The effect of interactions on Bose-Einstein condensation in a quasi two-dimensional harmonic trap

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A dilute bose gas in a quasi two-dimensional harmonic trap and interacting with a repulsive two-body zero-range potential of fixed coupling constant is considered. Using the Thomas-Fermi method, it is shown to remain in the same uncondensed phase as the temperature is lowered. Its density profile and energy are identical to that of an ideal gas obeying the fractional exclusion statistics of Haldane.

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I. INTRODUCTION

The quantum and thermodynamic properties of atom traps with reduced dimensionality have been studied by several groups [1–4]. In a recent review Dalfovo et al. [5] note that the phase transition of bosons in quasi two-dimensional atom traps is an important issue for future investigations. In this paper, we consider bosons which are trapped in a two-dimensional harmonic oscillator and interact by a repulsive zero-range pair potential of a fixed strength. Using the finite-temperature Thomas-Fermi (TF) method, we find that there is no strict phase-transition for such a system, no matter how weak the repulsion. As the temperature is lowered, the chemical potential rises smoothly, and only at zero temperature does it match the lowest energy level of the trap. By analyzing the equation of state of the interacting bose system in the complex fugacity plane, we show that the system remains in a single phase at all (real) temperatures. We demonstrate that the area integral of the interaction potential in two dimensions is related to the statistical parameter of Haldane’s fractional exclusion statistics (FES) [6]. In particular, the thermodynamic properties of the bose system interacting with a zero-range repulsive potential are found to be of the same form as that of an ideal FES gas.

Consider bosons in an oblate three-dimensional trap with the oscillator frequencies $\omega_x = \omega_y = \omega \ll \omega_z$. For a dilute Bose gas at low temperatures we take the usual three-dimensional delta function pseudo-potential \textsuperscript{[4,8]} with strength $(4\pi\hbar^2a/m)$, where $a$ is the s-wave scattering length, and which in first-order Born-approximation yields the correct low-energy quantum scattering result. For low enough temperatures, and assuming that the expectation value of the pseudo-potential is much smaller than $\hbar\omega_z$, we may restrict the Hilbert space in the $z$-direction by setting the oscillator quantum number $n_z = 0$. The quantum dynamics is then determined by an effectively two-dimensional Hamiltonian, given by
\[ H = \sum_{i=1}^{N} \left( \frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 r_i^2 \right) + \frac{2\pi \hbar^2}{m} g \sum_{i<j}^{N} \delta(r_i - r_j), \]  

where the momenta and coordinates are planar vectors. Such a Hamiltonian has been studied recently by several groups \[1,4,11\], and also by Mullin \[11,12\]. The dimensionless coupling constant \( g \) in the two-dimensional delta function interaction may be related to the scattering length \( a \) for \( s \)-wave scattering in three dimensions. This is done by taking the expectation value of the three-dimensional delta function with respect to the harmonic oscillator one-dimensional ground state wave function with \( n_z = 0 \). We then obtain the effective two-dimensional interaction given in Eq. (4), with the dimensionless coupling constant

\[ g = \sqrt{\frac{2}{\pi}} \left( \frac{a}{b_z} \right). \]  

Here \( b_z = \sqrt{\hbar/m\omega_z} \) is the length scale of confinement in the \( z \)-direction. This quasi two-dimensional description of the actual three-dimensional trap is valid only for a dilute system in which the scattering length \( a \ll b_z \ll b \) \[11\], where \( b = \sqrt{\hbar/m\omega} \) is the oscillator length scale in the \( x-y \) plane. It follows from Eq. (2), therefore, that \( g \ll 1 \) in Eq. (4). For an estimate of the parameter \( g \), take \( b = 3 \) micron, which corresponds to \( h\omega \approx 0.6 \) nK. An ideal gas in a two-dimensional harmonic trap would have BEC at the critical temperature \( T_c^0 = (6/\pi^2)^{1/2} N^{1/2} h\omega \). Taking \( N = 10^4 \) Rb\(^{87} \) atoms, this corresponds to \( T_c^0 \approx 48 \) nK. We must have \( \hbar\omega_z \gg k_B T_c^0 \) for the device to be effectively two-dimensional. Assuming \( \omega_z \approx 10^3 \omega \), and the scattering length \( a \) for Rb\(^{87} \) atoms to be 5.8 nm \[13\], the estimate of the interaction strength \( g \) from Eq. (2) is about 0.05. Thus the model Hamiltonian (2) is realizable experimentally for small \( g \), although we shall also present the results for \( g = 1 \) to see how the quantum statistics is altered. We emphasize that the two-dimensional delta function interaction in Eq. (2) is a dimensionally reduced form of the three-dimensional pseudo-potential, and is not to be regarded as a pseudo-potential derived from two-dimensional scattering theory. Later, we shall need to take the thermodynamic limit of this quasi two-dimensional system to investigate the question of strict phase transition. This is done by keeping \( \omega_z \) at a fixed appropriate value and letting \( N \to \infty, \omega \to 0 \), keeping \( N^{2}\omega \) constant. Note, however, that in the alternative scheme of keeping the ratio \( \omega_z/\omega \) fixed at a large value, and then taking the thermodynamic limit, would result in a three-dimensional geometry. This is because the condition \( \hbar\omega_z \gg k_B T_c^0 \) would not be satisfied. We now proceed to do a Thomas-Fermi calculation for this two-dimensional system.

II. THOMAS-FERMI CALCULATION

In BEC, it is customary to write the density of bosons to be \( n(r) = n_0(r) + n_T(r) \), where \( n_0 \) is the condensate density, and \( n_T \) the density of particles occupying states other than the ground state \[3\]. Consider temperatures above the critical \( T_c \) of the interacting system. Then there is no condensate, and \( n(r) = n_T(r) \). In this situation, the one-body potential generated by the above zero-range interaction is \( U(n(r)) = \frac{2\pi \hbar^2}{m} gn(r) \). Note that for \( T > T_c \), the more sophisticated Popov approximation \[14\] also reduces to the TF approximation:

\[ n(r) = \int \frac{d^2p/(2\pi\hbar)^2}{\exp[(\frac{p^2}{2m} + \frac{1}{2} m \omega^2 r^2 + \frac{2\pi \hbar^2}{m} gn(r) - \mu)\beta] - 1}. \]  

(3)
After performing the $p$-integration analytically, the number-density of particles ($\beta = 1/(k_B T)$) is given by

$$Z e^{-\beta \omega^2 r^2 / 2} = 2 e^{\alpha u} \sinh \frac{u}{2},$$  \hspace{1cm} (4)

where we have put $u(r) = 2\pi\hbar^2 n(r) \beta / m$, the fugacity $Z = \exp(\beta \mu)$, and $\alpha = (g - 1/2)$. The number of atoms in the trap is given by

$$N = \frac{m}{2\pi\hbar^2 \beta} \int u(r) d^2 r.$$  \hspace{1cm} (5)

To obtain $n(r)$ for a fixed $N$, Eqs. (4) and (5) have to be solved self-consistently. For $g = 0$, these cannot be satisfied for $T < T^0_c$, and the occupancy of the lowest quantum state (in this approximation at zero energy) has to be taken into account explicitly. This means that the condensate density $n_0$ occupying the lowest level is macroscopic below $T < T^0_c$. In Fig. 1, we show how this results in a discontinuity in $\mu$ at $T^0_c$ for $g = 0$. (In numerical work throughout, we use arbitrary units [a.u.] with $\hbar = m = 1$ and set $N = \omega = 1$.)

**FIG. 1.** Chemical potential $\mu$ versus temperature $T/T^0_c$. Self-consistent solutions of the temperature-dependent TF equations (4,5) are obtained for various values of the interaction strength $g$.

For a nonzero positive $g$, Eqs. (4) and (5) can be self-consistently solved right down to $T = 0$ (see Fig. 1). This contradicts Mullin’s claim [12] that there is no self-consistent solution of the TF equations below a nonzero $T_c$. Note that the $T \to 0$ limit of Eq. (4) yields a nonzero spatial density only within the classical turning point $r_0$:

$$n_0(r) = \frac{m}{2\pi\hbar^2 g} \left( \mu - \frac{1}{2} m \omega^2 r^2 \right), \quad r \leq r_0,$$  \hspace{1cm} (6)

where $r_0 = \sqrt{\frac{2\mu}{m \omega^2}}$. This gives $N = \mu^2 / 2g(\hbar \omega)^2$, so that the chemical potential at zero temperature is given by $\mu(T = 0) = \sqrt{2g} N^{1/2} \hbar \omega$. Thus, the self-consistent solution has
led to the $T \to 0$ TF result (Eq. (5)) for $n_0$ that one would obtain starting from the Gross-Pitaevskii density functional [3]. In passing we note that the zero-temperature density for a spin-less free Fermi gas in a two-dimensional harmonic potential is also given by Eq. (5), with the proviso that the occupancy of each quantum state is $1/g$ instead of unity. Indeed, even though it is not experimentally feasible to extrapolate $g$ to unity, it is amusing to note that putting $g = 1$ in Eq. (4) would yield exactly the finite temperature noninteracting fermionic result

$$n(r) = \frac{m}{2\pi \hbar^2 \beta} \ln \left(1 + \exp\left(\mu - \frac{1}{2}m\omega^2 r^2\beta\right)\right).$$

(7)

These results are not accidental, and their significance (specially for small $g$) will presently be discussed. It is also worth noting that the plots in our Fig. 1 are very similar to those of Fig. 2 for a noninteracting Haldane gas in Ref. [15].

It is important to note that the situation is very different for an interacting gas in a three-dimensional trap, where the TF equation analogous to Eq. (3) has no self-consistent solution for $T < T_c$. One then has to solve the Bogoliubov equations self-consistently, say in the Popov approximation [5]. For $T > T_c$, this procedure reduces to solving the temperature-dependent TF equation. Qualitatively, the calculated curves of $\mu$ vs $T$ for the three-dimensional trap (shown in Fig. 26 of [3]) look similar to our Fig. 1. This is somewhat deceptive, since the curves in our Fig. 1 are obtained in the TF approximation for all $T$, whereas the Popov approximation is used for $T < T_c$ in the three-dimensional case. The behavior of the so-called “release energy”, which is the total minus the harmonic oscillator energy, has a very interesting structure below and at $T_c$ in the three-dimensional case.

![FIG. 2. Release energy versus temperature $T/T_c^o$ from the self-consistent solution of the temperature-dependent TF equation. For comparison, the noninteracting $g = 0$ case is also shown.](image-url)
This is also confirmed experimentally by Ensher et al. [16] for Rb atoms, who find a discontinuous behavior of the deduced specific heat. By contrast, as is shown in Fig. 2 for the two-dimensional problem, no such structure is found for nonzero \( g \) in the calculated release energy. Experimentally, in three-dimensional traps, the appearance of a condensate is manifested as a sharp peak in the spatial density profile of the gas [17]. For the interacting two-dimensional gas, as shown in Fig. 3, the central density rises gradually rather than abruptly with the lowering of temperature. (This, however, may be a limitation of the TF model, see [2].)

\[\begin{align*}
\text{FIG. 3.} & \quad \text{Self-consistent TF density distribution, with unit normalization, as a function of the radial distance } r \text{ for temperatures above and below } T_c. \text{ The noninteracting } g = 0 \text{ case is shown for comparison.}
\end{align*}\]

We now show analytically, starting from Eqs. (4,5), that for \( g > 0 \) there can be no phase transition. Formally, these equations bear a striking similarity with Eqs. (29,30) of Sutherland’s classic paper [18] on the thermodynamics of the Calogero-Sutherland model (CSM) [19]. We exploit this for our proof, going to the thermodynamic limit \( N \to \infty, \omega \to 0 \), with \( N^{1/2} \omega = 1 \). In this limit, the \( r \)-dependence in Eq. (4) drops out, and we get

\[
Z = \left[ \exp(\mu) - \exp((\mu - 1)\omega) \right].
\]

From this, we see that for \( g = 0, \mu = -\ln(1 - Z) \), so \( u \) has a branch-point at \( Z = 1 \), i.e., at \( \mu = 0 \). This is where BEC takes place for the ideal Bose gas. For \( g = 1 \), on the other hand, Eq. (8) gives \( u = \ln(1 + Z) \), with a branch point at \( Z = -1 \). Similarly, for \( g = 1/2 \), it is easily checked that \( u \) has branch points at \( Z = \pm 2i \). More generally, the location of the branch points of \( u \) (which is proportional to the spatial density) in the complex \( Z \)-plane as a function of \( g \) are shown in Fig. 4, which is identical to Sutherland’s Fig. 1 for CSM in [18]. The only singularity on the positive real axis is at \( g = 0 \), and for \( g > 0 \) there is no phase transition.
III. EQUIVALENCE TO FRACTIONAL EXCLUSION STATISTICS

The two-dimensional delta function interaction considered in Eq. (1) is very special in the sense that it is scale-independent [9]. A two-body potential that varies as the inverse square of the distance between the two particles also shares this property. In one dimension, the latter is the much-studied exactly solvable $N$-particle CSM, which is known to obey [20–22] Haldane’s fractional exclusion statistics (FES). By this we mean that either one can solve the $N$-body interacting bosonic or fermionic problem with the pair-wise inverse square interaction, or map it onto a noninteracting set of $N$-particles obeying FES. The statistical occupancy factor for an ideal FES gas is given by [22,23] $\eta_i = (w_i + g)^{1-g}$, where

$$w_i^g(1 + w_i)^{1-g} = \exp[(\epsilon_i - \mu)\beta].$$  \hfill (9)

We note that FES is characterized by a “statistical factor” $g$, which will presently be identified with the dimensionless interaction strength of the delta function interaction in Eq. (1). The occupancy factor in FES reduces to the usual bosonic or the fermionic one for $g = 0$ or 1, respectively.

In order to demonstrate explicitly the equivalence between our two-dimensional interacting boson model and FES, let us consider the analogue of Eq. (3) for the number density of a gas of non-interacting “haldons”,

$$n(r) = \int \frac{d^2p/(2\pi\hbar)^2}{w + g}.$$  \hfill (10)

where $w$ depends on $p$ via Eq. (3). The number density can be rewritten as an integral over $w$ by noting that Eq. (3) gives $[g/w + (1-g)/(1+w)]dw = (\beta/2\pi m)d^2p$, so that

$$n(r) = \frac{m}{2\pi\hbar^2\beta} \int_{w_0}^{\infty} \frac{dw}{w(1 + w)} = \frac{m}{2\pi\hbar^2\beta} \ln \frac{1 + w_0}{w_0},$$  \hfill (11)
with \( w_0 \equiv w(p = 0) \) given by

\[
w_0^g (1 + w_0)^{1-g} = Z^{-1} e^{\beta m \omega^2 r^2/2}.
\] (12)

Eliminating \( w_0 \) from Eqs. (11) and (12) just gives Eq. (4), which shows that the number densities of the two models are the same. We proceed to prove that the same is the case for the energy density, which for the FES gas is given by

\[
E(r) = \frac{m^2 \pi \hbar^2}{2 \beta^2} \int_{w_0}^\infty \frac{dw}{w(1+w)} \left[ g \ln \frac{w}{1+w} + \ln(1+w) + \beta \mu \right].
\] (13)

Changing variables from \( p \) to \( w \) as above and using Eq. (9) to substitute

\[
\beta \left[ \frac{p^2}{2m} + m \omega^2 r^2 / 2 \right] = \beta \mu + g \ln w + (1 - g) \ln(1 + w),
\] (14)

the energy density takes the form

\[
E(r) = \frac{\pi \hbar^2 g}{m} \left( n(r) \right)^2 = \frac{m}{2 \pi \hbar^2 \beta^2} \int_{w_0}^\infty \frac{dw}{w(1+w)} \left[ y + \ln(1+w) + \beta \mu \right].
\] (15)

The first term of the integrand is a total derivative, giving a contribution

\[
(-mg/4\pi \hbar^2 \beta^2) \left( \ln \frac{w_0}{1+w_0} \right)^2 = (-\pi \hbar^2 g/m) \left( n(r) \right)^2 = -\frac{g}{2 \beta^2} \int_{w_0}^\infty \frac{dw}{w(1+w)} \left( n(r) \right)^2
\] (16)

to the energy density. With the variable substitution \( w = w_0 + (1 + w_0)(\exp(y) - 1) \), the remainder of the integral (15) takes the form

\[
E(r) + \frac{\pi \hbar^2 g}{m} \left( n(r) \right)^2 = \frac{m}{2 \pi \hbar^2 \beta^2} \int_0^\infty \frac{dy}{(1+w_0) e^y - 1} \left[ y + \ln(1+w_0) + \beta \mu \right].
\] (17)

Here, \( w_0 \) can be eliminated by using the relation

\[
1 + w_0 = \exp \left\{ \beta \left[ m \omega^2 r^2 / 2 + (2\pi \hbar^2 g/m) n(r) - \mu \right] \right\},
\] (18)

which is found by combining Eqs. (11) and (4). Further identifying \( y = \beta p^2 / 2m \) and collecting all terms, we find the final form of the energy density integral,

\[
E(r) = \int \frac{d^2p/(2\pi \hbar)^2 \left[ \frac{p^2}{2m} + \frac{1}{2} m \omega^2 r^2 + \frac{\pi \hbar^2}{m} g n(r) \right]}{\left[ \exp \left\{ (\frac{p^2}{2m} + \frac{1}{2} m \omega^2 r^2 + \frac{\pi \hbar^2}{m} g n(r) - \mu) / \beta \right\} - 1 \right]}.
\] (19)

But this is just the energy density of the interacting boson gas. Note that Eq. (18) brings in a term \( \sim g n(r) \) on the right-hand side of Eq. (17), which combines with the one in Eq. (16) to give the correct coefficient \( \pi \hbar^2 g/m \) in Eq. (19). Thus, we have demonstrated that the interacting bosons may be mapped on to noninteracting particles obeying FES. Although above we have assumed a harmonic trap, note that our proof holds for any shape of the confining trap potential.

For a dilute gas in the thermodynamic limit obeying FES in a \( D \)-dimensional system, the statistical factor \( g \) may be related \([24,25]\) to the high-temperature limit of the second virial coefficient \( B_2 \) \([26]\):
\[ g - \frac{1}{2} = 2^{D/2}B_2 . \]  

(20)

For the parameter \( g \) from Eq. (20) to be meaningful, it should be temperature-independent. This is possible if the interaction potential is scale-independent. This requirement is satisfied by an inverse-square potential in any dimension. In one dimension, the corresponding potential is the CSM mentioned before. Interestingly, the two-dimensional case is very special, since in this case the area-integral of any potential, when it exists, turns out to be proportional to the statistical parameter. To see this, consider, for \( (D = 2) \), the \( \beta \rightarrow 0 \) limit of \( B_2 \) given in [26]:

\[ B_2 = \frac{m}{4\pi\hbar^2}M_0 \pm \frac{1}{4} , \]  

(21)

where \( M_0 = \int d^2rV(r) \). We have assumed that the potential \( V \) is well-behaved, so that the expansion \( \exp(-\beta V) = [1 - \beta V + (\beta V)^2/2 - ...] \) is valid. Terms containing \( \int d^2rV^n \) for \( n \geq 2 \) do not contribute in the high-temperature limit, since \( \beta^{(n-1)} \rightarrow 0 \). Considering bosons in \( D = 2 \), Eq. (20) gives \( M_0 = (2\pi\hbar^2/m)g \). The zero-range effective potential in Eq. (1) has precisely this moment \( M_0 \), and its strength \( g \) is thus the statistical parameter for Haldane statistics.

**IV. DISCUSSION**

In summary, we have shown, using the Thomas-Fermi method, that the effect of a repulsive zero-range interaction between the atoms in the “two-dimensional” trap is more drastic than the corresponding three-dimensional case. Even in the thermodynamic limit, there is no strict phase transition with a repulsive zero-range two-body interaction, as shown by the behavior of the spatial density in the complex \( Z \)-plane. We have also demonstrated that such interacting bosons in a two dimensional trap have identical bulk thermodynamic properties as those of noninteracting “haldons” in the same trap, obeying FES.

The above conclusions have been reached using a two-dimensional zero-range interaction with a fixed coupling constant, which was obtained by a dimensional reduction of the three-dimensional pseudo-potential, as explained in the introduction. It should be noted, however, that in a strict two-dimensional problem, the pseudo-potential is more complicated. As emphasized by Schick [27], the scattering cross section for binary collision of two bosons due to a hard-disc potential of radius \( a \) diverges in the low-energy limit:

\[ \sigma \rightarrow \frac{\pi^2}{k(lnka)^2} , \quad (ka) << 1 , \]  

(22)

where \( k \) is the relative wave number. This is a very different behaviour from the three-dimensional problem, where the total cross section goes to a constant value proportional to \( a^2 \). Thus, in strictly two-dimensions, the strength of the pseudo-potential should be \( k \)-dependent.

Another way to define a pseudo potential for a very dilute gas would be to have a zero-range form with a density-dependent strength such that in Born approximation it reproduces the ground-state energy per particle to the lowest order. Schick had shown that this is given by \( E/N = -2\pi n(\ln na^2)^{-1} \), where \( n \) is the average number density of the bosons.
Shevchenko [28], in a detailed analysis of bosons in a trap, thus adopted a zero-range potential with the $g$ of our Eq.(2) replaced by the density-dependent factor $\ln^{-1}(1/(na^2))$. He came to the conclusion that whereas this repulsive interaction prevents strict BEC, superfluidity sets in at a temperature close to the critical value $T_{c}^{0} = (6/\pi^2)^{1/2}N^{1/2}\hbar\omega$ of the ideal gas. This transition to superfluidity for the compressed fraction of the gas near the center of the trap takes place through the Berezinskii-Kosterlitz-Thouless (BKT) phenomenon of bound vortex pairs, much as in the translationally invariant two-dimensional interacting gas.

In our simple Thomas-Fermi treatment of the two-dimensional problem with a zero-range pseudo potential of constant coupling strength, we cannot examine the fluctuations in the phase of the "quasi-condensate" [31], nor can we comment on the formation of BKT-vortices. Despite these limitations, we find, for our model, the transformation of Bose to Haldane statistics through the zero-range interaction. This, arguably, is the most interesting point of our paper.

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