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Temperature dependence of condensate fraction of weakly nonideal trapped Bose gas

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Abstract. Condensation of the weakly nonideal gas in an anisotropic parabolic trap was considered. The first order (with respect to the interaction parameter) correction $\Delta\bar n_0 = \bar n_0(T) - \bar n_0^0(T)$ to the temperature dependence of the ground state population $\bar n_0^0(T)$ of the ideal gas atoms was found using thermodynamic perturbation theory. The correction found $\Delta\bar n_0$ proved to be much larger than the one calculated within the mean field theory [see Giorgini S, Pitaevskii L P, Stringari S *Phys. Rev. A* 54 R4633 (1996)] at temperatures below critical. This correction tends to zero as the temperature approaches the critical one; i.e., the interaction of the atoms does not lead to variation in the critical temperature. A simple analytic expression was found that describes the smooth variation of $\bar n_0^0(T)$ as it approaches zero in the vicinity of the critical temperature. A new criterion for applicability of the thermodynamic limit is given.

The latest advances in the field of laser cooling of atoms allowed the implementation of new efficient loading methods for parabolic magnetic traps. As a result, the critical temperature of Bose condensation was achieved in such traps [1]. Since the first observations of the Bose condensation of atomic gases, the question of how the interatomic interaction affects the process of condensation has been actively studied (see, for example, [2]). From the conceptual viewpoint, this problem is currently one of the most important in the theory of Bose condensation.

At present, this problem is approached with the help of the mean field approximation [2, 3]. This approximation is based on the Gross-Pitaevskii equation, which describes the condensate wave function (the order parameter) and which follows from the assumption of spontaneously symmetry broken gauge. It was established within this approach [3] that, in the first order with respect to the interaction parameter a (a is the scattering length), the condensation temperature is shifted by $\Delta T_{\rm int}$ from its ideal-gas value $T_{\rm c}$,

$$\frac{\Delta T_{\rm int}}{T_{\rm c}} \approx -1.3\frac{a}{R}N^{1/6}, \tag{1}$$

Here, $R = (\hbar/m\omega)^{1/2}$ is the oscillator dimension; m is the mass of the atom; $\omega = (\omega_x\omega_y\omega_z)^{1/3}$, where ω_i are the frequencies of the parabolic trap; and N is the total number of trapped atoms.

In this paper, the thermodynamic perturbation theory is used to investigate the effect of the interatomic interaction on the temperature dependence of the ground-state population $\bar n_0(T)$ of the gas in an anisotropic parabolic trap. The main result of our approach is that, in the first order with respect to the interaction parameter a, this dependence has the form

$$\bar n_0(T) = \bar n_0^0(T)\left[1 - g\left(\frac{T}{T_{\rm c}}\right)^2\right],$$
$$g = \frac{2^{3/2}}{\pi^{1/2}}\frac{\zeta(2)}{\zeta^{2/3}(3)}\frac{a}{R}N^{2/3} \approx 2.3\frac{a}{R}N^{2/3}, \tag{2}$$

where $\zeta(x)$ is the Riemann zeta function. The function $\bar n_0^0(T)$ describes the ground-state population of the ideal gas [2, 4, 5]:

$$\frac{\bar n_0^0(T)}{N} = 1 - \varphi_0(T),\ \ \varphi_0(T) = \left(\frac{T}{T_{\rm c}^0}\right)^3 + \theta\left(\frac{T}{T_{\rm c}^0}\right)^2 N^{-1/3}, \tag{3}$$

where $T_{\rm c}^0 = N^{1/3}\hbar\omega\zeta^{-1/3}(3)$; $\theta = 1.5\,(\bar\omega/\omega)\,[\zeta(2)/\zeta^{2/3}(3)] \approx 2.18\bar\omega/\omega$; and $\bar\omega = (\omega_x + \omega_y + \omega_z)/3$. The second term in the expression for the function $\varphi_0(T)$ is the correction due to the finite number of atoms in the trap. As a result, $\bar n_0^0(T)$ vanishes at the temperature $T_{\rm c} = T_{\rm c}^0 + \Delta T_{\rm fin}$,, where $\Delta T_{\rm fin}/T_{\rm c}^0 = -(\theta/3)N^{-1/3}$ [4,5].

It is generally accepted that the ideal-gas dependence (3) holds in the thermodynamic limit (see, e.g., [2, 4])

$$N \to \infty, \quad \omega \to 0, \quad N\omega^3 \to {\rm const}\ . \tag{4}$$

Below, we show that the correct condition for the thermodynamic limit is not uniform in $\bar n_0^0$ and has the form

$$\bar n_0^0(T) \gg \sqrt{N}\ . \tag{5}$$

It is the fulfilment of condition (5) rather than (4), that determines validity of expressions (2) and (3). For any values of N and ω in the region $\bar n_0^0(T) \leqslant \sqrt{N}$, the corrections omitted in Eqns (2) and (3) become the leading terms and provide the smooth character of vanishing (with zero derivative) of $\bar n_0^0(T)$ when $T/T_{\rm c} \geqslant 1 - N^{-1/2}$ (see Fig. 1). Furthermore, these corrections play the decisive role in derivation of the dependence (2) in the region of the thermodynamic limit (5) as well.

A specific feature of Eqn (2) is a decrease in the correction $\Delta\bar n_0 = \bar n_0(T) - \bar n_0^0(T)$ with decreasing $\bar n_0$. As we show below, this feature is also preserved in the region $\bar n_0^0(T) \leqslant \sqrt{N}$. This means, that the curves $\bar n_0(T)$ and $\bar n_0^0(T)$ approach one another with increasing temperature at $T \to T_{\rm c}$ (see Fig. 1). This result, however, qualitatively

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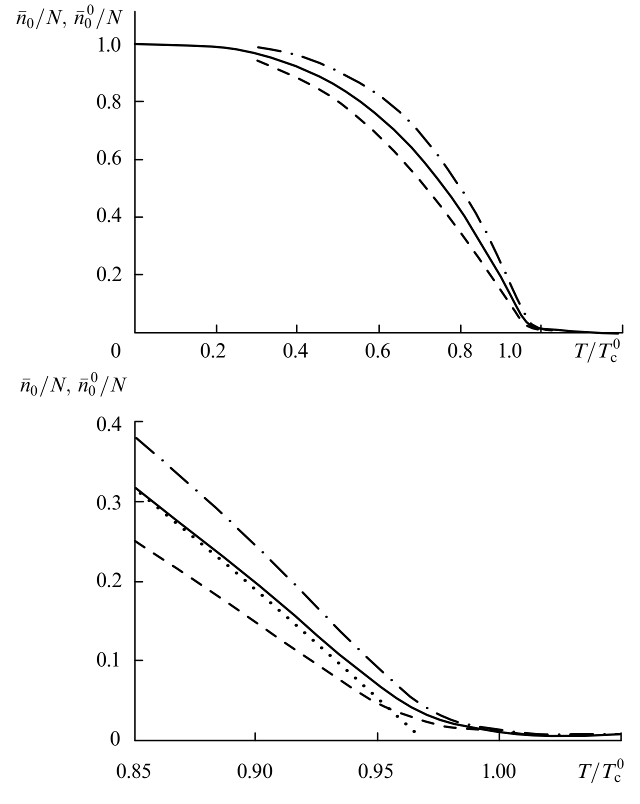

Figure 1. Temperature dependences of the condensed fraction of $\bar n_0^0/N$ of the ideal gas calculated by Eqn (16)(the solid curves) and Eqn (3) (the dotted curve) and of the condensed fraction $\bar n_0/N$ of the weakly nonideal gas calculated by Eqn (19) for $g = 0.25$ (the dashed curves) and $g = -0.25$ (the dash-dot curves). The total number of particles is $N = 10^3$.

contradicts the prediction of mean field theory (1). Another contradiction is that the correction parameter in Eqn (2) is $\sqrt{N}$ times larger than the corresponding parameter in Eqn (1); i.e., the correction in Eqn (2) is much larger than that in Eqn (1) when $T < T_c$.

The appearance of the parameter g in the thermodynamic perturbation theory can be qualitatively explained in the following way. The characteristic correction to the energy per particle induced by the interatomic interaction is determined by the parameter $\hbar\omega(a/R)N$ (see, e.g., [6, 7]). After introducing it into the Gibbs distribution, this correction is divided by T (the temperature in units of energy). Thereupon, one should take into account that $\hbar\omega/T \approx (\hbar\omega/T_c)(T_c/T) \approx (T_c/T) \times N^{-1/3}$.

We start our derivation by calculating, with the help of perturbation theory, the interaction-induced corrections to eigenvalues of the secondary quantisation Hamiltonian

$$\hat H = \hat H_0 + \hat U, \quad \hat H_0 = \sum_s \varepsilon_s a_s^+ a_s \ ,$$

$$\hat U = \frac{1}{2} \sum_{s_1', s_2', s_1, s_2} U_{s_1, s_2}^{s_1', s_2'} a_{s_1'}^+ a_{s_2'}^+ a_{s_1} a_{s_2} \ ,$$

Here, a_s^+ and a_s are, respectively, the creation and annihilation operators of a particle in the state s. In the case of an anisotropic trap, all levels are non-degenerate, and the first-order correction $\Delta E(n_0, n_1, ...)$ to the energy of the unperturbed Hamiltonian $E_0(n_0, n_1, ...) = \varepsilon_0 n_0 + \varepsilon_1 n_1 + ...$ has the form

$$\Delta E(n_0, n_1, ...) = \langle n_0, n_1, ...|\hat U|n_0, n_1, ...\rangle$$

$$= \frac{1}{2}\sum_k A_{kk} n_k (n_k - 1) + \sum_{k \neq l} A_{kl} n_k n_l \,. \tag{6}$$

In Eqn (6) we took into account that all the eigenfuctions are real in the absence of degeneration, and introduced the notation

$$A_{kl} = A_{lk} = U_{kl}^{kl} = U_{kl}^{lk} = \int \Psi_k^2(\boldsymbol{r}) U(\boldsymbol{r} - \boldsymbol{r}') \Psi_l^2(\boldsymbol{r}') \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{r}'.$$

Then, we insert $E_0 + \Delta E$ in the Gibbs distribution,

$$W(n_0, n_1, ...) = S^{-1} \exp\left[\frac{\mu}{T}(n_0 + n_1 + ...)\right.$$

$$\left. - \frac{1}{T}[E_0(n_0, n_1, ...) + \Delta E(n_0, n_1, ...)]\right]$$

$$\approx S^{-1} \exp\left[\frac{\mu}{T}(n_0 + n_1 + ...) - \frac{1}{T}[E_0(n_0, n_1, ...)\right]$$

$$\times \left[1 - \frac{1}{T}\Delta E(n_0, n_1, ...)\right] \tag{7}$$

and, using Eqn (6), calculate the normalisation constant

$$S = S_0\left(1 - \sum_{kl} B_{kl} \tilde n_k \tilde n_l\right), \ S_0 = \prod_i \left[1 - \exp\left(\tilde\mu - \frac{\varepsilon_i}{T}\right)\right]^{-1}, \tag{8}$$

$$\tilde n_i = \left[\exp\left(\frac{\varepsilon_i}{T} - \tilde\mu\right) - 1\right]^{-1}, \quad B_{kl} = \frac{A_{kl}}{T},$$

where $\tilde\mu = \mu/T$. Note that in presence of interatomic interaction ($B_{kl} \neq 0$), the quantities $\tilde n_i$ and $\tilde\mu$ are not the average number, in contrast to the case of ideal gas ($B_{kl} = 0$).

To calculate the average number $\bar n_i$ of atoms populating the level i when $B_{kl} \neq 0$, one has to perform the summation

$$\bar n_i = \sum_{n_0, n_1, ...} n_i W(n_0, n_1, ...) \ .$$

Using Eqns (7) and (8), we obtain

$$\bar n_i = \tilde n_i - 2\tilde n_i(\tilde n_i + 1) \sum_k B_{ik} \tilde n_k \,. \tag{9}$$

The parameter $\tilde\mu$ can then be determined from the relationship $N = \sum \bar n_i$. We rewrite this relationship in the following form to the separate terms that contain $\tilde n_0$

$$N = \tilde n_0 + \sum_{i \neq 0} \tilde n_i - 2B_{00}(\tilde n_0)^2(\tilde n_0 + 1)$$

$$-\tilde n_0(\tilde n_0 + 1)\Sigma_1 - \tilde n_0 \Sigma_2 - \Sigma_3, \tag{10}$$

$$\Sigma_1 = 2\sum_{k \neq 0} B_{0k} \tilde n_k, \ \ \Sigma_2 = 2\sum_{k \neq 0} B_{0k} \tilde n_k(\tilde n_k + 1),$$

$$\Sigma_3 = 2\sum_{k, l \neq 0} B_{kl} \tilde n_k \tilde n_l(\tilde n_l + 1),$$

Eqn (10) can be solved for the parameter $\tilde\mu$ using the iteration method. First, we need to calculate the sum

$$F = \tilde{n}_0 + \sum_{k \neq 0} \tilde{n}_k \,. \tag{11}$$

For that purpose, we introduce the vector index $\boldsymbol{k} = (k_x, k_y, k_z)$ (where $k_i = 0, 1, \ldots$, $i = x, y, z$) that enumerates the energy levels of the 3D oscillator $\varepsilon_{\boldsymbol{k}} = \hbar\omega(\boldsymbol{k}\boldsymbol{\Omega})$, where $\boldsymbol{\Omega} = (\Omega_x, \Omega_y, \Omega_z)$; $\Omega_i = \omega_i/\omega$ (the ground level $(3/2)\hbar\bar{\omega}$ is assumed to have zero energy). We therefore have

$$\tilde{n}_{\boldsymbol{k}} = \left[\exp(\boldsymbol{\beta}\boldsymbol{k} - \tilde{\mu}) - 1\right]^{-1} = \sum_{p=1}^{\infty} \exp[p(-\boldsymbol{\beta}\boldsymbol{k} + \tilde{\mu})]\,,$$
$$\boldsymbol{\beta} = \frac{\hbar\omega}{T}\boldsymbol{\Omega}\,. \tag{12}$$

The summation in Eqn (11) can then be easily performed [8], and we find

$$F = \tilde{n}_0 + \sum_{p=1}^{\infty} \mathrm{e}^{\tilde{\mu}p}\left[\prod_{i=1}^{3}\left(1 - \mathrm{e}^{-\beta_i p}\right)^{-1} - 1\right]. \tag{13}$$

Next, we derive from Eqn (8) the exact formula $\tilde{\mu} = -\ln(1 + 1/\tilde{n}_0)$, which can be approximated by $\tilde{\mu} = -1/\tilde{n}_0$ down to very small $\bar{n}_0 \geqslant 5$. The parameter $\beta \sim \hbar\omega/T \sim N^{-1/3}T_c/T$, which means that the inequality $\beta \ll 1$ holds for large values of N, beginning from temperatures T that are much lower than the condensation temperature ($T \ll T_c$) but still satisfy the condition

$$t \gg N^{-1/3}, \quad t = T/T_c\,. \tag{14}$$

In the following, we will assume condition (14) to always be fulfilled. The sum (13) can then be replaced by a series expansion to the second order with respect to $1/\beta$ and the first order with respect to $\tilde{\mu} = -1/\tilde{n}_0$ to obtain

$$F = \tilde{n}_0 + N\varphi_0(T) - \frac{1}{\tilde{n}_0}N\varphi_1(T),\ \varphi_1(T) = \gamma t^3,\ \gamma = \frac{\zeta(2)}{\zeta(3)}. \tag{15}$$

The passage to the thermodynamic limit corresponds to dropping the last term in the expression for F in Eqn (15). However, it is this term that ensures the smooth reduction of the ground-state population to zero (with the zero derivative) in the region $\bar{n}_0^0 \leqslant \sqrt{N}$ ($|1 - t| \leqslant N^{-1/2}$) and provides the correction that plays the decisive role in the following calculations in the region of the thermodynamic limit (5).

In the zeroth order with respect to interparticle interaction (the ideal gas), we insert $B = 0$ in Eqn (10), with the result that $F = N$ and, the quantities $\tilde{n}_i$ then describe populations of the states of the ideal gas. For the ground-state population $\tilde{n}_0 = \bar{n}_0^0$ of the ideal gas we find from (15) the expression

$$\frac{\bar{n}_0^0}{N} = \frac{1}{2}\left\{1 - \varphi_0(T) + \left\{[1 - \varphi_0(T)]^2 + 4\varphi_1(T)/N\right\}^{1/2}\right\}. \tag{16}$$

Near the critical temperature, $|t - 1| \ll 1$, this expression takes the form

$$\frac{\bar{n}_0^0}{N} = \frac{3}{2}\left\{1 - t + \left[(1 - t)^2 + \frac{4}{9}\frac{\gamma}{N}\right]^{1/2}\right\}.$$

The temperature dependence (3), usually called the thermodynamic limit, follows from Eqn (16) under the conditions $t < 1$ and $1 - \varphi_0(T) \gg N^{-1/2}$ [which are equivalent to condition (5)]. This decrease of $\bar{n}_0^0$ with increasing temperature continues up to temperatures that are very close to T_c but still satisfy the condition $1 - t \gg N^{-1/2}$, equivalent to Eqn (5).

Then, the character of the decrease of $\bar{n}_0^0(T)$ changes, and in the range $N^{-1/2} \ll t - 1 \ll 1$, it is given by the equation $\bar{n}_0^0(T) = (\gamma/3)(t - 1)^{-1}$, as follows from Eqn (16). In the intermediate region, $|t - 1| \leqslant N^{-1/2}$, the exact formula (16) must be used. Previously, this deviation of the function $\bar{n}_0^0(T)$ from the thermodynamic limit was studied only numerically [4, 5]). Thus, in the zeroth order with respect to the interatomic interaction, the ground-state population $\bar{n}_0^0$ (the ideal gas) is given by expression (16).

In the first order with respect to the interatomic interaction, we set

$$\tilde{n}_0 = \bar{n}_0^0 + \Delta\bar{n}_0,\ F(\tilde{n}_0) = F\left(\bar{n}_0^0\right) + \left(\frac{\partial F}{\partial \bar{n}_0^0}\right)\Delta\bar{n}_0$$
$$= N + \left[1 + N\varphi_1\left(\bar{n}_0^0\right)^{-2}\right]\Delta\bar{n}_0$$

and, using Eqns (10) and (9), obtain

$$\bar{n}_0 = \bar{n}_0^0 + \frac{\left(\bar{n}_0^0\right)^2}{\left(\bar{n}_0^0\right)^2 + \varphi_1 N}\big(-2B_{00}\varphi_1 N\bar{n}_0^0$$
$$-\varphi_1 N\Sigma_1 + \bar{n}_0^0\Sigma_2 + \Sigma_3\big). \tag{17}$$

Note that only by taking account of the last term in Eqn (15) (cor-rection to the thermodynamic limit) the term proportional to B_{00}, which becomes leading in the thermodynamic limit (5) is retained in the expression (17).

In the case of the harmonic oscillator and the contact interaction $U(\boldsymbol{r} - \boldsymbol{r}') = (4\pi\hbar^2 a/m)\delta(\boldsymbol{r} - \boldsymbol{r}')$, the values of B_{00} and the sums $\Sigma_{1,2,3}$ can be calculated exactly. In particular, B_{00} can be found by a simple integration: $2B_{00} = g(\gamma N t)^{-1}$, where we took into account that $\hbar\omega/T = t^{-1}N^{-1/3}\zeta^{1/3}(3)$. In order to calculate the sums $\Sigma_{1,2,3}$ the numbers $\tilde{n}_k$ must first be represented in the form (12) and then summed over k using the well-known formula for Hermite polynomials [9]

$$\sum_{k=0}^{\infty}\frac{y^k}{k!}H_k^2(x) = \frac{1}{(1 - 4y^2)^{1/2}}\exp\left(\frac{4y}{1 + 2y}x^2\right)\ ;$$

finally, integration completes the calculation. The result, a sum of functions over one or two scalar indices (m_1, m_2), becomes much simpler in the considered case $\beta \ll 1$:

$$\Sigma_1 = g\frac{\zeta(3/2)}{\zeta(2)}\left[\frac{\zeta(3)}{N}\right]^{1/2}t^{1/2},\ \Sigma_3 = g\zeta^{-1}(2)t^{7/2}\left[\frac{N}{\zeta(3)}\right]^{1/2}M, \tag{18}$$

$$\Sigma_2 = g\zeta^{-1}(2)t\left[\frac{\zeta(3)}{N}\right]^{1/3}\int_0^{\infty}\mathrm{d}u\,u\left[\prod_{i=x,y,z}\left(1 - \mathrm{e}^{-\Omega_i u}\right)^{-1/2} - 1\right],$$

where

$$M = \sum_{m_1, m_2 = 1}^{\infty} m_1^{-3/2}m_2^{-1/2}(m_1 + m_2)^{-3/2} \approx 1.2\,.$$

One can see from Eqn (18) that, under condition (14), the term in Eqn (17) that contains Σ_2 is much smaller than the term containing B_{00}; therefore, the former term can be neglected. We then obtain the following expression for the ground-state population

$$\bar{n}_0 = \bar{n}_0^0 - gt^2 \frac{\left(\bar{n}_0^0\right)^2}{\left(\bar{n}_0^0\right)^2 + \gamma t^3 N} \left(\bar{n}_0^0 + \delta t^{3/2} N^{1/2}\right) (19)$$

where $\bar{n}_0^0$ is given by Eqn (16), and $\delta = \zeta(3/2)\zeta^{-1/2}(3)[1 - M\zeta^{-1}(2)\zeta^{-1}(3/2)] \approx 1.74$.

In the thermodynamic limit (5) $(1 - t \gg N^{-1/2})$, this expression takes the form

$$\frac{\bar{n}_0}{N} = [1 - \varphi_0(T)]\left(1 - gt^2\right) - g\delta t^{7/2} N^{-1/2} \, . \qquad (20)$$

When $T = T_{\mathrm{c}}$, it follows from Eqn (19) that

$$\frac{\bar{n}_0}{N} = \left(\frac{\gamma}{N}\right)^{1/2} \left[1 - \frac{1}{2} g \left(1 + \delta \gamma^{-1/2}\right)\right]. \qquad (21)$$

Finally, under the conditions $N^{-1/2} \ll t - 1 \ll 1$ ($\bar{n}_0^0 \ll N^{1/2}$), we find from Eqn (19) that

$$\frac{\bar{n}_0}{N} = \frac{1}{3} \frac{\gamma}{N(t-1)} \left[1 - \frac{\delta}{3} g N^{-1/2} (t-1)^{-1}\right]. \qquad (22)$$

In the thermodynamic limit (20), the correction $\Delta\bar{n}_0$ given by the last term in the right-hand side is much smaller than the one given by the first term, which appears, as mentioned above, only as a result of the difference in value of $\bar{n}_0^0$ and its value given by Eqn (3) in the thermodynamic limit (5). Therefore, formula (2) should be used instead of formula (20). This means that, in all the cases given by Eqns (20)–(22), the correction $\Delta\bar{n}_0$ is proportional to $\bar{n}_0^0$ and tends to zero, together with $\bar{n}_0^0$, in the region $t - 1 \gg N^{-1/2}$ (see Fig. 1). The result given by Eqn (1) can be obtained only by taking a formal limit of $\bar{n}_0^0$ approaching zero ($\bar{n}_0^0 \ll N^{-1/2}$) in Eqn (20). This formal passsage to the limit, however, violates the condition (5) of validity of Eqn (20) (in this region, $\bar{n}_0$ has the form (22) rather than (20)). An important property of expression (2) is that it depends only on the term $(A_{00}/2)\bar{n}_0^2$ of the sum (6), which preserves its form in traps of any shape.

Note that calculation of the dependence $\bar{n}_0(T)$ according to Eqns (3) or (16) with the critical temperature correction given by the mean field theory equation (1) does not lead to any noticeable changes in the plot due to that correction.

Weakness of the interatomic interaction imposes new, other than condition (14), restrictions on the validity of the derived expression (19). The first constraint follows from the fact that the correction to $\bar{n}_0^0$ in Eqn (19) should be small compared to both $\bar{n}_0^0$ and the difference $N - \bar{n}_0^0$. Only in this case, the thermodynamic perturbation theory can be used to calculate the populations of excited states as well as the ground-state population. The second constrain is related to the condition of smallness of the energy correction (6) (per particle) compared to the energy level difference $\hbar\omega$. In the thermodynamic limit (20), both of these restrictions are important, which leads to the conditions $g \ll 1, (a/R)\bar{n}_0 \ll 1$, and $t \gg g$. For the case given by Eqn (21), only the first requirement is important, which corresponds to the constraint $g \ll 1$. Conversely, for the case given by Eqn (22), the second requirement plays the dominant role, resulting in the restriction $(a/R)N^{1/2} \ll 1$, which is the weakest of all the mentioned constraints. The only experimental measurement of $\bar{n}_0(T)$ [10] we are aware of was performed with a large number of particles and, therefore, did not satisfy the above constraints.

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