Bose–Einstein condensates: recent advances in collective effects/Avancées récentes sur les effets collectifs dans les condensats de Bose–Einstein

Thermodynamics of a dilute Bose gas with condensate

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Abstract

The partition function of a dilute Bose gas with repulsive interaction, fixed number of particles and in the presence of a condensate is computed up to first order in the interactions. An equilibrium condition appears for the fraction of particles in the condensate and the chemical potential of the particles. We show that for a dilute gas the Bose–Einstein transition is not of second order. Moreover, the thermodynamical quantities obtained may look different from those in the literature, because the chemical potential enters in a nontrivial way in the quasi particle spectrum.***To cite this article: S. Rica, C. R. Physique 5 (2004).***

Résumé

Thermodynamique d'un gaz de Bose dilué en présence d'un condensat. La fonction de partition d'un gaz de Bose dilué avec des interactions répulsives à nombre de particules fixé en présence d'un condensat est calculée au premier ordre du paramètre d'interactions. Une condition d'équilibre apparaît pour la fraction de particules condensées et pour le potentiel chimique des particules. On montre que pour un gaz dilué la transition de Bose–Einstein n'est pas de second ordre. De plus, les quantités thermodynamiques qui apparaîssent dans cette approche sont différentes de celles présentes dans la littérature sur le sujet du fait d'une dépendance non triviale du potentiel chimique avec le spectre des quasiparticules. ***Pour citer cet article : S. Rica, C. R. Physique 5 (2004).***

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According to Landau quasiparticle theory [1], the momentum density of the normal fluid, moving with a speed **v** relative to the superfluid part, is

$$\mathbf{j}_n = \frac{1}{(2\pi\hbar)^3}\int \mathrm{d}^3p\, p\, \frac{\mathbf{p}}{\mathrm{e}^{\beta(\varepsilon(p)-\mathbf{v}\cdot\mathbf{p})}-1}. \tag{1}$$

This relation could be expanded around $\mathbf{v}=0$ (if $|v| \ll \min \frac{\varepsilon(p)}{p}$), leading to $\mathbf{j}_n = m\rho_n\mathbf{v} + \mathrm{O}(v^2)$. $m\rho_n$ is called the normal matter density. After (1) one has that the number density of the normal component in a superfluid at temperature T is (hereafter we shall use the word density for a number density, that is, the number of particles per unit volume)

$$\rho_n = \frac{1}{3mk_BT}\frac{1}{(2\pi\hbar)^3}\int \mathrm{d}^3p\, p p^2 \frac{\mathrm{e}^{\beta\varepsilon(p)}}{(\mathrm{e}^{\beta\varepsilon(p)}-1)^2}. \tag{2}$$

In (2) $\varepsilon(p)$ is the excitation spectrum (that is, the energy of a quasiparticle as a function of its momentum p). Let ρ be the total fluid density. As usual, one defines the superfluid density by $\rho_s \equiv \rho - \rho_n$. In the case of helium, the normal density vanishes at

$T = 0$ K ($\rho_s = \rho$) and grows as T increases. Actually, the formula for ρ_n (2) has sense only if $\rho_n \leqslant \rho$ ($\rho_s \geqslant 0$). Using the roton shape part, Landau estimated the critical temperature where the normal density becomes the total fluid density. As he noted, this critical temperature is not exact in real liquid helium because the interactions between the quasiparticles were omitted.

Atomic vapours that undergo a Bose–Einstein transition are described in the framework of the Bogoliubov theory for a weakly interacting Bose gas [2]. For such a dilute system one finds an analytic expression for the spectrum:

$$\varepsilon(p) = \frac{1}{2m}\sqrt{p^4 + 2f\hbar^2\rho_0 p^2}, \tag{3}$$

where m is the particle mass, f the scattering length, $2\pi\hbar$ the Planck constant and ρ_0 is the number density of particles in the condensate (see later for a precise definition). In this case the normal density depends on the energy spectrum, that depends itself on the density of the condensate. Although there is no simple relation between the normal density and the condensate one, we shall set the superfluid density equal to the condensate one: $\rho_0 = \rho - \rho_n$ to illustrate the solutions of Eq. (2). A rapid evaluation says that $\rho_0 = 0$ at $T = T_{\mathrm{BE}} = \frac{2\pi}{\zeta(3/2)^{2/3}}\frac{\hbar^2}{mk_B}\rho^{2/3}$, and suggests that there is no change in the critical temperature as soon as we turn-on interactions. However, as was shown by Huang, Lee, Luttinger and Yang in a series of papers [3–6] the condensate density ρ_0 posses a subcritical behavior around T_{BE}, indicating that transition is not of second order.

Naturally, in our reasoning we have added the relation $\rho_0 = \rho - \rho_n$ mixing two quantities that have no direct connection; ρ_n defined by Landau is a hydrodynamical variable and ρ_0 is a thermodynamical variable with a very precise definition in the framework of the Bogoliubov theory [2]. Therefore, we shall leave out Landau's definition (2) and consider the Bogoliubov theory for a weakly interacting gas as a starting point. Although subcriticality does not disappear, the Bose distribution changes dramatically.

Let us consider a system with N interacting non-relativistic bosons in a volume Ω. Let $a_\alpha^\dagger$ (a_α) be the creation (annihilation) operators for the state of momentum p_α. Naturally they obey the commutation rule: $a_\alpha a_\beta^\dagger - a_\beta^\dagger a_\alpha = \delta_{\alpha\beta}$. The Hamiltonian is

$$H = \sum_p \frac{p^2}{2m} a_p^\dagger a_p + \frac{4\pi f\hbar^2}{2m\Omega} \sum_{\alpha,\beta,\nu,\omega} a_\alpha^\dagger a_\beta^\dagger a_\nu a_\omega \delta(p_\alpha + p_\beta - p_\nu - p_\omega), \tag{4}$$

where Ω is the total volume and the δ-function is Kronecker discrete function, equal to zero if its argument is not zero and to 1 otherwise.

Following the principles outlined by Bogoliubov, at zero temperature the interaction part of the energy is split into a part involving the condensate and a part not involving this condensate. If there is condensation in the state of zero momentum, the operators of index zero become c-numbers: $a_0 = \Psi_0\Omega^{1/2}$, $a_0^\dagger = \bar{\Psi}_0\Omega^{1/2}$, where Ψ_0 is the ground state wavefunction, practically a complex constant here, $\bar{\Psi}_0$ being its complex conjugate. The condensate number density appears to be $\rho_0 \equiv |\Psi_0|^2 = |a_0|^2/\Omega$.

The sum $\sum_{\alpha\ldots\omega}$ may be decomposed in five terms, depending on the way the condensate wavefunction enters into those terms: first, the one with four zero wavenumbers: $\frac{2\pi\hbar^2 f}{m\Omega}|a_0|^4$. The terms with three zero wavenumbers do not exist because of the δ-function. The terms such that two wavenumbers are zero contribute with $\frac{2\pi\hbar^2 f}{m\Omega}\sum_p'(a_0^2 a_p^\dagger a_{-p}^\dagger + \bar{a}_0^2 a_p a_{-p} + 4|a_0|^2 a_p^\dagger a_p)$; here $\sum_p'$ excludes the $p = 0$ term. This term is precisely the one kept by Bogoliubov, allowing him to describe a perfect gas of quasi-particles with a well defined energy spectrum at $T = 0$ K. The cubic terms on the a_p are always negligible compared to the other interaction terms except near the transition. This is because it has the lowest order in a_0, with respect to any other term involving a_0, and so becomes the most important term involving a_0 as the superfluid density tends to zero. However, outside this neighborhood of the transition, this term may be neglected. In a regular perturbation scheme, the effect of the third term would require us to go to the second order in f^2 (because any combination cubic in creation annihilation operators brings no first order contribution), although we shall deal with terms of at most first order in f. Finally, we have the terms such that all four wavenumbers $p_{\alpha\ldots\omega}$ differ from zero. One could expect that those are of higher order, but, after a rapid inspection, one sees that the particular terms where $p_\alpha = p_\nu$, $p_\beta = p_\omega$ and $p_\alpha = p_\omega$ with $p_\beta = p_\nu$ contributes up to a first order. Other terms introduce quantum correlations which we neglect. The final sum can be written

$$\frac{4\pi f\hbar^2}{m\Omega}\left(\sum_\alpha{}' a_\alpha^\dagger a_\alpha\right)\left(\sum_\beta{}' a_\beta^\dagger a_\beta\right) = \frac{4\pi f\hbar^2}{m\Omega}(N - n_0)^2,$$

where n_0 is by definition the total number of particles with zero momentum, i.e., $n_0 = |a_0|^2 = |\Psi_0|^2\Omega = \rho_0\Omega$.

Finally, the Hamilton operator that we are going to use can be written as:

$$H = \sum_p \frac{p^2}{2m} a_p^\dagger a_p + \frac{2\pi\hbar^2 f}{m\Omega}\left[2(N - n_0)^2 + n_0^2\right] + \frac{2\pi\hbar^2 f}{m}\sum_p{}'\left(\Psi_0^2 a_p^\dagger a_{-p}^\dagger + \bar{\Psi}_0^2 a_p a_{-p} + 4|\Psi_0|^2 a_p^\dagger a_p\right). \tag{5}$$

We shall compute the partition function $Z_N = \mathrm{Tr}(\mathrm{e}^{-H/(k_B T)})$, for a given total number of particles N in a box of volume Ω. Following now the same general method as outlined in Huang's book [7] we decompose the trace into a sum over states with n_0 particles in the condensate (depending only on n_0) and sums over states with non-zero momentum. Therefore one has

$$Z_N = \sum_{n_0=0}^{N} \mathrm{e}^{-((2\pi\hbar^2 f)/(mk_B T\Omega))[2(N-n_0)^2+n_0^2]}\,\mathrm{Tr}'\big(\mathrm{e}^{-H'/(k_B T)}\big),$$

where

$$H' = \sum_p{}' \left[\left(\frac{p^2}{2m} + \frac{8\pi\hbar^2 f}{m}|\Psi_0|^2\right)a_p^\dagger a_p + \frac{2\pi\hbar^2 f}{m}\left(\Psi_0^2 a_p^\dagger a_{-p}^\dagger + \bar{\Psi}_0^2 a_p a_{-p}\right)\right].$$

The trace $\mathrm{Tr}'(\mathrm{e}^{-H'/(k_B T)})$ is sum over states where $N - n_0 = N' = \sum_p' a_p^\dagger a_p$ is fixed. This trace could be performed directly adding a Lagrange multiplier $\mu(N' - \sum_p' a_p^\dagger a_p)$. In a sense, this trace represents the partition function of a fictitious non-interacting gas in equilibrium. Let us call this partition function $Z'_N(n_0, \mu)$. Therefore the full partition function could be written as

$$Z_N = \sum_{n_0=0}^{N} Z_N(n_0,\mu) = \sum_{n_0=0}^{N} \mathrm{e}^{-((2\pi\hbar^2 f)/(mk_B T\Omega))[2(N-n_0)^2+n_0^2]} Z'_N(n_0,\mu).$$

Huang's method uses the following inequality for Z_N:

$$\mathrm{Max}\big[Z_N(n_0,\mu)\big] < Z_N < (N+1)\mathrm{Max}\big[Z_N(n_0,\mu)\big],$$

where $\mathrm{Max}[Z_N(n_0,\mu)]$ is the global maximum of $Z_N(n_0,\mu) = \mathrm{e}^{-((2\pi\hbar^2 f)/(mk_B T\Omega))[2(N-n_0)^2+n_0^2]} Z'_N(n_0,\mu)$ in $n_0 \in [0, N]$ and $\mu \in \Re$. Let $\bar{n}_0$ and $\bar{\mu}$ be the maximal values. The preceding inequality says that

$$\frac{1}{N}\ln Z_N(\bar{n}_0,\bar{\mu}) < \frac{1}{N}\ln Z_N < \frac{1}{N}\ln Z_N(\bar{n}_0,\bar{\mu}) + \frac{1}{N}\ln(N+1),$$

therefore as $N \to \infty$ one has the following limit for the partition function

$$\frac{1}{N}\ln Z_N \to \frac{1}{N}\ln Z_N(\bar{n}_0,\bar{\mu}).$$

Let us now compute $Z'_N(n_0,\mu)$. As we said, we use the grand canonical ensemble with a Lagrange multiplier $\mu(N' - \sum_p' a_p^\dagger a_p)$. Therefore we should compute the trace

$$Z'_N(n_0,\mu) = \mathrm{e}^{-\mu(N-n_0)/(k_B T)}\,\mathrm{Tr}\exp\left(\frac{-1}{k_B T}\sum_p{}'\left[\left(\frac{p^2}{2m} + 4\frac{2\pi\hbar^2 f}{m}|\Psi_0|^2 - \mu\right)a_p^\dagger a_p + \frac{2\pi\hbar^2 f}{m}\left(\Psi_0^2 a_p^\dagger a_{-p}^\dagger + \bar{\Psi}_0^2 a_p a_{-p}\right)\right]\right).$$

The trace computation is made possible by transforming the operator in the exponential into its diagonal form using the Bogoliubov transformation:

$$\begin{aligned} a_p &= u_p b_p + v_p b_{-p}^\dagger, \\ a_p^\dagger &= \bar{u}_p b_p^\dagger + \bar{v}_p b_{-p}, \\ 1 &= |u_p|^2 - |v_p|^2, \end{aligned} \tag{6}$$

where the third relation follows from the commutation relation $[a_p, a_p^\dagger] = 1$. Imposing the condition that the resulting Hamiltonian is diagonal in $b_p^\dagger b_p$ one has that

$$\frac{v_p}{\bar{u}_{-p}} = \frac{-T_p \pm \sqrt{T_p^2 - 4g^2|\Psi_0|^4}}{2g\bar{\Psi}_0^2},$$

where $g = 2\pi\hbar^2 f/m$ and $T_p = p^2/(2m) + 4g|\Psi_0|^2 - \mu$. Finally, the operator in the exponential in its diagonal form is

$$\sum_p{}' \big(T_p^2 - 4g^2|\Psi_0|^4\big)^{1/2} b_p^\dagger b_p.$$

Therefore, if

$$\varepsilon_B\big(p,\mu,|\Psi_0|^2\big) \equiv \sqrt{\left(\frac{p^2}{2m}+4g|\Psi_0|^2-\mu\right)^2-4g^2|\Psi_0|^4} \tag{7}$$

one has in the end that

$$\ln Z'_N(n_0,\mu)=\frac{-\mu(N-n_0)}{k_BT}-\Omega\int\frac{\mathrm{d}^Dp}{(2\pi\hbar)^D}\ln\big(1-\mathrm{e}^{-\varepsilon_B(p,\mu,|\Psi_0|^2)/k_BT}\big). \tag{8}$$

We need now to find the maxima of

$$Z_N(n_0,\mu)=\mathrm{e}^{-((2\pi\hbar^2f)/(mk_BT\Omega))[2(N-n_0)^2+n_0^2]} \times\exp\left[\frac{-\mu(N-n_0)}{k_BT}-\Omega\int\frac{\mathrm{d}^Dp}{(2\pi\hbar)^D}\ln\big(1-\mathrm{e}^{-\varepsilon_B(p,\mu,|\Psi_0|^2)/k_BT}\big)\right] \tag{9}$$

through the conditions

$$\frac{\partial Z_N(n_0,\mu)}{\partial\mu}=\frac{\partial Z_N(n_0,\mu)}{\partial n_0}=0,$$

giving

$$\rho'=\frac{N-n_0}{\Omega}=-\int\frac{\mathrm{d}^Dp}{(2\pi\hbar)^D}\frac{1}{\mathrm{e}^{\varepsilon_B(p,\mu,|\Psi_0|^2)/k_BT}-1}\frac{\partial\varepsilon_B(p,\mu,|\Psi_0|^2)}{\partial\mu}. \tag{10}$$

Although this equation means that we obtain a perfect gas of quasi-particles in thermodynamical equilibrium with a well defined number of excitations, the total number of quasi-particles is not the usual Bose–Einstein factor. The second condition (note that $\varepsilon_B(p,\mu,|\Psi_0|^2)$ depends explicitely on n_0 because $n_0=|\Psi_0|^2\Omega$) implies:

$$\mu+\frac{2\pi\hbar^2f}{m}(4\rho-6\rho_0)-\Omega\int\frac{d^Dp}{(2\pi\hbar)^D}\frac{1}{\mathrm{e}^{\varepsilon_B(p,\mu,\rho_0)/(k_BT)}-1}\frac{\partial\varepsilon_B}{\partial n_0}=0. \tag{11}$$

From (7) $\partial\varepsilon_B/\partial\mu=-T_p/\varepsilon_B$ and $\partial\varepsilon_B/\partial n_0=(4gT_p-8g^2\rho_0)/\varepsilon_B$, and putting those derivatives into (10) and (11) one transforms (10), (11) into:

$$\rho-\rho_0=\int\frac{\mathrm{d}^Dp}{(2\pi\hbar)^D}\frac{1}{\mathrm{e}^{\varepsilon_B(p,\mu,|\Psi_0|^2)/k_BT}-1}\frac{T_p}{\varepsilon_B(p,\mu,|\Psi_0|^2)}, \tag{12}$$

$$\mu-2\frac{2\pi\hbar^2f}{m}\rho_0=-8\left(\frac{2\pi\hbar^2f}{m}\right)^2\rho_0\int\frac{d^Dp}{(2\pi\hbar)^D}\frac{1}{\mathrm{e}^{\varepsilon_B(p,\mu,\rho_0)/(k_BT)}-1}\frac{1}{\varepsilon_B}. \tag{13}$$

Eqs. (12) and (13) solve, in principle, the problem. These equations differ from the ones in [8] by changing $\mu\to\mu+2(2\pi\hbar^2f/m)\rho_0$.

One may study numerically the solutions of (12) and (13), after a correct reduction to dimensionless quantities. This reduction depends on the thermodynamical process. In [8] we have considered an isothermal process and we explored the $P-V$ diagram arriving to the conclusion that the transition is not of second order. In that case it was useful to use the thermal de Broglie wavelength $\lambda=\sqrt{2\pi\hbar^2/(mk_BT)}$ as unit length. Densities are made dimensionless by $\tilde\rho=\rho\lambda^D$, $\tilde\rho_0=\rho_0\lambda^D$ and $\tilde\rho'=\tilde\rho-\tilde\rho_0=\rho'\lambda^D$, and the interaction parameter $\alpha=f\lambda^{2-D}$.

Here we shall consider a constant density ρ. In this case it is useful to define a characteristic temperature depending on the particle density: the transition temperature of an ideal Bose gas in 3D is a good candidate

$$T_{\mathrm{BE}}=\frac{2\pi}{\zeta(3/2)^{2/3}}\frac{\hbar^2}{mk_B}\rho^{2/3}.$$

Let us define the dimensionless interaction parameter $\alpha=\zeta(3/2)^{2/3}f\rho^{1/3}$, $y=(\mu/(k_BT_{\mathrm{BE}})-2\alpha\rho_0/\rho)$, $t=T/T_{\mathrm{BE}}$ and $\xi=\rho_0/\rho$, then Eqs. (12) and (13) become

$$1=\xi+t^{3/2}\frac{4}{\sqrt{\pi}\zeta(3/2)}\int_0^\infty\frac{1}{\mathrm{e}^{\hat\varepsilon(x,y,t,\xi)}-1}\frac{\big(x^2-y/t+2\alpha\xi/t\big)}{\hat\varepsilon(x,y,t,\xi)}x^2\,\mathrm{d}x, \tag{14}$$

$$y=-8\alpha^2\xi t^{1/2}\frac{4}{\sqrt{\pi}\zeta(3/2)}\int_0^\infty\frac{1}{\mathrm{e}^{\hat\varepsilon(x,y,t,\xi)}-1}\frac{x^2\,\mathrm{d}x}{\hat\varepsilon(x,y,t,\xi)}, \tag{15}$$

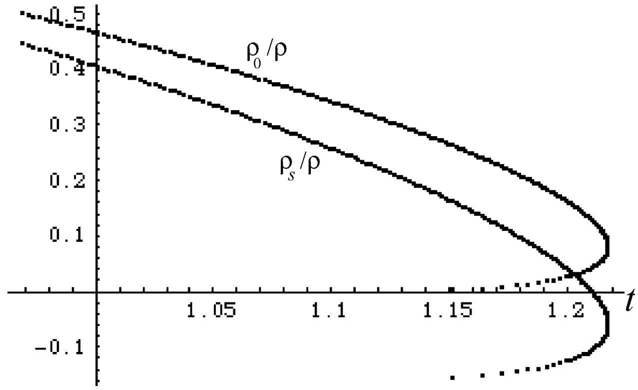

Fig. 1. Condensate fraction: ρ_0/ρ and superfluid fraction: ρ_s/ρ, as functions of the dimensionless temperature $t \equiv T/T_{\mathrm{BE}}$.

where $\hat{\varepsilon}(x, y, t, \xi) = \sqrt{(x^2 - y/t + 2\alpha\xi/t)^2 - 4\alpha^2\xi^2/t^2}$.

We have solved numerically (see Fig. 1 for $\alpha = 0.1$) these coupled equations in terms of the functions $y(\xi)$ and $t(\xi)$ instead of $y(t)$ and $\xi(t)$ because condensate density is a multivalued function of temperature. Solutions are found by iterating the map:

$$y_{n+1} = -8\alpha^2 \xi t_n^{1/2} \frac{4}{\sqrt{\pi}\zeta(3/2)} \int_0^\infty \frac{1}{\mathrm{e}^{\hat{\varepsilon}(x,y_n,t_n,\xi)} - 1} \frac{x^2\,\mathrm{d}x}{\hat{\varepsilon}(x, y_n, t_n, \xi)}$$

and

$$t_{n+1} = \left(\frac{1-\xi}{(4/(\sqrt{\pi}\zeta(3/2)))\int_0^\infty (1/(\mathrm{e}^{\hat{\varepsilon}(x,y_n,t_n,\xi)} - 1))((x^2 - y_n/t_n + 2\alpha\xi/t_n)/\hat{\varepsilon}(x, y_n, t_n, \xi))x^2\,\mathrm{d}x}\right)^{2/3},$$

that converges easily to a fixed point.

Coming from high temperature region we observe that the condensate density jumps from zero value to a finite one at a temperature $Tc > T_{\mathrm{BE}}$ depending only on α. This is because the curve ρ_0/ρ versus t possesses a turning point characteristic of a subcritical behavior.

Finally, let us go back to the Landau's expression for the normal density. The momentum of the quasiparticle gas of excitations moving with a speed $\mathbf{v}$ with respect to the condensate is

$$\mathbf{j}_n = \mathrm{Tr}\left(\sum_p{}' \mathbf{p} a_p^\dagger a_p \frac{\mathrm{e}^{-(H - \sum_p{}' \mathbf{v}\cdot\mathbf{p} a_p^\dagger a_p)/(k_B T)}}{Z_N}\right) = k_B T \frac{\partial \ln Z_N}{\partial \mathbf{v}},$$

where the second equality holds because energy and momentum commutes and Z_N is the trace $Z_N(n_0, \mu, \mathbf{v}) = \mathrm{Tr}(\mathrm{e}^{-(H-\sum_p{}'\mathbf{v}\cdot\mathbf{p}a_p^\dagger a_p)/(k_B T)})$. This trace and the thermodynamical stability are considered by Pomeau in this volume [9]; the leading result is that the partition function (9) remains as stated but changing the Bogoliubov spectrum (7): $\varepsilon_B(p, \mu, |\Psi_0|^2) \to \varepsilon_B(p, \mu, |\Psi_0|^2) - \mathbf{v} \cdot \mathbf{p}$. Moreover, Landau's formulas for the flux of mass and the normal density (2) remain unchanged, but take $\varepsilon_B(p, \mu, |\Psi_0|^2)$ as the energy spectrum. The superfluid density $\rho_s \equiv \rho - \rho_n$ differs quantitatively from the condensate density and does not enter the equations of state (12) and (13). It depends explicitly on the temperature, condensate density and chemical potential in a passive way. In terms of the normalization used in (14) and (15) one obtains:

$$\frac{\rho_s}{\rho} = 1 - \frac{8t^{3/2}}{3\sqrt{\pi}\zeta(3/2)} \int_0^\infty \frac{x^4\,\mathrm{e}^{\hat{\varepsilon}(x,y,t,\xi)}}{(\mathrm{e}^{\hat{\varepsilon}(x,y,t,\xi)} - 1)^2}\,\mathrm{d}x.$$

In Fig. 1 it the superfluid fraction ρ_s/ρ is added as a function of temperature. Although the condensate density jumps from zero to a finite value at the returning point T_c, the superfluid density posses a negative fictitious value at T_c. As said previously Landau's formula makes sense only if $\rho_s \geqslant 0$ and this happens only below a temperature T_s such that $T_{\mathrm{BE}} < T_s < T_c$. In conclusion, the appearence of a Bose–Einstein thermodynamical phase does not means that a superfluid state, in the sense that the fluid could realize a flow without dissipation, appears at the same temperature. Going back to Landau's seminal work [1], perhaps, superfluidity is not directly related to Bose–Einstein condensation, at least in the limit of a dilute gas $f\rho^{1/3} \to 0$.

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