Momentum Distribution for Bosons with Positive Scattering Length in a Trap

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Abstract

The coordinate-momentum double distribution function $\rho(\mathbf{r}, \mathbf{p})d^{3}r d^{3}p$ is calculated in the local density approximation for bosons with positive scattering length $a$ in a trap. The calculation is valid to the first order of $a$. To clarify the meaning of the result, it is compared for a special case with the double distribution function $\rho_{w}d^{3}r d^{3}p$ of Wigner.
Using the local density approximation (LDA) [1,2], which is a straightforward adaptation of the Thomas-Fermi method, the density distribution $\rho(r)d^3r$ in coordinate space for BEC for $a > 0$ in a trap has been obtained. We want to calculate in this paper the coordinate-momentum distribution $\rho(r, p)d^3rd^3p$ in the same approximation. We follow the notation of Ref. [2] throughout. In particular, the fugacity $z$ of the system is

$$z = \exp[\mu/kT]$$

where $\mu$ is the chemical potential. We introduce a local fugacity $\zeta(r)$ defined as

$$\zeta = z \exp[-\beta V(r)].$$

1. The Gaseous Phase

By the gaseous phase we include both the system before BEC sets in, and the system at high densities for the cells outside of $r_0$ [2], i.e., outside of the region where BEC takes place. We consider such a cell of volume $V$ in which the local fugacity is $\zeta$. Using the method of Ref.[3] we write the grand partition function in the cell as

$$Q = \sum N \zeta^N Tr[\exp(-\beta H_0 - \beta H')]$$

The average occupation number $\ll n_k \gg$ of the state with momentum $\hbar k$ can be computed from

$$Q \ll n_k \gg = \sum N \zeta^N Tr[(a_k^\dagger a_k)\exp(-\beta H_0 - \beta H')]$$

We shall drop all terms beyond the first order of $H'$. Since $H_0$ commutes with $a_k^\dagger a_k$, we find

$$Q = \sum N \zeta^N Tr[\exp(-\beta H_0)(1 - \beta H')] = Q_0 + Q_1$$

and

$$Q \ll n_k \gg = \sum N \zeta^N Tr[\exp(-\beta H_0)(a_k^\dagger a_k)(1 - \beta H')] = A_0 + A_1$$

where

$$Q_0 = \sum N \zeta^N Tr[\exp(-\beta H_0)] = \prod[1 - \zeta e^{-\beta \epsilon}]^{-1}$$
is the term in $Q$ without the perturbation term. $Q_1$ has been evaluated in Ref.[3].

$$Q_1/Q_0 = -\beta \frac{4\pi a h^2}{m V} \left[ \sum_{\alpha \neq \beta} \bar{n}_\alpha \bar{n}_\beta + \sum_\alpha \frac{1}{2} \bar{n}_\alpha^2 - \sum_\alpha \frac{1}{2} \bar{n}_\alpha \right]$$  \tag{8}

where the bar means average over the grand canonical ensemble $Q_0$:

$$\bar{n}_\alpha = \frac{\zeta e^{-\beta \epsilon_\alpha}}{1 - \zeta e^{-\beta \epsilon_\alpha}} .$$  \tag{9}

Similarly

$$A_0/Q_0 = \bar{n}_k$$  \tag{10}

and

$$A_1/Q_0 = -\beta \frac{4\pi a h^2}{m V} \left\langle n_k \left[ \sum_{\alpha \neq \beta} n_\alpha n_\beta + \sum_\alpha \frac{1}{2} n_\alpha^2 - \sum_\alpha \frac{1}{2} n_\alpha \right] \right\rangle$$  \tag{11}

where the symbol $\langle \rangle$ means the same average as the bar. The coefficient in (8) and (11), $-\beta 4\pi a h^2 (mV)^{-1}$, is equal to $-2a\lambda^2 V^{-1}$. Now (11) can be rewritten as

$$A_1/Q_0 = -2a\lambda^2 V^{-1} \left\langle n_k - \bar{n}_k \left[ \sum_{\alpha \neq \beta} n_\alpha n_\beta + \sum_\alpha \frac{1}{2} n_\alpha^2 - \sum_\alpha \frac{1}{2} n_\alpha \right] \right\rangle + \bar{n}_k Q_1/Q_0.$$  \tag{12}

Notice that $Q_0$ is a product distribution function according to (7). Thus $\bar{n}_\alpha n_\beta = \bar{n}_\alpha \bar{n}_\beta$ if $\alpha \neq \beta$. Using this and similar identities we find that in the sum over $\alpha$ and $\beta$ in (12), the bracket $\langle \rangle$ vanishes unless $k = \alpha$ or $k = \beta$. Thus

$$A_1/Q_0 = -2a\lambda^2 V^{-1} \left\langle \sum_{\beta \neq k} n_k n_\beta (n_k - \bar{n}_k) + \frac{1}{2} (n_k^3 - \bar{n}_k n_k^2 - n_k^2 + \bar{n}_k^2) \right\rangle + \bar{n}_k Q_1/Q_0.$$  \tag{13}

Now $V^{-1} \left\langle \sum_{\beta \neq k} n_k n_\beta (n_k - \bar{n}_k) \right\rangle \to \rho(\bar{n}_k^2 - \bar{n}_k^2)$ as $V \to \infty$, yielding

$$A_1/Q_0 = -4a\lambda^2 \rho(\bar{n}_k^2 - \bar{n}_k^2) + \bar{n}_k Q_1/Q_0.$$  \tag{14}

Adding this to (10) and dividing by $1 + Q_1/Q_0$ we obtain, to order $a$,

$$\ll n_k \gg = \bar{n}_k - 4a\lambda^2 \rho(\bar{n}_k^2 - \bar{n}_k^2).$$  \tag{15}

The number of modes $k$ in a cell of volume $V$ is $(8\pi^3)^{-1} V d^3 k$. Thus the combined coordinate-momentum distribution $\rho(r, p)$ is given by

$$h^3 \rho(r, p) = \ll n_k \gg = \frac{\zeta e^{-\beta \epsilon_\alpha}}{1 - \zeta e^{-\beta \epsilon_\alpha}} - 4\pi \lambda^2 \rho(r) \frac{\zeta e^{-\beta \epsilon_\alpha}}{(1 - \zeta e^{-\beta \epsilon_\alpha})^2}$$  \tag{16}
where $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$ and $\zeta$ is given by (2). In (16) we have evaluated $\overline{n_k^2}$ in a straightforward way from the product partition function (7).

Integrating (16) over $d^3p$ we should get the density $\rho(r)$ times $\hbar^3$. This can be done without much difficulty, yielding Eq. (3) of Ref. [2].

2. The Region with Condensate

For high densities, BEC forms in some cells of the trap. In those cells $\rho = \rho_0 + \rho_s > \rho_0$, where [4],

$$\rho_0 = \lambda^{-3} g_{3/2}(1)$$

(17)

and

$$V(r) + 4\pi a \rho_s(r) \hbar^2 / m = V(r_0).$$

(18)

Here $\rho_s$ denotes superfluid density, i.e., density of particles with $p = 0$. An important parameter $\xi_5 = \rho_s / \rho$, a function of the location of the cell, with value between 0 and 1, describes *incomplete occupation* of the ground state, and was studied in detail in Ref. [5]. [Notice that $\xi_5$ and $\xi$ are totally different quantities.] For cells without BEC, $\xi_5 = 0$.

It was shown in Ref. [5] that the system in a cell with BEC has an energy given by (5.16) with a phonon spectrum (for $k \neq 0$) given by (5.18):

$$\hbar \omega_k = \frac{\hbar^2}{2m} (k^4 + 2k_0^2 k^2)^{1/2}, \quad k_0^2 = 8\pi a \xi_5 \rho = 8\pi a \rho_s.$$  

(19)

Notice that for the gaseous phase, $\xi_5 = 0$ and the phonon spectrum is quadratic for small $k$.

The phonon creation operator $b_k^\dagger$ and the particle creation operator $a_k^\dagger$ are related to each other through a Bogoliubov transformation [6]:

$$a_k = (b_k - \alpha_k b_{-k}^\dagger)(1 - \alpha_k^2)^{-1/2}$$

(20)

where

$$\alpha_k = k_0^{-2}(k^2 + k_0^2 - \sqrt{k^4 + 2k_0^2 k^2}).$$

(21)
For a state with $m_k$ phonons we can compute the average occupation number $\langle n_k \rangle$ of atoms in the state $p = \hbar k$ using (20) above. The result is linear in $m_k$. Now the average number of $m_k$ is given by Eqs.(5.27) and (5.31). Thus

$$\rho(r, p) = h^{-3}[\alpha_k^2 + (1 + \alpha_k^2)(e^{\beta \hbar \omega_k} - 1)^{-1}](1 - \alpha_k^2)^{-1}, \quad (k \neq 0), \quad (22)$$

where $\omega_k$ is given by (19), and $\alpha_k$ is given by (21).

For $k \gg k_0 = \sqrt{8\pi a \rho_s}$, the phonon energy (19) can be expanded in powers of $a$ and (22) becomes

$$\rho(r, p) = h^{-3}(e^{\beta E_k} - 1)^{-1}, \quad (k \gg k_0), \quad (23)$$

where

$$E_k = \frac{p^2}{2m} + \frac{\hbar^2}{2m}[8\pi a \rho_s(r)].$$

For other values of $k > 0$, Eq.(22) gives the distribution. It is a complicated function of $k$. For $0 < k \ll k_0$, it reduces to

$$\rho(r, p) \approx h^{-3}m\beta^{-1}p^{-2}, \quad (0 < k \ll k_0). \quad (24)$$

Notice that this differs by a factor of 2 from the corresponding distribution when $a = 0$.

3. Wigner Double Distribution

What is the meaning of the double distribution $\rho(r, p)$? It, of course, should only be used [2] for $d^3r > (L_2)^3$, and for $d^3rd^3p > \hbar^3$. But does it have a clear meaning in quantum mechanics? We discuss this by examining Eq.(16) in the limit of $a = 0$, for the case of a spherically symmetrical harmonic trap $V(r) = \frac{1}{2}m\omega^2r^2$. In such a case we can compute exactly the matrix element of $\langle r'|ze^{-\beta H}|r \rangle = \sum_{\ell=1}^{\infty}\langle r'|\ell^\ell e^{-\beta \ell H}|r \rangle$, by using, e.g., the result of Ref.[9]. Using Wigner’s idea [10], we put $r' = R - \frac{1}{2} \eta$, and $r = R + \frac{1}{2} \eta$ and evaluate the above, and then make a Fourier transform to the variable $P$ conjugate to $\eta$.

The resultant double distribution $a \ell a$ Wigner becomes

$$\rho_w(R, P) = h^{-3}\sum_{\ell=1}^{\infty}z^\ell(\text{sech} \frac{\ell \varepsilon}{2})^3 \exp \left\{-\frac{2\beta}{\varepsilon}(\text{tanh} \frac{\ell \varepsilon}{2})(\frac{P^2}{2m} + \frac{1}{2}m\omega^2R^2)\right\} \quad (25)$$
where $\varepsilon = \beta \hbar \omega$. In the limit that $\varepsilon \to 0$, this is exactly Eq.(16) for $a = 0$, [noticing that the local fugacity $\zeta$ is given by (2)] which is in agreement with the discussion in Ref. [2] for the single distribution function $\rho(r)$.

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