

Thermodynamic properties of trapped, two-dimensional interacting Bose gases in Hartree–Fock approximation

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Abstract. We demonstrate the importance of the consistent treatment of mutual interaction between the condensate and the thermal component by applying the semiclassical Hartree–Fock model to the 2D trapped interacting Bose system. In contrast to the case where the interaction from the thermal component is neglected, the present system shows a lowering of the critical temperature and increase of the critical chemical potential due to the short-range repulsive interaction.

Recent experimental observations of Bose–Einstein condensation (BEC) [1, 2] in dilute atomic gases confined in a magnetic trap have created great theoretical interest in weakly interacting Bose gases. At zero temperature the Gross–Pitaevskii (GP) equation [3] provides satisfactory ground state properties of the condensate. For finite temperature the Hartree–Fock–Bogoliubov–Popov (HFBP) theory has been developed to describe the finite-temperature properties of BEC [4,5]. Moreover, since the elementary collective excitations do not contribute significantly to the thermodynamics [6], the HFBP theory has been further simplified to the Hartree–Fock (HF) model where the condensate is described by the GP equation combined with the Thomas–Fermi (TF) approximation, and thermal components are treated as non-interacting bosons in an effective mean potential [7]. Recently, this simple and intuitive two-fluid model has been applied to obtain a semi-analytic expression of 3D BEC by further neglecting atomic interaction from the thermal component [8]. The validity of the two-fluid model has been confirmed by comparisons with the more elaborate self-consistent calculations for the 3D case [9].

All BEC experiments on trapped Bose gases to date have been naturally performed on the 3D system. However, over the last few years, several schemes for the preparation of atomic quasi-2D gases by using various planar waveguides for atoms have been proposed [10]. Theoretical study of the 2D system is also interesting, because even though the 2D homogeneous ideal boson system does not undergo BEC, a number of studies have indicated that it might be possible if a proper confining potential is applied [11–13]. Recently, Bayindir *et al* showed that 2D interacting Bose gases have BEC-like behaviour similar to those of an ideal system for weak interaction by applying a simplified form of the two-fluid model which neglects the interaction from the thermal component [14]. The results of the quantum Monte Carlo (QMC) study by Pearson *et al* [15] also strongly support the idea that there exists BEC in two dimensions for finite N , even though, as pointed out by Krauth [16], the effect of interaction is largely underestimated.

In this paper, we have calculated the analytical results of thermodynamics of 2D interacting Bose gases within the framework of a semiclassical HF model without neglecting the effect of atomic interaction from the thermal component. Our system, which considers mutual interaction between the condensate and the thermal component in a consistent manner, develops realistic thermodynamic behaviours including the lowering of the critical temperature and a corresponding increase of the critical chemical potential. Note that the Bayindir system, which corresponds to the zeroth order of the HF model with respect to $g\rho_1$ in equations (1) and (2), shows no changes in the critical temperature and the critical chemical potential compared with the non-interacting system irrespective of the strength of the interaction [14]. Moreover, we present an analytical form of the critical temperature and corresponding critical chemical potential for small interaction parameter even though $g\rho_1$ is no longer an appropriate perturbation parameter in the case of two dimensions.

In the 2D HF model, the condensate wavefunction ψ_0 has been obtained by the time-independent GP equation as

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{trap}}(r) + g_0^{2\text{D}}(\psi_0^2 + 2\rho_1) \right] \psi_0 = \mu\psi_0$$

where $V_{\text{trap}}(r) = m\omega^2 r^2/2$, $g_0^{2\text{D}}$ represents a short-range repulsive pseudo-potential between atoms in two dimensions, and ρ_1 corresponds to the density of the thermal component. In the large- N limit, the kinetic term of the GP equation can be neglected compared with the self-interaction term $g_0^{2\text{D}}\psi_0^2$ so that the condensate density $\rho_0 = \psi_0^2$ can be obtained as a simple algebraic form. On the other hand, if the thermal component is treated as a semiclassical ideal boson in the effective mean-field potential $V_{\text{trap}}(r) + 2g_0^{2\text{D}}(\psi_0^2 + \rho_1)$, ρ_1 can be expressed as

$$\rho_1(r) = \int \frac{d^2p}{(2\pi\hbar)^2} \frac{1}{e^{(p^2/2m + V_{\text{eff}} - \mu)/k_B T}}.$$

After some straightforward calculations, the above equations can be transformed to the following coupled equations:

$$\rho_0 = \frac{1}{g}(\mu - t^2/2 - 2g\rho_1)\theta(\mu - t^2/2 - 2g\rho_1), \quad (1)$$

$$\rho_1 = \frac{1}{\lambda_{T'}^2} g_1(e^{(\mu - t^2/2 - 2g(\rho_0 + \rho_1))/T'}) \quad (2)$$

where $\theta(x)$ is a Heaviside step function. In the derivation of equations (1) and (2) we used the critical temperature of an ideal boson confined in the harmonic potential $k_B T_0^{2\text{D}} = \hbar\omega[N/\zeta(2)]^{1/2} = \hbar\omega\lambda^2$, $\zeta(n)$ being the Riemann zeta function, and the harmonic oscillator length $l = \sqrt{\hbar/m\omega}$ as natural scaling parameter. Then the length, temperature, and interaction parameter are also scaled as $t = r/l\lambda$, $T' = T/T_0^{2\text{D}}$, and $g = mg_0^{2\text{D}}/\hbar^2$, respectively. The densities of the condensate and thermal component ρ_0 and ρ_1 are scaled with respect to λ^2/l^2 . Finally, $\lambda_{T'}$ is the scaled thermal wavelength $\lambda_{T'} = \sqrt{2\pi/T'}$, and g_1 is the Bose function defined as $g_n(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^n}$. The scaled chemical potential $\mu = \mu/k_B T_0^{2\text{D}}$ is determined by the constraint of a total number of particles as

$$\zeta(2) = \int d^2t [\rho_0 + \rho_1] = N_0 + N_1^{\text{BEC}}. \quad (3)$$

It should be noted that equations (1)–(3) are independent of the total number of particles N by scaling if $g_0^{2\text{D}}$ does not depend on N , in contrast to the 3D case where the scaled interaction parameter g has N -dependence as $g = 4\pi a/l [N/\zeta(3)]^{1/6}$ by scaling with respect to $k_B T_0^{3\text{D}}$ and l for $g_0^{3\text{D}} = 4\pi\hbar^2 a/M$, a being the s-wave scattering length [17]. The explicit form of $g_0^{2\text{D}}$ has not been obtained yet. The experiment of 2D BEC can be realized on the quasi-2D trap

by suppressing the excitation in the z -direction of the 3D trap using the optical dipole trap or highly anisotropic magnetic trap ($\omega_x = \omega_y \ll \omega_z$). In this situation, g_0^{2D} is influenced by the length scale of confinement in the z -direction since this length scale becomes comparable to the s -wave scattering length a . In this work we consider g as a small parameter which covers the finite-size effect of the quasi-2D trap as well as the atomic interaction.

To solve the coupled equations (1)–(3), let us introduce a new variable α , which may be termed the local effective chemical potential, as

$$\begin{aligned}\alpha &= \mu - t^2/2 - 2g(\rho_0 + \rho_1) \\ &= -|\mu - t^2/2 - 2gf(\alpha)|\end{aligned}\quad (4)$$

where $f(\alpha) = T'/2\pi g_1[e^{\alpha/T'}] = -T'/2\pi \ln(1 - e^{\alpha/T'})$. Then $\rho_0 = -(\alpha/g)\theta(\mu - t^2/2 - 2gf(\alpha))$ and $\rho_1 = f(\alpha)$. Note that α is always less than zero and $0 < f(\alpha) < \infty$. This guarantees that there is at least one intersection point α_s satisfying equation (4) for the whole range of t ($t \geq 0$). The solutions can be classified into two cases depending on whether the tangent point α^* exists between $y = \alpha$ and $y = -|\mu - t^2/2 - 2gf(\alpha)|$ for a given point t^* ($t^* > 0$) or not. We first consider the case where there is a tangent point α^* for a given t^* . The condition to have a tangent point is $2gf'(\alpha^*) = 1$ from equation (4), where $f'(\alpha) = df/d\alpha$. This gives $\alpha^* = -T' \ln(1 + g/\pi)$ and a corresponding t^* becomes $\sqrt{2(\mu - \mu_c^{2D})}$, μ_c^{2D} being $2gf(\alpha^*) - \alpha^*$. Then, from the graph of equation (4), the solution α_s is determined, depending on the range of t , as

$$\alpha_s = \begin{cases} -\mu + t^2/2 + 2gf(\alpha_s), & t < t^*; \quad \rho_0 \neq 0 \\ \mu - t^2/2 - 2gf(\alpha_s), & t > t^*; \quad \rho_0 = 0. \end{cases}\quad (5)$$

Therefore, t^* corresponds to the boundary between the condensate and the thermal component. At $t = t^*$, α_s has a jump discontinuity since $\alpha_s(t^{*-}) \neq \alpha_s(t^{*+})$. So we define $\alpha_s(t^{*+}) = \alpha_m$ as $\alpha_m = \mu_c^{2D} - 2gf(\alpha_m)$. In fact, μ_c^{2D} is the critical chemical potential where the condensate begins to disappear in the centre of trap. If $\mu < \mu_c^{2D}$, t^* cannot be defined, and therefore the condensate does not exist. Next, we consider the case where α^* does not exist. In this case, α_s is determined uniquely from $\alpha_s = \mu - t^2/2 - 2gf(\alpha_s)$. As t increases from zero, α_s decreases monotonically. In this case $\rho_0 = 0$ for the whole range of t . Summarizing all these results, ρ_0 and ρ_1 can be expressed by α as

$$\begin{aligned}\rho_0 &= -\frac{\alpha}{g}\theta(t^* - t), \\ \rho_1 &= \frac{1}{2g}(\mu - t^2/2 + \alpha)\theta(t^* - t) + \frac{1}{2g}(\mu - t^2/2 - \alpha)\theta(t - t^*).\end{aligned}$$

The gap of density profile at the boundary $t = t^*$, $\Delta\rho$, defined as $\rho(t^{*-}) - \rho(t^{*+})$, is $(\alpha_m - \alpha^*)/2g$. If equations (1) and (2) are expanded in a series with respect to the perturbation parameter $g\rho_1$, the zeroth order corresponds to the Bayindir model. But $g\rho_1$ is no longer the appropriate perturbation parameter for two dimensions, since the zeroth-order $\rho_1 = 1/\lambda_{T'}^2 g_1[e^{-|\mu - t^2/2|}]$ is divergent at the boundary $t^* = \sqrt{2\mu}$. Notice that $g\rho_1$ is small and uniformly bounded for the whole range of t for three dimensions, so that the first-order correction is accurate enough for small g compared with the full numerical calculation [7].

To determine μ for a given g and T' , we first calculate the number of particles in the condensate, N_0 , and that in the thermal component, N_1^{BEC} , respectively. For this purpose, the integration with respect to t in equation (3) is transformed into one with respect to α using $d\alpha/dt$. From equation (5) $d\alpha/dt$ can be uniquely defined as

$$\frac{d\alpha}{dt} = \begin{cases} t/(1 - 2gf'(\alpha)), & t < t^* \\ -t/(1 + 2gf'(\alpha)), & t > t^*. \end{cases}\quad (6)$$

Then the number of atoms in the condensate N_0 is

$$N_0 = -\frac{2\pi}{g} \int_{\alpha_0}^{\alpha^*} [1 - 2gf'(\alpha)]\alpha d\alpha \\ = \frac{\pi}{g} [\alpha_0^2 - \alpha^{*2}] + 2T'[\alpha^*g_1(\alpha^*) - \alpha_0g_1(\alpha_0)] - 2T'^2[g_2(\alpha^*) - g_2(\alpha_0)] \quad (7)$$

where $g_n(\alpha) = g_n(e^{\alpha/T'})$, and α_0 means the value of α at $t = 0$ determined from $\alpha_0 = -\mu + 2gf(\alpha_0)$. Here we have used the simple relation $dg_n(\alpha)/d\alpha = 1/T'g_{n-1}(\alpha)$. The number of atoms in the thermal component N_1^{BEC} becomes

$$N_1^{\text{BEC}} = T'^2 \left[g_2(\alpha^*) + g_2(\alpha_m) - g_2(\alpha_0) + \frac{g}{2\pi} \{g_1^2(\alpha_0) + g_1^2(\alpha_m) - g_1^2(\alpha^*)\} \right]. \quad (8)$$

Note that N_0 and N_1^{BEC} are expressed as functions of α^* , α_m , and α_0 only. α^* and α_m are fixed values independent of μ , and α_0 is the one to be calculated for a trial μ . If the temperature of the system is above the critical temperature, only the thermal component exists. So $N_0 = 0$ and, in this case, N_1^{th} can be obtained straightforwardly as

$$N_1^{\text{th}} = T'^2 [g_2(\alpha_0) + g/2\pi g_1^2(\alpha_0)] \quad (9)$$

where $\alpha_0 = \mu - 2gf(\alpha_0)$. Therefore, we have to solve different sets of equations to determine μ , depending on whether the system is below the critical temperature or not.

The critical temperature for a given g can be determined by considering the critical chemical potential μ_c^{2D} . For $\mu < \mu_c^{2D}$ there is no condensate. Therefore a saturation of the thermal component occurs when $N_1^{\text{th}}(\alpha_0^c) = \alpha_0^c$ being determined from $\alpha_0^c = \mu_c^{2D} - 2gf(\alpha_0^c)$, since N_1^{th} increases monotonically as μ increases. Then the critical temperature is given from the condition $N_1^{\text{th}}(\alpha_0^c) = \zeta(2)$ as

$$T_c = T_0^{2D} \left(\zeta(2) / \left[\sum_{j=1}^{\infty} e^{jx_c} / j^2 + g/2\pi \{ \ln(1 - e^{x_c}) \}^2 \right] \right)^{1/2} \quad (10)$$

where $x_c - g/\pi \ln(1 - e^{x_c}) = g/\pi \ln(1 + \pi/g) + \ln(1 + g/\pi)$, x_c being α_0^c/T' . It should be noted that α_0^c/T' is fixed for a given g independent of T' . For small g , considering a lowest-order correction of μ_c^{2D} and T_c with respect to g , we have

$$\mu_c^{2D} = gT'/\pi \ln(g/\pi) - gT'/\pi \\ T_c = T_0^{2D} \left[1 - \frac{g}{4\pi\zeta(2)} (\ln |gy_c/\pi|)^2 + \frac{gy_c}{2\pi\zeta(2)} (\ln |gy_c/\pi| - 1) \right]$$

where the non-algebraic form of μ_c^{2D} and T_c emphasize that a straightforward perturbation with respect to $g\rho_1$ cannot work for two dimensions. Here x_c becomes gy_c/π for small g , where $y_c = -0.278$ is determined from $y_c = 1 + \ln(-y_c)$. On the other hand, if we consider only the thermal component from the start, we cannot find the critical point until the temperature approaches zero since $N_1^{\text{th}}(\alpha_0) = \zeta(2)$ can be always satisfied with a suitable μ due to the divergence of the second term in equation (9). If the interaction from the thermal component is neglected, equations (7)–(9) become reduced as $N_0 = \pi\mu^2/g$, $N_1^{\text{BEC}} = T'^2[2\zeta(2) - g_2(-\mu)]$, and $N_1^{\text{th}} = T'^2g_2(\mu)$. In this case, substituting the critical chemical potential $\mu_c^{2D} = 0$ into N_1^{th} , we always have the same critical temperature T_0^{2D} as with the ideal case irrespective of the strength of the interaction. In figure 1 we plot the condensate fraction N_0/N with respect to T' for $g = 0.001$ and 0.1 . It shows that the critical temperature T_c decreases and the condensate fraction becomes reduced as g increases compared with the non-interacting case due to the repulsive nature of the interaction. Note that, as T approaches T_c , the thermal atoms become dominant, and the depletion of the condensate is more significant in the HF model than in the

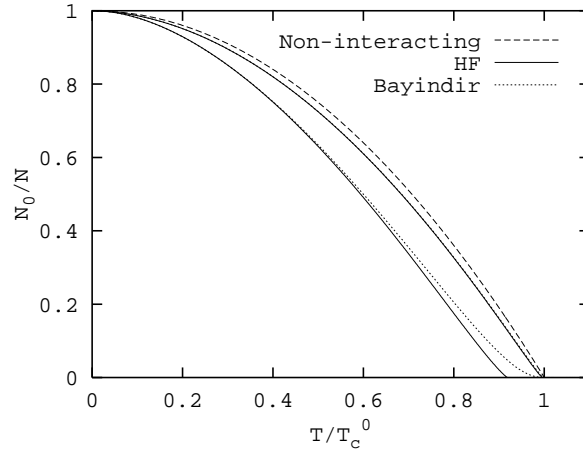


Figure 1. The condensate fraction N_0/N as a function of temperature for $g = 0.001$ and $g = 0.1$.

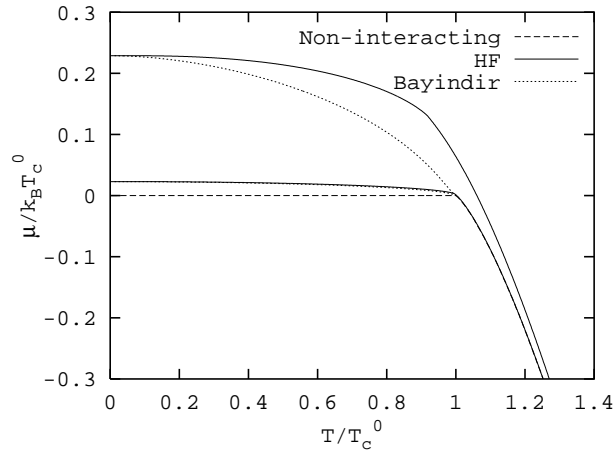


Figure 2. The scaled chemical potential μ as a function of temperature for $g = 0.001$ and $g = 0.1$.

Bayindir model because of the interaction between the condensate and the thermal component. The behaviour of μ with respect to temperature for given g is plotted in figure 2. It shows that μ_c^{2D} in the HF model increases from zero as g increases. The results of QMC calculation by Pearson *et al* [15] also show that the transition temperature decreases as the hard core radius increases even though the effects of interaction were underestimated in their results [16].

The internal energy defined as $E = (E_{th}(N - N_0)/2 + E_c)/N$, consists of the contribution from the thermal component E_{th} and that from the condensate component E_c . E_{th} is further divided into kinetic energy K_{th} and effective potential energy V_{th} , respectively. By applying equation (6), K_{th} is given by

$$K_{th} = \hbar\omega\lambda^6 T'^3 \left[g_3(\alpha^*) + g_3(\alpha_m) - g_3(\alpha_0) + \frac{g}{\pi} \{g_1(\alpha_m)g_2(\alpha_m) + g_1(\alpha_0)g_2(\alpha_0) - g_1(\alpha^*)g_2(\alpha^*)\} - \frac{g}{\pi T'} \left\{ \int_{\alpha^*}^{\alpha_m} g_1^2(\alpha) d\alpha + \int_{-\infty}^{\alpha_0} g_1^2(\alpha) d\alpha \right\} \right], \quad (11)$$

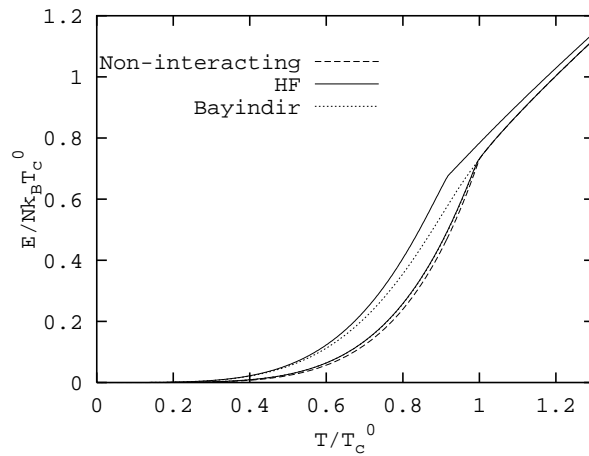


Figure 3. The ground state energy E as a function of temperature for $g = 0.001$ and $g = 0.1$.

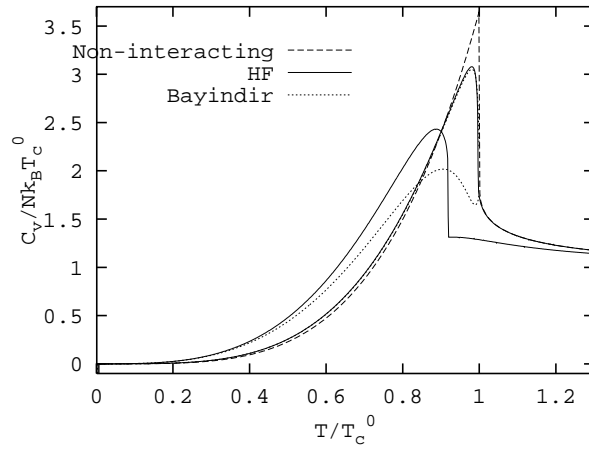


Figure 4. The specific heat $C_v = dE/dT'$ as a function of temperature for $g = 0.001$ and $g = 0.1$.

and V_{th} becomes

$$V_{th} = \hbar\omega\lambda^6 T'^2 \left[\mu \{g_2(\alpha_m) + g_2(\alpha^*) - g_2(\alpha_0)\} + \{F_1(\alpha_0) - F_1(\alpha^*) - F_1(\alpha_m)\} + \frac{g\mu}{\pi} \{F_2(\alpha_m) - F_2(\alpha^*) + F_2(\alpha_0)\} + \frac{g}{\pi} \{F_3(\alpha^*) - F_3(\alpha_0) - F_3(\alpha_m)\} \right] \quad (12)$$

where

$$F_1(\alpha) = \alpha g_2(\alpha) - T' g_3(\alpha), \quad F_2(\alpha) = g_1^2(\alpha)/2$$

$$F_3(\alpha) = \alpha g_1^2(\alpha)/2 - \frac{1}{2} \int_{-\infty}^{\alpha} g_1^2(\alpha) d\alpha.$$

On the other hand E_c is given by

$$E_c = \hbar\omega\lambda^6 \frac{\pi}{g} \left[\frac{1}{3} (\alpha^{*3} - \alpha_0^3) - \frac{gT'}{\pi} \{ \alpha^{*2} g_1(\alpha^*) - \alpha_0^2 g_1(\alpha_0) \} \right]$$

$$\left. + \frac{2gT'^2}{\pi} \{\alpha^* g_2(\alpha^*) - \alpha_0 g_2(\alpha_0)\} - \frac{2gT'^3}{\pi} \{g_3(\alpha^*) - g_3(\alpha_0)\} \right] \quad (13)$$

since the kinetic energy of the condensate is ignored due to the TF approximation. If we neglect the interaction from the thermal component, E_c and E_{th} become, respectively,

$$E_c^0 = \hbar\omega \frac{\pi}{3g} \left(\frac{\mu}{\hbar\omega} \right)^3$$

$$E_{th}^0 = \hbar\omega \lambda^6 [4T'^3 \zeta(3) - 2T'^3 g_3(-\mu) + 2\mu T'^2 \xi(2) - 2\mu T'^2 g_2(-\mu)],$$

which are identical to the results of Bayindir and Tanatar [14]. The behaviour of the internal energy as a function of temperature is plotted in figure 3, which shows that the internal energy increases as g increases due to the repulsive interaction. In figure 4 we also plot the specific heat $C_v = dE/dT'$ versus T' . For nonzero g , figure 4 shows the smoothing of a sharp peak and a significant reduction of the increase in the specific heat with respect to the non-interacting case across the critical temperature. Notice the unrealistic oscillation of the specific heat in the Bayindir model for $g = 0.1$. The deviation of the Bayindir model from the fully interacting HF model diminishes as g decreases or T goes to zero since the effect of the thermal component vanishes.

In summary, we have applied the semiclassical HF model to the 2D trapped interacting Bose gases and calculated the thermodynamic properties of the system for various interaction strengths. By considering the mutual interaction between the condensate and the thermal component in a consistent manner, we observe the lowering of the critical temperature and the condensate fraction compared with the ideal case, and the smoothing of the specific heat across the critical temperature.

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