the trapped gases is not a phase transition. In practice, the macroscopic occupation of the lowest state occurs rather abruptly as the temperature lowered and can be observed. For an ideal Bose gas in a general trap potential $V_{ext}(r) = \frac{m}{2}(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2)$, the transition temperature is

$$T_c^0 = \frac{\hbar\omega}{k_B} \left(\frac{N}{\zeta(3)} \right)^{1/3}, \quad (1)$$

where $\omega = (\omega_1\omega_2\omega_3)^{1/3}$ is the geometrical mean of the frequencies and N is the number of total particle. ζ is the Riemann's Zeta function. The transition temperature is under the condition of the thermodynamic limit ($N \rightarrow \infty$). The effect of finite N is called the finite-size effect. For noninteracting atoms in the general trap potential, the fractional change of transition temperature T_c relative to the ideal Bose gas due to the finite-size effect is [3]

$$\Delta t_c \equiv \frac{T_c - T_c^0}{T_c^0} = -\frac{\zeta(2)}{2[\zeta(3)]^{2/3}} \frac{\bar{\omega}}{\omega} N^{-1/3}, \quad (2)$$

where $\bar{\omega} = (\omega_1 + \omega_2 + \omega_3)/3$ is the arithmetic mean of the oscillator frequencies. The transition temperature is down shifted with respect to the ideal Bose gas in the thermodynamic limit and vanishes in the large N limit.

In the current BEC experiments, there are weakly interactions among the ultracold atoms. The mutual interactions change the density profile drastically from the noninteracting trapped Bose gas [4]. Thus, the role of interactions on critical phenomena is an important problem. Specially, the differences between the behavior of uniform and nonuniform Bose gases are interested. Holzmann *et al.* studied the case with uniform Bose gases (YM : ??). The case of nonuniform gas has not been treated in details. Bagnato *et. al.*[6] first consider the effect of two-body collision on the transition temperature in trap. Giorgini, Pitaevskii, and Stringari [7, 8] pointed out that the repulsive interaction in trapped Bose gas reduce the condensate fraction and critical temperature, and results the shift of T_c in opposite direction compared to the uniform case. (YM : ??) [9, 10].

We present in this paper an improvement to the theory of the BEC near T_c including the interactions. A simple physical picture called *Relative Shift Approximation* (RSA) which describes the shifts of energy is proposed. The shift of eigen-energy of the thermal state can be absorbed into the chemical potential, and the collisional effect is represented as an effective shift of the eigen-energy of the condensate state. In the theory of Giorgini *et al.* [7, 8], the variation of the condensate profile was neglected. We find that near T_c the shift of condensate energy is sensitively depends on density profile (*YM : correct ?*). We consider the variation of the effective condensate energy and calculate the Bose distribution function carefully and determine the number of condensate and its energy.

The remainder of this paper is organized as follows. In Sec.II, we describe the finite-temperature generalization of the Gross-Pitaevskii equation. In Sec.III, comparing to the ideal Bose gas equation, we estimate the energy eigenvalue shift due to the interactions. We find that the energy eigenvalue shift is dependent on condensation fraction. The explanation of upward shift or downward shift of energy is given. Having obtained the energy spectrum, we derive the number distribution in Sec.IV. Combining the condition of well-defined transition temperature and energy eigenvalue shift, the transition temperature shift is self-consistent obtained. Finally, some concluding remarks are given in Sec. V.

II. RELATIVE SHIFT APPROXIMATION

In ideal Bose gas, it is well known the energy spectrum and its thermodynamic behavior. In the harmonic oscillators trap, the ideal Bose gas energy eigenvalues are

$$\epsilon_{\{n_i\}}^{ide} = \sum_{i=1}^3 \left(n_i + \frac{1}{2} \right) \hbar\omega_i \quad (n_i = 0, 1, 2, \dots), \quad (3)$$

where ω_i is the frequency of harmonic at i -dimension.

But in real Bose gas, the energy spectrum has shift due to the interaction. In the two-fluid model, we separate the gases into thermal part and condensate part, which energy level express as ϵ_T and ϵ_c .

In a simple case, suppose the thermal state energy unchange $\epsilon_T = \epsilon_T^{ide}$ and the condensate state energy has a shift due to the interaction

$$\epsilon_c = \epsilon_c^{ide} + \Delta\epsilon_c. \quad (4)$$

We want to know how does this change affect the T_c ?

By the Bose-Einstein distribution in eigen space

$$N = \sum_{\{n_i\}} \frac{1}{e^{(\epsilon_{\{n_i\}} - \mu)/k_B T} - 1}, \quad (5)$$

where μ is the chemical potential, hereafter μ is the parameter of this system. $z = e^{\mu/k_B T}$ is the fugacity.

At $kT \gg \hbar\omega_i$, Expression Eq.(5) then takes the form

$$\begin{aligned} N &= \sum_{j=1}^{\infty} z^j \prod_{i=1}^3 \sum_{n_i=0}^{\infty} e^{-j\hbar(n_i+1/2)\omega_i/k_B T} \\ &= \left(\frac{k_B T}{\hbar\omega} \right)^3 g_3(z), \end{aligned} \quad (6)$$

where $g_\nu(x) = \sum_{n=1}^{\infty} x^n/n^\nu$ is the Bose-Einstein function. Eq.(6) is exactly to first order, the shift of condensate state no contribute in the distribution function. Then the calculation is as usually, but near the T_c the chemical potential is around ϵ_c . We denote the reduce fugacity

$$z' = e^{(\mu - \epsilon_c)/k_B T} \quad (7)$$

notice near T_c , $z' \rightarrow 1$, we should substitute z by z' , thus

$$N = \left(\frac{k_B T}{\hbar\omega} \right)^3 g_3(z') + \frac{\epsilon_c^{ide} + \Delta\epsilon_c}{\hbar\omega} \left(\frac{k_B T}{\hbar\omega} \right)^2 g_2(z'), \quad (8)$$

In general, the interaction also make the thermal energy change, which has shift of energy $\Delta\epsilon_T$. The shift can be absorbed by chemical potential μ , and the condensate state remain the relative shift

$$\epsilon_c^{RSA} = \Delta\epsilon_c - \Delta\epsilon_T \quad (9)$$

Thus Eq.(8) be modified as

$$N = \left(\frac{k_B T}{\hbar\omega} \right)^3 g_3(z') + \frac{\epsilon_c^{ide} + \epsilon_c^{RSA}}{\hbar\omega} \left(\frac{k_B T}{\hbar\omega} \right)^2 g_2(z'), \quad (10)$$

where z' also be defined as Eq.(7).

Here we can modify the Eq.(2) as

$$\Delta t_c = -\frac{\zeta(2)}{3[\zeta(3)]^{2/3}} \left(\frac{\epsilon_c^{ideal} + \epsilon_c^{RSA}}{\hbar\omega} \right) N^{-1/3}, \quad (11)$$

In this approximation, we allow $\epsilon_c^{RSA} > \epsilon_c^{ide}$, but need $\epsilon_c^{RSA} \ll k_B T$.

In usually, we divided the shift into two parts : $\Delta t_c = \Delta t_c^{fin} + \Delta t_c^{int}$. The first term Δt_c^{fin} is the finite size effect, which due to the finite number of bose gases and ideal ground-state-eigenvalue and the second term is due to relative shift energy ϵ_c^{RSA} , which is cause by the interaction of the atoms. The following sections, we will calculate the shift $\Delta \epsilon_c$ and $\Delta \epsilon_T$ by the Gross-Pitaevskii equation(GPE).

III. ENERGY SPECTRUM SHIFT

A. Hartree-Fock-Bogoliubov Approximation

Our starting point is the finite-temperature generalization of the Gross-Pitaevskii equation with Hartree-Fock-Bogoliubov (HFB) approximation[20] :

$$\left(-\frac{\nabla^2}{2m} + V_{ext}(r) - \mu\right) \Phi_c(r) + g[n_c(r) + 2n_T(r)]\Phi_c(r) = 0, \quad (12)$$

and

$$i\frac{\partial \Phi_T(r,t)}{\partial t} = \left(-\frac{\nabla^2}{2m} + V_{ext}(r) - \mu\right) \Phi_T(r,t) + 2gn(r)\Phi_T(r,t). \quad (13)$$

The first equation describes the space variations of the condensate wave function $\Phi_c(r) = \langle \psi(r) \rangle$ at statistical equilibrium, where $\psi(r)$ is the particle field operator. The second one is the equation for the fluctuations of the condensate $\Phi_T(r,t) = \langle \psi(r,t) \rangle - \Phi_c(r)$, which give the elementary excitations of the system. In the coupled equations, $V_{ext}(r)$ is the external potential, μ is the chemical potential, $g = 4\pi\hbar^2 a/m$ is the interaction coupling constant fixed by the s -wave scattering length a , $n_c(r) = |\Phi_c(r)|^2$ is the equilibrium condensate density, $n(r) = \langle \phi(r)^\dagger \phi(r) \rangle$ is the particle density, and $n_T(r) = n(r) - n_c(r)$ is the thermally excited particles density. We neglected the anomalous density $m_T(r) = \langle \phi(r)\phi(r) \rangle - \Phi_c(r)^2$, for high temperature $m_T \ll n_T$ and in the low-temperature n_T and m_T both are negligible. The present mean-field approach is expected to provide correctly the thermodynamic properties of the system, apart from the critical behavior near T_c where the mean-field approach is known to fail.

B. In uniform potential

The collisional shifts of spectral lines in a uniform gas by the Eq.(12) and Eq.(13) can be written as

$$\text{uniform gas} \begin{cases} \epsilon_T = \epsilon_T^{ide} + 2gn(0), \\ \epsilon_c = \epsilon_c^{ide} + 2gn_T(0) + gn_c(0), \end{cases} \quad (14)$$

where $n(0)$ is the density function $n(r)$ at $r = 0$. Note that the eigenvalue of condensate state ϵ_c and the chemical potential μ is different in non-zero temperature, but in large number of condensation particle they are go to the same. Eq.(14) shows the relative shift energy lever is $\epsilon_c^{RSA} = -gn_c(0)$. This effect increase the energy gap between the condensation and excitation, then raising the transition temperature. Note that the energy eigenvalue not the energy per particle[1][9]. In uniform bose gas, the total energy of condensate state is $E = N\epsilon_c^{ide} - Ngn_c(0)/2$. The energy per particle E/N compare with Eq.(14) in right hand side second term has 1/2 factor, it is come form the particle exchange.

C. in trapped potential

By the *local density approximation*(LDA)[21], the spacial distribution of thermal state n_T can be obtained as

$$n_T(r) = \frac{1}{\lambda_T^3} g_{3/2}(ze^{-[V_{ext}(r)-\mu]/k_B T}), \quad (15)$$

where $\lambda_T = \hbar(2\pi/mk_B T)^{1/2}$ is the thermal wavelength.

How does the nonlinear terms affect the spectrum ? Giorgini, Pitaevskii and Stringari(GPS)[7] consider the Bose distribution in $p - r$ phase space

$$f(p, r) = \frac{1}{\exp[\epsilon(p, r)/k_B T] - 1}, \quad (16)$$

where $\epsilon(p, r)$ is the semiclassical excitation spectrum. According the Bose distribution Eq.(13), we get

$$\epsilon(p, r) = \epsilon^{ide}(p, r) + 2gn_T(r) - \mu \quad (17)$$

we using Taylor expansion for g to the first order in Eq.(16)

$$\begin{aligned} f &= f|_{g=0} + g \frac{\partial f}{\partial g}|_{g=0} \\ &= f_0 - 2gn_T \frac{\partial f_0}{\partial \mu}, \end{aligned} \quad (18)$$

where f_0 is $g = 0$, which reduce to the noninteracting ideal gases. Integral the momentum space get the modification of $n_T(r, \mu)$ by interacting is

$$n_T^{int}(r, \mu) \simeq n_T - 2gn_T \frac{\partial n_T}{\partial \mu}. \quad (19)$$

Integral Eq.(19) both side get the number of thermal particle

$$N_T^{int} = \int n_T d^3r - 2g \int n_T \frac{\partial n_T}{\partial \mu} d^3r. \quad (20)$$

Eq.(17) is dependent of r . We denote the eigen energy spectrum of thermal part are

$$\epsilon_T = \epsilon_T^{ide} + 2g\bar{n}_T - \mu \quad (21)$$

Our concern is how large the shift of the eigen energy $2g\bar{n}_T$? Eq.(17) and Eq.(21) must have the same distribution in Eq.(16), including same number of excited particles and chemical potential. To calculate the \bar{n}_T , we substitute Eq.(21) into Eq.(20) may get the same number of thermal particle, then get \bar{n}_T is the average in the phase space by

$$\bar{n}_T = \frac{\int d^3r \frac{\partial n_T}{\partial \mu} n_T}{\int d^3r \frac{\partial n_T}{\partial \mu}} = S n_T(0), \quad (22)$$

where $n_T(0)$ is the thermal density $n_T(r)$ at trap center $r = 0$, and S is a constant. For finding S , use Eq.(15) and assume $\mu = 0$, it is easy to obtain $S = \sum_{n,m=1}^{\infty} (1/n^{1/2} m^{3/2}) [1/(n+m)^{3/2}] / \zeta(3/2)\zeta(2) \simeq 0.281$.

GPS assume the condensate density n_0 at T_c can be neglect, then $n(r) \sim n_T(r)$. Further, the condensate part is much smaller than thermal part and focus on the center of the thermal part. By the Eq.(12), $n(r)$ can substitute by $n_T(0)$, then the energy shift is $2gn_T(0)$ than the ideal gases.

Thus we obtain the physical picture by the energy spectrum shift of the GPS :

$$\text{GPS picture : } \begin{cases} \epsilon_T = \epsilon_T^{ideal} + 2g\bar{n}_T, \\ \epsilon_c = \epsilon_c^{ideal} + 2gn_T(0), \end{cases} \quad (23)$$

we denote the relative shift of the condensate energy level as $\epsilon^{GPS} = 2g(n_T(0) - \bar{n}_T) = 2\alpha gn_T(0)$, where $\alpha = (1 - S) = 0.719$.

D. The condensate state

In 1998, Pathria analyse the chemical potential and number of particle in condensate state N_c at T_c get [14]

$$N_c = \frac{1}{1 - z'} = \left(\frac{\zeta(2)N}{\zeta(3)} \right)^{1/2}. \quad (24)$$

At this temperature, n_c is very rare, we may use the one particle ideal eigenfunction of condensate state

$$\phi(r) = \left(\frac{1}{\pi a_{ho}^2} \right)^{3/4} e^{-m[x^2/(2a_1^2) + y^2/(2a_1^2) + z^2/(2a_1^2)]/2\hbar}, \quad (25)$$

the condensate density can be written as $n_c(r) = |\Phi_c(r)|^2 = N_c |\phi(r)|^2$. We can get $n_c(0) = \zeta(2)^{1/2} N^{1/2} / (\zeta(3)^{1/2} \pi^{3/2} a_{ho}^3)$. By the Eq.(15), one can get $n_T(0) = \zeta(\frac{3}{2}) N^{1/2} / (\zeta(3)^{1/2} (2\pi)^{3/2} a_{ho}^3)$. We find out $n_c(0)/n_T(0) = \zeta(2)^{1/2} 2^{3/2} / \zeta(3/2) = 1.3885$, The density $n_c(0)$ is large than $n_T(0)$, then the condensate density $n_c(r)$ can not be arbitrarily neglected.

In this section, first we want to know how the n_c affect ϵ_T ? Considering two lengths in harmonic traps : $\xi_{iT} = (2\pi m \omega_i^2 / k_B T)^{-1/2}$ is the classical oscillation amplitude of a particle in the trap with energy $k_B T$, it is the size of $n_T(r)$ at i -direction, $\xi_{ic} = \sqrt{\hbar / m \omega_i}$ is the size of the ground state in the oscillator at i -direction. We notice that

$$\frac{\xi_{iT}}{\xi_{ic}} = \frac{k_B T}{2\pi \hbar \omega_i} \sim O(N^{1/3}) \gg 1. \quad (26)$$

this is saying even $n_c(0) \sim n_T(0)$, in the thermal range ξ_T but far the center we still have $n_T(r) \gg n_c(r)$, we can also omit the effect of $n_c(r)$.

The second, how the n_c affect ϵ_c in Eq.(12) ?

In very large number of condensate particle N_c , *Thomas-Fermi approximation* is an accurate expression, but not suit for very few N_c when near T_c . Here we use *Gaussian variational calculation*[?].

We adopt our trial function for Φ_c the same form as Eq.(25)

$$\phi(r) = \frac{1}{\pi^{3/4} (b_1 b_2 b_3)^{1/2}} e^{-m[x^2/(2b_1^2) + y^2/(2b_2^2) + z^2/(2b_3^2)]/2\hbar}, \quad (27)$$

where the lengths b_i are variational parameters. Substitution of Eq.(27) into Eq.(12) yields the total condensate energy expression

$$E = N \sum_i \hbar \omega_i \left(\frac{a_i^2}{4b_i^2} + \frac{b_i^2}{4a_i^2} \right) + 2Ngn_T(0) + \frac{N^2 g}{2(2\pi)^{3/2} b_1 b_2 b_3}. \quad (28)$$

In very rare n_c , we can putting the b_i equal to a_i , and finds

$$E = N\epsilon_c^{ide} + 2Ng n_T(0) + \frac{N^2}{2} \langle 00|v|00 \rangle. \quad (29)$$

where

$$\langle 00|v|00 \rangle = g \int dr |\psi(r)|^4 \quad (30)$$

is the interaction energy for two particles in the condensate state of the oscillator. The energy level is

$$\epsilon_c = \epsilon_c^{ide} + 2gn_T(0) + g\bar{n}_c, \quad (31)$$

where $\bar{n}_c = \beta n_c(0)$, $\beta = 2^{-3/2} \simeq 0.35$.

By numerical simulation, the factor $\beta = 0.35$ is suit for few hundreds condensate number which is correspond to $N \sim 10^5$ (See Fig.1). Then our modification is

$$\text{trapped gas} \begin{cases} \epsilon_T = \epsilon_T^{ideal} + 2g\bar{n}_T, \\ \epsilon_c = \epsilon_c^{ideal} + 2gn_T(0) + g\bar{n}_c, \end{cases} \quad (32)$$

thus $\epsilon_c^{RSA} = 2\alpha gn_T(0) + g\bar{n}_c$. In next paragraph we will show the amount $n_T(0)$ and $n_c(0)$ near T_c is same order. However, our prediction of RSA is large than GPS, thus the effect in transition temperature is much obvious.

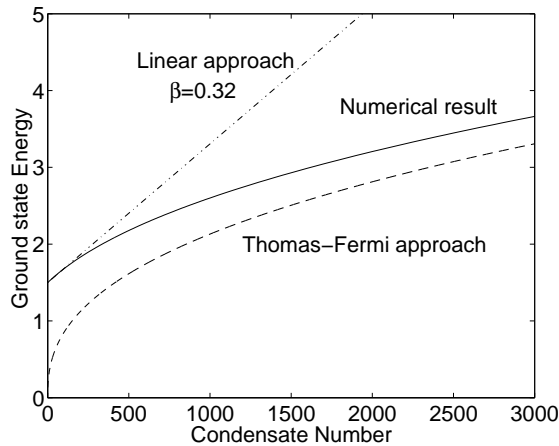


FIG. 1: The comparison of the energy eigenvalue approximation.

IV. TRANSITION TEMPERATURE

The RSA emphasizes single particle behaviour and shows how the collisional effects come about, then can treat the system analogous to ideal gas. In the grand canonical emsemble, the total number of particle in Bose-Einstein distribution is

In Eq.(8) the leading term obtain the transition temperature in the thermodynamic limit ($N \rightarrow \infty$) is Eq.(1). Considering the third term on the right-hand-side of Eq.(8), obtain the finite- N transition temperature shift ratio is Eq.(2). We divided the shift into two parts : $\Delta t_c = \Delta t_c^{fin} + \Delta t_c^{int}$. The first term Δt_c^{fin} is due to the finite number of bose gans and ideal ground-state-eigenvalue and the second term is due to the RSA. It also divided into two parts : $\Delta t_c^{int} = \Delta_T + \Delta_c$, the first term is due to the thermal state, the second term is dut to the condensate state. Near T_c , by the LDA, $n_T(0) = \zeta(\frac{3}{2})N^{1/2}/(\zeta(3)^{1/2}(2\pi)^{3/2}a_{ho}^3)$, where $a_{ho} = \sqrt{\hbar/m\omega}$ is the harmonic oscillator length, thus the transition temperature shift ratio Δ_T by GPS is

$$\begin{aligned}\Delta_T &= -\frac{\zeta(2)}{3[\zeta(3)]^{2/3}} \frac{\Delta E^{GPS}}{\hbar\omega} N^{-1/3} \\ &= -1.33 \frac{a}{a_{ho}} N^{1/6}.\end{aligned}\quad (33)$$

For get the Δ_c , need to calculate the particle number in condensation N_c . At temperature $T = T_c$, the reduce fugacity constraint by second and fourth terms on right-hand-side of Eq.(8), which can get $1 - z' = \sqrt{\zeta(3)/(N\zeta(2))}$, thus N_c at T_c is

$$N_c \sim \frac{1}{1 - z'} = \left(\frac{\zeta(2)N}{\zeta(3)} \right)^{1/2}.\quad (34)$$

Using the ideal eigenfunction of condensate state

$$\phi(r) = \left(\frac{1}{\pi a_{ho}^2} \right)^{3/4} e^{-m(\omega_1 x^2 + \omega_2 y^2 + \omega_3 z^2)/2\hbar},\quad (35)$$

the equilibrium condensate density can be written as $n_c(r) = |\Phi_c(r)|^2 = N_c |\phi(r)|^2$. Thus the transition temperature shift ratio cause by the condensation is

$$\begin{aligned}\Delta_c &= -\frac{\zeta(2)}{3[\zeta(3)]^{2/3}} \frac{2g\beta n_c(0)}{\hbar\omega} N^{-1/3} \\ &= -0.41 \frac{a}{a_{ho}} N^{1/6},\end{aligned}\quad (36)$$

and

$$\Delta t_c^{int} = \Delta_T + \Delta_c = -1.74 \frac{a}{a_{ho}} N^{1/6}.\quad (37)$$

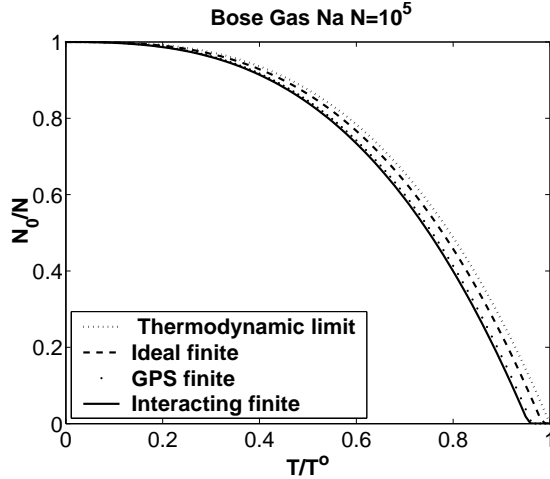


FIG. 2: The condensate fraction of the Na Bose gases, where $a/a_{ho} = 2.56 \times 10^{-3}$.

V. DISCUSSION

The shift $\Delta t_c^{fin} = O(N^{-1/3})$ originating from finite-size effects is always negative and vanishes in the large- N limit. In small- N , the shift $\Delta_c = O(N^{1/6})$ is negative and increases with N . But when $N_c \simeq 2 \times 10^2$ (corresponding to $N \sim 10^5$), the linear approximation needs to be corrected. Applying TFA $n_c(0) = O(N^{1/5})$ thus $\Delta_c = O(N^{-2/15})$ it also vanishes in the large- N limit. $\Delta_T = O(N^{1/6})$ always increases with N .

Although the correction is small, but we provide a simple physical picture related to n_c and n_T to describe the variation of the eigenenergy near the T_c and using fewer assumptions. Under T_c , $N_c = O(N)$, $n_c(0) \gg n_T(0)$, the dominant term affecting E_c is N_c . In large- N_c using TFA has been discussed by Ref.[8], but N_c from hundreds to thousands are not a simple analytic relation.

The fluctuation in T_c is $O(g^2)$ has been discussed by GPS, meaning the mean-field approach can be reliable in the linear scattering length. The difference of the chemical potential μ and eigenenergy of the condensate state in T_c is

$$\mu - E_c = -\frac{\hbar\omega}{\sqrt{\zeta(2)}} \left(\frac{\zeta(3)}{N} \right)^{1/6}, \quad (38)$$

comparison with the interacting shift is $O(N^{-1/3}a/a_{ho})$, it is very small when $N < 10^7$, it means the E_c substitute the μ is reliable.

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