# Quantum corrections to the thermodynamic potential of trapped bosons

Subhasis Sinha

*The Institute of Mathematical Sciences, Madras 600 113, India*

We calculate the quantum corrections of the thermodynamic quantities of a system of confined bosons at finite temperature. Systematically quantum corrections are written in a series of $\hbar$, which is convergent when $kT$ is much larger than the spacing between energy levels of the system. We apply this method to the different physical systems. First we calculate the thermodynamic potential of spin-1 bosons confined in a general power-law potential, and calculate the paramagnetic susceptibility of the gas including the quantum corrections. Local-density approximation for charged bosons in the weak magnetic field is improved by the semiclassical expansion. Diamagnetic susceptibility of a system of confined charged bosons is calculated using this method. Finally we apply this method to calculate analytically the thermodynamic potential of a weakly interacting Bose-gas confined in at three-dimensional harmonic-oscillator potential. For a large number of particles, quantum corrections become small, and contribute to the finite-size corrections to scaling. [S1050-2947(98)03810-4]

PACS number(s): 03.75.Fi, 32.80.Pj

## I. INTRODUCTION

There has been renewed interest in the Bose-Einstein condensation (BEC) after its experimental demonstration by Anderson *et al.* [1,2]. It has now become possible to measure the relevant thermodynamic quantities of a system of weakly interacting bosons in a magnetic trap [3,4]. In these experiments, the temperature dependence of the condensate fraction and the release energy are measured. Theoretically, the thermodynamic properties of homogeneous Bose gas were studied by several authors starting with London [5]. The thermodynamic properties of the inhomogeneous Bose gas were studied by Legget *et al.* [6,7]. After the recent experimental developments, there is a new impetus to understand the thermodynamic properties of interacting inhomogeneous Bose gas. Within the local-density approximation (LDA), Stringari *et al.* [8] have calculated the thermodynamic quantities numerically and shown scaling properties of strongly interacting bosons in a trap. Since then, several calculations have been reported by various authors [9,10]. In these papers the thermodynamic properties of inhomogeneous gas have been calculated within the LDA, neglecting the quantum corrections.

In this paper we develop a systematic semiclassical $\hbar$ expansion for thermodynamic quantities of an interacting Bose gas, which takes into account the quantum corrections. Since the self-consistent potential is quite complicated and device-dependent, the formalism is kept as general as possible. We follow a method analogous to the highly successful extended Thomas-Fermi method (ETF), which has been successfully applied in the case of finite fermion systems, such as nuclei, atoms, clusters, etc. It is well known that the smooth part of the quantum density of states can be semiclassically expanded in powers of $\hbar$. The leading term in this expansion is the Thomas-Fermi level density. Systematic $\hbar$ corrections to the leading approximation may then be obtained using the well known Wigner-Kirkwood (WK) expansion [11]. In the case of finite fermion systems this is what is usually referred to as the extended Thomas-Fermi approxi-

mation [12]. Following this procedure, we develop a semiclassical expansion for finite Bose systems at finite temperature. The method is simple and can be effectively used even when the bosons are interacting. To demonstrate the usefulness of the method, we first apply it to noninteracting bosons confined in a general trap potential. In the case of a harmonic potential we compare the results obtained with the known results obtained using exact calculations and check the correctness of the method. We then extract physically relevant thermodynamic quantities at finite temperature including the quantum corrections to the leading order.

The paper is organized as follows. In Sec. II, we develop the formalism of semiclassical expansion and apply it to the case of noninteracting bosons in complicated trap potentials in Sec. III. Motivated by the recent experiment on spin-1 $^{23}$Na atoms [2], in Sec. IV we also calculate the paramagnetic susceptibility of the gas, including the quantum corrections. Section V is devoted to the application of the semiclassical expansion for a system of charged bosons in a homogeneous magnetic field, and the diamagnetic susceptibility of the Bose gas above the critical temperature is calculated. Here we show that the diamagnetic susceptibility comes entirely from the quantum corrections. In Sec. VI, we analytically calculate the thermodynamic quantities of an ensemble of weakly interacting Bose gas confined in at three-dimensional harmonic-oscillator potential including the leading-order quantum corrections. We show that the leading-order thermodynamic quantities are functions of only two scaling parameters. The quantum corrections, however, give rise to small but finite-size corrections to scaling $O(1/N^{2/3})$. Section VII contains a summary and conclusions.

## II. EXTENDED THOMAS-FERMI APPROXIMATION FOR BOSONS

We first develop a systematic $\hbar$ expansion using the Wigner-Kirkwood (WK) method [11]. Consider the single-particle Hamiltonian $H$ for a system of particles, which satisfies the Schrödinger equation,

$$H\psi_n = E_n\psi_n, \tag{1}$$

where $E_n$ are eigenvalues and $\psi_n$ are corresponding wave functions. The canonical partition function of the system is defined as

$$Z_0(\beta) = \sum_n e^{-\beta E_n}, \tag{2}$$

where $\beta$ is, for our purposes, a parameter with the dimension of inverse energy and should not be confused with the physical temperature of the system.

We first briefly review the semiclassical method as applied to the finite fermion system [12], which is well known. To extract thermodynamic quantites of the finite fermion system from the canonical partition function, a weight function is defined as

$$w_F = \frac{\pi\beta kT}{\sin(\pi\beta kT)}. \tag{3}$$

By using this weight function, one can write the thermodynamic potential of the system in the following way:

$$kTq(T,z) = \mu N - E + TS = L_\mu^{-1}\left(\frac{Z_0(\beta)w_F}{\beta^2}\right). \tag{4}$$

In the integral representation,

$$kTq(T,z) = \frac{1}{2\pi i}\int_{\epsilon-i\infty}^{\epsilon+i\infty} e^{\beta\mu}\frac{Z_0(\beta)w_F}{\beta^2}d\beta, \tag{5}$$

where the contour is closed from the left for $E_n < \mu$ and from the right for $E_n > \mu$. Summing over all residues, we obtain the well known result [13]

$$q(T,z) = \sum_n \ln(1 + ze^{-E_n/kT}), \tag{6}$$

where $z = e^{\mu/kT}$ is the fugacity and $T$ is the temperature. Using this thermodynamic potential all the relevant thermodynamic quantities related to the finite fermion system may be obtained.

The method can now be extended to the case of bosons. Here we propose a form of the weight function for bosons, so that all calculations done for finite fermion systems can be extended to the finite Bose systems at finite temperature. The weight function for bosons is given by

$$w_B = \frac{-\cos(\pi\beta kT)\pi\beta kT}{\sin(\pi\beta kT)}. \tag{7}$$

The thermodynamic potential of an ensemble of bosons can therefore be written in terms of the following integral, as in the case of fermions:

$$kTq(T,z) = \frac{1}{2\pi i}\int_{\eta-i\infty}^{\eta+i\infty} e^{\beta\mu}\frac{Z_0(\beta)w_B}{\beta^2}d\beta, \tag{8}$$

where $Z_0(\beta)$ is the same as in Eq. (2). The line of integration is chosen in such a way that all the positive poles (excluding

zero) are to the right side of the line. This integral is well defined and convergent. Since the chemical potential $\mu < E_n$ (for all $n$) for bosons, we close the contour from the right. Summing over all the residues at the positive poles inside the contour, we obtain the well known result for the thermodynamic potential [13],

$$q(z,T) = -\sum_n \ln(1 - ze^{-E_n/kT}). \tag{9}$$

This immediately checks the correctness of the weight function $w_B$ for bosons. From the above thermodynamic potential we can calculate all thermodynamic quantities. One important difference between the finite fermion and the finite boson systems is the existence of a critical temperature in the latter. Care must therefore be exercised in using the semiclassical formalism close to the critical temperature. We clarify this point as we go along.

To do a systematic $\hbar$ expansion of bosons, we start from the high-temperature limit. Neglecting the zero point energy and the occupation number of the ground state, we can do the WK expansion of a canonical partition function. For the semiclassical expansion of the partition function, it is most convenient to take the plane-wave basis for calculation of the canonical partition function,

$$Z_0(\beta) = \frac{1}{h^3}\int d^3p \int d^3r\, e^{-i\vec{p}\cdot\vec{r}/\hbar}e^{-\beta H}e^{i\vec{p}\cdot\vec{r}/\hbar}, \tag{10}$$

where $H$ is the single particle Hamiltonian. To evaluate the partition function, we introduce the function

$$u(\vec{r},\vec{p},\beta) = e^{-\beta H}e^{i\vec{r}\cdot\vec{p}/\hbar},$$

$$= e^{-\beta H_{\mathrm{cl}}}e^{i\vec{r}\cdot\vec{p}/\hbar}w(\vec{r},\vec{p},\beta), \tag{11}$$

where $H_{\mathrm{cl}}$ is the classical Hamiltonian, $H_{\mathrm{cl}} = p^2/2M + V(\vec{r})$, and $V(r)$ is the self-consistent single-particle potential. It is easy to see that the function $u$ obeys the Bloch equation

$$\frac{\partial u}{\partial\beta} + Hu = 0 \tag{12}$$

with the boundary condition

$$\lim_{\beta\to 0} u = e^{i\vec{p}\cdot\vec{r}/\hbar}. \tag{13}$$

Substituting $u$ in the above equation, we obtain the following equation for $w$:

$$\frac{\partial w}{\partial\beta} = -i\hbar\left(\frac{\beta}{M}(\vec{p}\cdot\nabla V)w - \frac{1}{M}(\vec{p}\cdot\nabla w)\right) + \frac{\hbar^2}{2M}[\beta^2(\nabla V)^2 w$$
$$- \beta(\nabla^2 V)w + \nabla^2 w - 2\beta(\nabla V\cdot\nabla w)]. \tag{14}$$

The above equation can be solved order by order in $\hbar$, by expanding $w$ as a power series in $\hbar$,

$$w = 1 + \hbar w_1 + \hbar^2 w_2 + \cdots, \tag{15}$$

where $w_1, w_2, \ldots$ are determined at each order using the Bloch equation. Up to the order $\hbar^2$, the canonical partition may then be written as [12]

$$Z_{\text{WK}}(\beta) = \frac{1}{(2\pi\hbar)^3} \int d^3p \, e^{-\beta p^2/2M} \int d^3r \, e^{-\beta V(\vec{r})} \left[ 1 - \frac{\beta^2 \hbar^2}{12M} \left( \nabla^2 V(\vec{r}) - \frac{\beta}{2} (\nabla V(\vec{r}))^2 \right) \right] + O(\hbar^4). \qquad (16)$$

After doing integration by parts, the above expression can be written in the following form:

$$Z_{\text{WK}}(\beta) = \frac{1}{(2\pi\hbar)^3} \int d^3p \, e^{-\beta p^2/2M} \int d^3r \, e^{-\beta V(\vec{r})} \left( 1 - \frac{\beta^2 \hbar^2}{24M} \nabla^2 V(\vec{r}) \right) + O(\hbar^4), \qquad (17)$$

where $V(r)$ is the effective single-particle potential. We note that at this stage the above result is true for both fermions and bosons because the statistics has not yet been imposed.

Inserting the expression for $Z_{\text{WK}}$ for the canonical partition function in Eq. (8), we obtain the thermodynamic potential of the normal state of the Bose system,

$$q(z,T) = -\frac{1}{(2\pi\hbar)^3} \int d^3p \int d^3r \left( \ln(1 - z e^{-[p^2/2M + V(\vec{r})]/kT}) - \frac{\hbar^2}{24M} \nabla^2 V(\vec{r}) \frac{\partial^2}{\partial\mu^2} \ln(1 - z e^{-[p^2/2M + V(\vec{r})]/kT}) \right) + O(\hbar^4). \qquad (18)$$

After substituting Eq. (16) into Eq. (8), we get the following form of the density of the thermodynamic potential or the local thermodynamic potential up to order $\hbar^2$:

$$F(\vec{r}) = \frac{1}{\lambda^3} \left( g_{5/2}(\tilde{z}) - \frac{\hbar^2}{24M(kT)^2} \{ \nabla^2 V(\vec{r}) g_{1/2}(\tilde{z}) + \nabla \cdot [\nabla V(\vec{r}) g_{1/2}(\tilde{z})] \} \right), \qquad (19)$$

where the $g_n(x)$ and the thermal wavelength $\lambda$ are defined as

$$\lambda = \frac{2\pi\hbar}{\sqrt{2\pi M kT}}, \quad g_n(x) = \sum_{i=1}^{\infty} \frac{x^i}{i^n}, \qquad (20)$$

and the effective fugacity is $\tilde{z} = z e^{-V(r)/kT}$. Equation (19) is the central result of the paper, and in the following sections we use this expression to calculate the quantum corrections of various thermodynamic quantities of the Bose system. Here we have calculated the local thermodynamic potential up to $\hbar^2$ order, but $\hbar^4$ and higher-order terms can also be calculated easily following the same procedure. Unlike the calculation of the Wigner distribution function, this method provides a much simpler way to calculate the quantum corrections order by order in $\hbar$.

From the thermodynamic potential, we can derive the number of particles and the energy of the normal state,

$$N_e = z \left( \frac{\partial q}{\partial z} \right)_T, \qquad (21)$$

$$U = (kT)^2 \left( \frac{\partial q}{\partial (kT)} \right)_z. \qquad (22)$$

This completes our discussion of single-particle properties of a finite Bose system using a systematic semiclassical expansion. While we have given the results up order $(\hbar^2)$, in principle the method can be continued to higher orders. In the next section we consider a simple application of this formalism to noninteracting bosons confined in an arbitrary power-law potential.

## III. APPLICATION TO NONINTERACTING BOSONS

We first apply the formalism to a system of noninteracting but confined bosons and check its correctness. To show the simplicity as well as the usefulness of the method, we first consider a general power-law-type confinement and specialize to the harmonic traps later. The general power-law potential is given by [9]:

$$V(\vec{r}) = \epsilon_1 \left( \frac{x}{L} \right)^{2p} + \epsilon_2 \left( \frac{y}{L} \right)^{2l} + \epsilon_3 \left( \frac{z}{L} \right)^{2q}, \qquad (23)$$

where $L$ is a length parameter and $\epsilon_i$ have the dimensions of energy. The exponents $p, q, l$ are positive but arbitrary. Notice that since the potential is complicated, it is not, in general, possible to get the exact spectrum and therefore exact results are not known except in special cases. To calculate the thermodynamic potential including the leading-order quantum correction, we use the expression of the local thermodynamic potential derived earlier in Eq. (19). Substituting for $V(r)$, and after doing some algebra, we obtain the following expression for the thermodynamic potential including corrections up to order $\hbar^2$:

$$q(z,T) = q_0(z,T) + q_2(z,T). \qquad (24)$$

$q_0(z,T)$ denotes the leading contribution in the semiclassical expansion, which is given by

$$q_0(z,T) = \frac{C_0}{\lambda^3} g_{5/2 + \eta'}(z), \qquad (25)$$

where

$$C_0 = \frac{L^3 \Gamma(1/2p)\Gamma(1/2l)\Gamma(1/2q)}{pql(\epsilon_1/kT)^{1/2p}(\epsilon_2/kT)^{1/2l}(\epsilon_3/kT)^{1/2q}}, \quad (26)$$

$$\eta' = \frac{1}{2p} + \frac{1}{2q} + \frac{1}{2l}, \quad (27)$$

and $\lambda$ is the thermal wavelength given in the preceding section. Further, $q_2(z,T)$ is the second-order quantum correction $[O(\hbar^2)]$ of the thermodynamic potential, and is given by

$$q_2(z,T) = -\frac{C_0}{\lambda^3} \frac{E_0}{24kT} \left\{ \left[ f(p)\left(\frac{\epsilon_1}{kT}\right)^{1/p} g_{3/2+\eta'-1/p}(z) \right. \right.$$

$$+ f(l)\left(\frac{\epsilon_2}{kT}\right)^{1/l} g_{3/2+\eta'-1/l}(z)$$

$$\left. \left. + f(q)\left(\frac{\epsilon_3}{kT}\right)^{1/q} g_{3/2+\eta'-1/q}(z) \right] \right\}. \quad (28)$$

The parameters in the above equation are

$$f(x) = \frac{2x(2x-1)\Gamma(1-1/2x)}{\Gamma(1/2x)}, \quad (29)$$

$$E_0 = \frac{\hbar^2}{ML^2}. \quad (30)$$

Thus for any given $p,q,l$, it is possible to obtain the relevant thermodynamic quantities from the closed form for the thermodynamic potential given above.

As an example, we choose the parameters of the potential so that it specializes to the harmonic trap. This can be done by setting $p=l=q=1$, $\epsilon_1=\epsilon_2=\epsilon_3=\hbar\omega/2$, and $L^2 = \hbar/M\omega$, so that the potential becomes an isotropic simple harmonic potential. By substituting the values of the parameters of the potential in the above expressions for the thermodynamic potential, we obtain

$$q(z,T) = \left(\frac{kT}{\hbar\omega}\right)^3 \left[ g_4(z) - \frac{1}{8}\left(\frac{\hbar\omega}{kT}\right)^2 g_2(z) \right]. \quad (31)$$

From this thermodynamic potential we can derive the number of particles and the energy of the normal state. Using the definitions given in Eqs. (21) and (22), we have

$$N_e = \left(\frac{kT}{\hbar\omega}\right)^3 \left[ g_3(z) - \frac{1}{8}\left(\frac{\hbar\omega}{kT}\right)^2 g_1(z) \right], \quad (32)$$

$$U = kT\left(\frac{kT}{\hbar\omega}\right)^3 \left[ 3g_4(z) - \frac{1}{8}\left(\frac{\hbar\omega}{kT}\right)^2 g_2(z) \right]. \quad (33)$$

Indeed, the above expression may also be derived from the exact quantum-mechanical density of states of a three-dimensional (3D) harmonic oscillator (HO). The exact canonical partition function of the 3D HO is given by

$$Z(\beta) = \frac{1}{[2\sinh(\beta\hbar\omega/2)]^3}. \quad (34)$$

Density of states can be calculated by taking the inverse Laplace transform of the canonical partition function with respect to $\beta$ from which the above expressions for the number and energy follow up to order $\hbar^2$. Similar results may be obtained by the Eular-Maclaurin summation method [10].

It is therefore clear that thermodynamic quantities may be expanded in a series of a dimensionless parameter $\hbar\omega/kT$ when the trap potential is harmonic. The expansion parameter is in fact $\hbar\omega/kT$. Therefore, the series converges only when $\hbar\omega/kT \leq 1$. However, at low temperatures $\beta\hbar\omega \approx 1$, and hence the Wigner-Kirkwood expansion breaks down. At these temperatures, only a few low-energy states are occupied, so energy levels cannot be taken as continuous. Obviously one should treat the semiclassical expansion derived in this section as a high-tempertaure expansion.

## IV. QUANTUM CORRECTIONS TO THE PARAMAGNETISM OF SPIN-1 BOSONS

As an application of the formalism developed in the preceding sections, we do the semiclassical expansion of free energy of the spin-1 bosons in a general power-law-type confinement. Very recently it has become possible to observe Bose-Einstein condensation of dilute $^{23}$Na atoms in an optical dipole trap. Total spin of a $^{23}$Na atom is $F=1$, and it has three degenerate states labeled by the $z$ component of the total spin, $F_z=0,1,-1$. In the previous experiments in magnetic trap spin degrees of freedom of alkali atoms are frozen. But in the optical trap, Stamper-Kurn et al. [2] have produced a stable condensate of three spin states of $^{23}$Na atoms. This experiment opens a new window to study the spin dynamics of the trapped bosons. In this section, we consider the trapped spin-1 bosons in a weak magnetic field and calculate the magnetic properties of the gas and the quantum corrections in the high-temperature limit.

The Hamiltonian of the system in a uniform weak magnetic field $B$ can be written as

$$H = \frac{p^2}{2M} + V(\vec{r}) - \mu_z B m_f, \quad (35)$$

where $\mu_z$ is the magnetic moment of the atom and $m_f$ is the $z$ component of the spin of the atom. Simkin and Cohen [14] have recently shown that the $z$ component of the magnetic moment of a $^{23}$Na atom is $\mu_z = \mu_b/2$, where $\mu_b$ is the Bohr magneton. In the noninteracting case the three spin states of spin-1 boson behave as a three-component fluid, and therefore their thermodynamic potential will add up. Generalizing the expression for the thermodynamic potential to spin-1 bosons and including the Zeeman term, we obtain the following expression for the thermodynamic potential:

$$q_{\text{tot}}(z,T,B) = q(ze^y,T) + q(z,T) + q(ze^{-y},T), \quad (36)$$

where $q(z,T)$ is the thermodynamic potential of one-component gas, which we have already derived, and $y = \mu B/kT$. Here we investigate the magnetization and paramagnetic susceptibility of the gas above the critical temperature. Therefore, all the atoms are in the normal state. Magnetization of the gas is defined as

$$M = \mu_z \frac{N(1) - N(-1)}{N}, \qquad (37)$$

where $N(1), N(-1)$ are the number of spin-up ($m_f = +1$) and spin-down ($m_f = -1$) particles. In terms of the grand potential of each spin state, magnetization and paramagnetic susceptibility can be written as

$$M = \frac{\mu_z}{N} \left( z \frac{\partial q(z e^y, T)}{\partial z} - z \frac{\partial q(z e^{-y}, T)}{\partial z} \right), \qquad (38)$$

$$\chi = \frac{\partial M}{\partial B} \Big|_{B=0}. \qquad (39)$$

The paramagnetic susceptibility of the gas confined in a power-law potential described in Eq. (23) is given by

$$\chi = \frac{\mu_z^2}{kT} \frac{2}{N} \frac{C_0}{\lambda^3} \left\{ g_{1/2 + \eta'}(z) - \frac{E_0}{24kT} \left[ \sum_{x=p,l,q} f(x) \left( \frac{\epsilon_x}{kT} \right)^{1/x} g_{\eta' - 1/2 - 1/x}(z) \right] \right\}, \qquad (40)$$

where $C_0$, $f(x)$, $E_0$, and $\eta'$ are given by Eqs. (26), (29), (30), and (27), respectively. It is an interesting point to note that for $\eta' \leqslant 1/2$, susceptibility diverges at critical temperature. Susceptibility of Bose gas in an anisotropic harmonic oscillator potential is given by

$$\chi = \frac{2\mu_z^2}{\delta N kT} \left( \frac{kT}{\hbar \omega_\perp} \right)^3 \left( g_2(z) - \frac{(\hbar \omega_\perp / kT)^2}{24} (2 + \delta) \frac{z}{1 - z} \right), \qquad (41)$$

where $\omega_\perp, \omega_z$ are the frequencies of the harmonic-oscillator potential in the $x$-$y$ plane and in the $z$ direction, respectively, and $\delta = \omega_z / \omega_\perp$. The second term in the expression for susceptibility is the quantum correction. In the high-temperature limit, susceptibility can be expanded as a power series in the fugacity variable $z$,

$$\chi = \frac{2}{3} \frac{\mu_z^2}{kT} \left( 1 + \frac{z}{2^{\eta' + 3/2}} (1 - \alpha) + O(z^2) \right), \qquad (42)$$

where

$$\alpha = \frac{\beta E_0}{24} \sum_{x=p,l,q} f(x) (\beta \epsilon_x)^{1/x} (2^{1 + 1/x} - 1). \qquad (43)$$

As to be expected in the high-temperature limit, the leading term in susceptibility does not depend on the nature of confinement or quantum corrections.

## V. CHARGED BOSONS IN MAGNETIC FIELD

The local-density approximation (LDA) has been widely used [8] to calculate thermodynamic quantities, albeit numerically. However, the major limitation of the local-density approximation is that it fails to describe the physical quantities correctly for a system of charged particles in a magnetic field. The effect of a magnetic field is incorporated only through the quantum corrections.

The situation, however, may be rectified in the case of charged bosons in a weak magnetic field where the strength is used as an expansion parameter. Consider a system of charged bosons in a weak magnetic field applied along the $z$ axis. Here we consider the system of bosons above the critical temperature, so that there is no macroscopic occupation

of the ground state. To include the effect of a magnetic field in the thermodynamic potential, we first do the Wigner-Kirkwood expansion of the canonical partition function. In the symmetric gauge, the vector potential can be written as

$$\vec{A} = \left( -\frac{1}{2} By, \frac{1}{2} Bx, 0 \right), \qquad (44)$$

where $B$ is the magnitude of the field. The Hamiltonian of the system is then given by

$$H = \frac{1}{2M} [\vec{p} + (e/c)\vec{A}]^2 + V(\vec{r}) = H_0 + H_1, \qquad (45)$$

where

$$H_0 = \frac{p^2}{2M} + V(\vec{r}) \qquad (46)$$

$$H_1 = \frac{e^2 B^2}{8M c^2} r_\perp^2 + \frac{eB}{2Mc} l_z, \qquad (47)$$

and

$$r_\perp^2 = (x^2 + y^2), \qquad (48)$$

$$l_z = -i\hbar \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right). \qquad (49)$$

For simplicity, here we consider only the spherically symmetric trap. The Wigner-Kirkwood expansion of the canonical partition function in the magnetic field has been done by Jennings and Bhaduri [15]. Here we use their result, and briefly mention the steps needed for the calculation of the partition function. In terms of the single-particle Hamiltonian, the canonical partition function can be written as

$$Z(\beta, B) = \text{Tr}\, e^{-\beta(H_0 + H_1)} \approx \text{Tr}\, e^{-\beta H_0} e^{-\beta H_1} + O(B^4). \qquad (50)$$

To the leading order in a magnetic field, the partition function can be written as

$$Z(\beta, B) = Z(\beta, 0) + \frac{\beta^2 e^2 B^2}{8 M^2 c^2} \text{Tr}(e^{-\beta H_0})[l_z^2 - M r_\perp^2 / \beta],$$

$$(51)$$

where $\beta$ is a parameter as in Sec. I with energy dimensions. Performing the Wigner-Kirkwood expansion, the canonical partition function up to order $B^2$ and $\hbar^2$ is given by

$$Z(\beta, B) = \frac{1}{8 \pi^{3/2} \beta^{3/2}} \left( \frac{2M}{\hbar^2} \right)^{3/2} \int d^3 r e^{-\beta V(\vec{r})} \left[ 1 - \frac{\beta^2 \hbar^2}{24 M} \right.$$

$$\left. \times \left( \nabla^2 V(\vec{r}) - \frac{e^2 B^2}{24 M c^2} \right) \right].$$

$$(52)$$

The thermodynamic potential of the charged boson system can be written as

$$q(z, T) = \frac{1}{kT} \frac{1}{2 \pi i} \int_{\eta - i\infty}^{\eta + i\infty} e^{\beta \mu} \frac{Z(\beta, B)}{\beta^2} w_B d\beta, \quad (53)$$

where the weight factor $w_B$ is given by Eq. (7). The thermodynamic potential is given by

$$q(z, T) = \frac{1}{\lambda^3} \int d^3 r \left( g_{5/2}(\tilde{z}) - \frac{\hbar^2}{24 M (kT)^2} [\nabla^2 V(\vec{r}) + M \omega_c^2] g_{1/2}(\tilde{z}) \right), \quad (54)$$

where,

$$\tilde{z} = z e^{-V(\vec{r})/kT}, \quad \omega_c = \frac{eB}{Mc}. \quad (55)$$

The diamagnetic susceptibility of the trapped Bose gas can then be written as

$$\chi = \frac{kT \partial^2 q(z, T, B)}{N} \bigg|_{B=0} = \frac{-e^2 \hbar^2}{12 N M^2 c^2 kT} \frac{1}{\lambda^3} \int g_{1/2}(\tilde{z}) d^3 r. \quad (56)$$

Since $\chi$ is proportional to $\hbar^2$, the susceptibility (diamagnetic contribution) is entirely due to the quantum corrections.

The diamagnetic susceptibility of ideal Bose gas confined in an isotropic harmonic-oscillator potential is then given by

$$\chi = -\frac{e^2 \hbar^2}{12 M^2 c^2 kT} \frac{g_2(z)}{g_3(z)}. \quad (57)$$

Since $z \to 1$ near the critical point, the susceptibility becomes

$$\chi(T_c) = -\frac{e^2 \hbar^2}{12 M^2 c^2 kT_c} \frac{\zeta(2)}{\zeta(3)}. \quad (58)$$

In the high-temperature limit it reduces to the usual Landau diamagnetic susceptibility,

$$\chi(T \to \infty) = -\frac{e^2 \hbar^2}{12 M^2 c^2 kT}. \quad (59)$$

Thus the semiclassical expansion as applied to noninteracting Bose systems reproduces the know limits correctly. We next apply the formalism to the weakly interacting Bose gas.

## VI. APPLICATION TO WEAKLY INTERACTING BOSE GAS

Having checked the formalism, we now apply the semiclassical method to nonideal Bose gas. This is much closer to the realistic case. For example, in a recent experiment, Ensher et al. [3] measured the thermodynamic quantities of an interacting Bose system consisting of 40 000 $^{87}$Rb atoms, for which the s-wave scattering length is $\approx 100 a_0$, where $a_0$ is the Bohr radius.

In the preceding sections we dealt with the Bose system in the high-temperature limit, where the system is in the normal (or noncondensate) phase. However, at $T < T_C$, we have to consider the system in both condensate and noncondensate phases. The usual procedure is to treat the condensate and noncondensate mixture as two fluids. Small amplitude fluctuations may then be described by a set of coupled Bogoliubov's equations,

$$[H_0 - \mu + 2 u \rho(\vec{r})] u_\lambda(\vec{r}) + u \phi^2 v_\lambda = \hbar \omega_\lambda u_\lambda(\vec{r}), \quad (60)$$

$$[H_0 - \mu + 2 u \rho(\vec{r})] v_\lambda(\vec{r}) + u \phi^{*2} u_\lambda(\vec{r}) = \hbar \omega_\lambda v_\lambda(\vec{r}), \quad (61)$$

where $\phi(\vec{r})$ is the condensate wave function and $H_0$ is the noninteracting part of the full Hamiltonian, given by

$$H_0 = \frac{p^2}{2M} + V(\vec{r}). \quad (62)$$

The total density of the gas is $\rho = |\phi|^2 + \rho_{nc}$, where $\rho_{nc}(\vec{r})$ is the noncondensate density. The interaction strength is given by $u = 4 \pi \hbar^2 a / M$. The particle ($u_\lambda$) and the hole ($v_\lambda$) excitations are necessary to describe the low-lying excitations of the system. These excitations are important in describing the low-temperature properties of the system. Classical phase-space dynamics of such a quasiparticle and a hole was recently investigated by Fliesser et al. [16]. They have also

discussed the validity of Bogoliubov equations as well as Hartree-Fock equations to describe the excitations.

As is generally known, the single-particle-like excitations are described by the Hartree-Fock(HF) equation, which is given by [6,7,17]

$$[H_0 + 2u\rho(\vec{r})]\psi_i(\vec{r}) = e_i\psi_i(\vec{r}). \tag{63}$$

Unlike in the bulk, in the case of a confined Bose system, condensate density vanishes beyond the turning point and locally the Bogoliubov equations reduce to the HF equation. For this reason the density of states of the excitations calculated from these two different equations match almost exactly, except for a few low-lying excitations [17]. In this paper, therefore, we use the HF approximation hereafter to describe the thermodynamic properties of the weakly interacting Bose gas.

Within the Hartree-Fock theory of bosons, noncondensate density is given by

$$\rho_{nc}(\vec{r}) = \sum_i \frac{|\psi_i|^2}{e^{(e_i - \mu)/kT} - 1}. \tag{64}$$

The condensate density, for a Bose system in an isotropic harmonic trap, is obtained as a solution of the Gross-Pitaevskii equation [18],

$$\left(-\frac{\hbar^2}{2M}\nabla^2 + \frac{1}{2}M\omega^2 r^2 + 2u\rho_{nc}(r) + u\rho_c(r)\right)\phi(r) = \epsilon_0\phi(r), \tag{65}$$

where $\rho_{nc}(r)$ and $\rho_c(r)$ are the densities of the noncondensate and condensate part. Neglecting the kinetic energy of the condensate, the lowest energy eigenvalue may be approximated by

$$\epsilon_0 \approx \epsilon_1 + 2u\rho_{nc}(0), \tag{66}$$

where $l = \sqrt{\hbar/M\omega}$ and $\epsilon_1 = \frac{1}{2}\hbar\omega(15N_0(a/l))^{2/5}$. Further within the same approximation, condensate density can be written as

$$\rho_c(r) = \frac{1}{u}[\epsilon_1 - V(r)]. \tag{67}$$

The above approximation is valid for a large number of condensate atoms $N_0$ and for strong repulsive interaction between the atoms in the condensate. This approximation, however, breaks down within a small region near the critical temperature, where the number of condensate atoms becomes very small. For the noncondensate part we may use the semiclassical formalism developed earlier for the normal Bose fluid. Using Eq. (19), the local thermodynamic potential of the noncondensate atoms may be written as,

$$F(r) = \frac{1}{\lambda^3}\left(g_{5/2}(\tilde{z}_{eff}) - \frac{\hbar^2}{24M(kT)^2}\nabla^2 V_{eff}g_{1/2}(\tilde{z}_{eff})\right), \tag{68}$$

where $\tilde{z}_{eff} = e^{[\mu - V_{eff}(r)]/kT}$ and $V_{eff}(r) = V(r) + 2u\rho(r)$.

The perturbative expansion is best done by writing the effective fugacity in the following form:

$$\tilde{z}_{eff} = \tilde{z}\exp(\{\epsilon_1 - V(r) - 2u\rho_c(r) + 2u[\rho_{nc}(0) - \rho_{nc}(r)]\}/kT), \tag{69}$$

where $\tilde{z} = e^{(\mu - \epsilon_0)/kT}$, which is always less than 1 since $\mu < \epsilon_0$. Assuming weak coupling, we expand the functions in terms of the small parameter $2u[\rho_{nc}(0) - \rho_{nc}(r)]$. The perturbative expansion in this method turns out to be well behaved [9]. Excluding the noncondensate part, the leading term in the effective fugacity can be written as

$$\tilde{z}_{eff} = \tilde{z}e^{[V(r) - \epsilon_1]/kT} \quad \text{for } r < r_0, \tag{70}$$

$$= \tilde{z}e^{[\epsilon_1 - V(r)]/kT} \quad \text{for } r > r_0,$$

where $r_0$ is the turning point of the Thomas-Fermi density $\rho_c$. From the above expression it is easy to see that there is no expansion parameter for the condensate part. We therefore approximate the local chemical potential within the condensate by its mean value. To calculate the free energy of the system within mean-field theory, we subtract the self-energy from the total energy of the system. The self-energy contribution is given by

$$E_s = u\int \rho_{nc}^2(r)d^3r. \tag{71}$$

In the following calculation, we replace the coupling by a dimensionless parameter $\eta = [\sqrt{(2/\pi)}(a/l)N^{1/6}]^{2/5}$. Up to order $\eta^{5/2}$ and $\hbar^2$, the thermodynamic potential is given by

$$q(z,T)/N = q_0(\tilde{z},t,\eta) + \frac{1}{N^{2/3}}q_2(\tilde{z},t,\eta). \tag{72}$$

The first term $q_0(\tilde{z},t,\eta)$ is the leading-order scale invariant part of the thermodynamic potential and is given by

$$q_0(\tilde{z},t,\eta) = t^3\tilde{g}(4,\tilde{z},1/2,\alpha\eta\tilde{\beta}) + \frac{2}{\sqrt{\pi}}t^3\sqrt{(\alpha\eta\tilde{\beta})}$$

$$\times\left(g_{7/2}(\tilde{z}) + \frac{2}{3}\alpha\eta\tilde{\beta}g_{5/2}(\tilde{z}e^{-2/5\alpha\eta\tilde{\beta}})\right)$$

$$+ 2\eta^{5/2}t^{7/2}\left(\zeta(3/2)g_3(\tilde{z}) - \frac{1}{2}F(3/2,3/2,3/2,\tilde{z})\right). \tag{73}$$

The scale noninvariant part is due to the quantum corrections and is given by

$$q_2(\tilde{z},t,\eta) = -\frac{1}{8}t\left[\tilde{g}(2,\tilde{z},1/2,\alpha\eta\tilde{\beta}) + \frac{2}{\sqrt{\pi}}\sqrt{(\alpha\eta\tilde{\beta})}\right.$$

$$\times\left(g_{3/2}(\tilde{z}) - \frac{2}{3}\alpha\eta\tilde{\beta}g_{1/2}(\tilde{z}e^{-2/5\alpha\eta\tilde{\beta}})\right)$$

$$+ 2\eta^{5/2}t^{1/2}[\zeta(3/2)g_1(\tilde{z}) - F(1/2,-1/2,5/2,\tilde{z})$$

$$\left. - F(3/2,-1/2,3/2,\tilde{z})]\right], \tag{74}$$

where the new functions and parameters are defined by

$$\tilde{g}(s,x,t,y) = \sum_{i=1}^{\infty}\frac{x^i}{i^s}I(t,iy);$$

$$I(t,y) = \frac{1}{\sqrt{\pi}}\int_0^{\infty}dx\, e^{-x}(x+y)^{(t-1)}, \tag{75}$$

$$F(\alpha',\beta',\gamma',x) = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\frac{x^{(i+j)}}{i^{\alpha'}j^{\beta'}(i+j)^{\gamma'}}, \tag{76}$$

$$\alpha = \frac{1}{2}\left(15\sqrt{\frac{\pi}{2}}N_0/N\right)^{2/5}; \quad t = 1/\tilde{\beta} = kT/(\hbar\omega N^{1/3}). \tag{77}$$

The condensate fraction can now be calculated from the thermodynamic potential as

$$N_0/N = 1 - z\frac{\partial[q(z,T)/N]}{\partial z}. \tag{78}$$

Close to the critical temperature, the condensate fraction goes to zero, i.e., $N_0 \to 0$, and using Eq. (77) we get $\alpha \to 0$. Then the function $\tilde{g}(s,\tilde{z},1/2,\alpha\eta\tilde{\beta})$ can be written as $g_s(\tilde{z})$. Therefore, above the critical temperature the thermodynamic potential of the full system is given by

$$q(z,T)/N = q_0(\tilde{z},t,\eta) + \frac{1}{N^{2/3}}q_2(\tilde{z},t,\eta). \tag{79}$$

Again $q_0(\tilde{z},t,\eta)$ denotes the leading term in the semiclassical expansion, which is given by

$$q_0(z,T) = t^3 g_4(z) + 2\eta^{5/2}t^{7/2}$$

$$\times\left(\zeta(3/2)g_3(\tilde{z}) - \frac{1}{2}F(3/2,3/2,3/2,\tilde{z})\right), \tag{80}$$

and the term $q_2(\tilde{z},t,\eta)$ coming from the second-order quantum correction $[O(\hbar^2)]$ is given by

$$q_2(\tilde{z},t,\eta) = -\frac{1}{8}t\{g_2(\tilde{z}) + 2\eta^{5/2}t^{1/2}[\zeta(3/2)g_1(\tilde{z})$$

$$- F(1/2,-1/2,5/2,\tilde{z}) - F(3/2,-1/2,3/2,\tilde{z})]\}, \tag{81}$$

where $\tilde{z} = ze^{-2u\rho(0)/kT}$. In the noninteracting limit, $\eta = 0$, and Eq. (79) for the thermodynamic potential reduces to the thermodynamic potential of noninteracting Bose gas [Eq. (31)].

For $T < T_c$, $\tilde{z} \approx 1$, then some terms in the series defined in Eqs. (75) and (76) become divergent. To regulate some divergent terms appearing in the $\hbar^2$ corrections, we set $\tilde{z} \approx e^{-\beta\hbar\omega}$, which is the natural energy gap from the ground state [19]. From the above expression we can see that the condensate fraction and other thermodynamic quantities are not fully scale invariant with respect to the dimensionless scaling parameters $\eta$ and $t$. But the extra terms coming from the quantum corrections contain a factor $1/N^{2/3}$. These terms depend on the number of particles in the system, and give finite-size corrections to the scaling form of the thermodynamic quantities. In the large-$N$ limit and also in the high-temperature phase, quantum corrections are negligible. But for small quantum confined systems the corrections to the free energy are finite and non-negligible.

For the physical systems under consideration, the typical value of the parameter $\eta$ that determines the two-body interaction strength varies from 0.1 to 0.25. In recent experiments, the number of trapped atoms is $N \approx 10^4 - 10^5$. We have estimated the quantum corrections of the condensate fraction for such systems, and the order of magnitude of the quantum corrections is $\delta N_0/N \approx 10^{-3}$, which is typically two orders smaller than the leading-order contribution. Our calculation shows that for confined systems containing a large number of atoms ($\approx 10^5$), the LDA is sufficient for the calculation of the thermodynamic properties and the hydrodynamics of the system. But for the systems with a smaller number of atoms, quantum corrections become important and, further, their magnitude depends on the shape of the trap.

## VII. CONCLUSION

To summarize, in this paper, we have developed an extended Thomas-Fermi method at finite temperature for a system of bosons. This is done by introducing a weight function $w_B$ given in Eq. (7), which facilitates the extension of the well known methods for the finite fermion systems to the case of bosons also. Systematic quantum corrections may then be written as a series in powers of $\hbar$, which converges for temperatures larger than the average spacing between energy levels. This method can be applied to calculate the thermodynamic quantities of the noncondensed Bose gas at finite temperature, including the quantum corrections. Yet another difficulty in the systems that show macroscopic occupation of ground state at finite temperature is that the chemical potential of the system tends to zero, i.e., $z \to 1$. As a result, the higher-order terms in $\hbar$ expansion show infrared divergence. To regulate such divergences, fugacity of the system can be replaced by $ze^{-\Delta E/kT}$, where $\Delta E$ is the natural energy gap of finite-size systems [19]. This is equivalent to introducing an infrared momentum cutoff $\approx 1/L$, where $L$ is the system size and does not cause any problem. We have demonstrated the utility of the semiclassical expansion with several applications: We first calculate the quantum correction to a system of spin-1 bosons trapped in a general power-law potential. In general, an exact quantum-mechanical spectrum of such a

system is not known except in special cases, but our method provides a simple way of calculating the quantum corrections systematically. At $T>T_c$, the paramagnetic susceptibility of the gas is obtained including the leading-order quantum correction. Semiclassical expansion is then applied to improve the local-density approximation for a system of charged bosons in a homogeneous magnetic field. Within the simple Thomas-Fermi approximation it is not possible to calculate the susceptibility of the system, because energy and free energy do not depend on the magnetic field. We have calculated the diamagnetic susceptibility of the gas in a normal state and it is shown that only quantum corrections contribute to the susceptibility. This method may also be applied to the interacting Bose system at finite temperature to estimate the effect of interaction on the susceptibility. Lastly, we have used our method to calculate the thermodynamic potential of a system of weakly interacting Bose gas confined in an isotropic harmonic-oscillator potential. The thermodynamic potential and condensate fraction are calculated analytically up to order $\hbar^2$. Leading terms in $\hbar$ are the functions of scaling parameters $t$ (or temperature) and $\eta$ only, but the leading-order quantum corrections give $N$-dependent corrections to the scaling form. In the present situation, quantum corrections are negligibily small when the number of particles is large, of the order of $10^5$. However, quantum corrections may be important for a small number of particles and in low-dimensional systems. Further, its magnitude depends on the nature of the confinement potential.

## ACKNOWLEDGMENTS

[1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Science **269**, 198 (1995).

[2] D.M. Stamper-Kurn, M. R. Andrews, A. P. Chikkartur, S. Inouye, H. J. Miesner, J. Stenger, and W. Ketterle, Phys. Rev. Lett. **80**, 2027 (1998).

[3] J. R. Ensher, D. S. Jin, M. R. Matthews, C. E. Weiman, and E. A. Cornell, Phys. Rev. Lett. **77**, 416 (1996).

[4] M. O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, D. S. Durfee, and W. Ketterle, Phys. Rev. Lett. **77**, 416 (1996).

[5] F. London, Nature (London) **141**, 643 (1938); L. Landau, J. Phys. (Moscow) **5**, 71 (1941).

[6] V. V. Goldman, I. F. Silvera, and A. J. Leggett, Phys. Rev. B **24**, 2870 (1981).

[7] J. Oliva, Phys. Rev. B **39**, 4197 (1989).

[8] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Phys. Rev. Lett. **78**, 3987 (1996).

[9] H. Shi and W. M. Zheng, Phys. Rev. A **56**, 2984 (1997).

[10] H. Haugerud, T. Haugset, and F. Ravndal, Phys. Lett. A **225**, 18 (1997).

[11] E. Wigner, Phys. Rev. **40**, 749 (1932); J. G. Kirkwood, *ibid.* **44**, 31 (1933).

[12] Matthias Brack and Rajat K. Bhaduri, *Semiclassical Physics* (Addison-Wesley, New York, 1997).

[13] R. K. Pathria, *Statistical Mechanics* (Pergamon Press, New York, 1972).

[14] M.V. Simkin and E.G.D. Cohen, e-print cond-mat/9803199.

[15] B.K. Jennings and R.K. Bhaduri, Phys. Rev. B **14**, 1202 (1976).

[16] M. Fliesser, A. Csordas, R. Graham, and P. Szepfalusy, Phys. Rev. A **56**, 4879 (1997).

[17] F. Dalfovo, S. Giorgini, M. Guilleumas, L. Pitaevskii, and S. Stringari, Phys. Rev. A **56**, 3840 (1997).

[18] L. P. Pitaevskii, Zh. Éksp. Teor. Fiz. **40**, 646 (1961) [Sov. Phys. JETP **13**, 451 (1961)]; E. P. Gross, Nuovo Cimento **20**, 454 (1961); J. Math. Phys. **4**, 195 (1963).

[19] R. Masut and W. J. Mullin, Am. J. Phys. **47**, 493 (1979).