Theory of Bose-Einstein condensation with pair correlations

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Abstract

We study the thermodynamic properties of an interacting Bose gas with condensate using the energy-functional formulation of the Hartree-Fock-Bogoliubov (HFB) approach. For contact interaction, we obtain a solution with self-eliminating divergence to the coupled equations describing a condensate of correlated pairs of particles in equilibrium. We analyze the temperature dependencies of thermodynamic quantities such as condensate density, chemical potential, and pressure and compare them with those of Popov approximation. Our results show a first-order phase transition from the normal to the paired condensate state, with a higher transition temperature than that of an ideal Bose gas.

Energy-functional formulation of HFB approach

The non-equilibrium state of a quasiparticle Bose gas in the presence of anomalous averages is characterized by the following non-equilibrium statistical operator:

$$\rho = \exp(Z - F), \quad F = a^\dagger_{\mathbf{p}} A_{\mathbf{pp}'} a_{\mathbf{p}'} + \frac{1}{2}(a_{\mathbf{p}} B_{\mathbf{pp}'} a_{\mathbf{p}'} + a^\dagger_{\mathbf{p}} B^*_{\mathbf{pp}'} a^\dagger_{\mathbf{p}'}) + a^\dagger_{\mathbf{p}} C_{\mathbf{p}} + C^*_{\mathbf{p}} a_{\mathbf{p}}, \tag{1}$$

In equilibrium, $A_{\mathbf{pp}'}$ and $B_{\mathbf{pp}'}$ are determined through the self-consistency procedure. This statistical operator modifies Wick's rule, producing both normal and anomalous averages,

$$f_{\mathbf{p}_2\mathbf{p}_1} = \operatorname{Sp}\rho a^\dagger_{\mathbf{p}_1} a_{\mathbf{p}_2}, \quad g_{\mathbf{p}_2\mathbf{p}_1} = \operatorname{Sp}\rho a_{\mathbf{p}_1} a_{\mathbf{p}_2}, \quad g^\dagger_{\mathbf{p}_2\mathbf{p}_1} = \operatorname{Sp}\rho a^\dagger_{\mathbf{p}_1} a^\dagger_{\mathbf{p}_2}, \quad \operatorname{Sp}\rho a_{\mathbf{p}} = b_{\mathbf{p}}, \quad \operatorname{Sp}\rho a^\dagger_{\mathbf{p}} = b^*_{\mathbf{p}}. \tag{2}$$

The normal and anomalous distribution functions are conveniently combined into a block matrix, and the condensate amplitudes into a column vector:

$$\hat f = \begin{pmatrix} f & -g \\ g^\dagger & -1-\tilde f \end{pmatrix}, \quad \hat b = \begin{pmatrix} b \\ b^* \end{pmatrix}.$$

According to (2), the matrices A, B and $B^\dagger$ in (1) are expressed through f, g and $g^\dagger$. Hence, the statistical operator and the non-equilibrium entropy $S = -\operatorname{Sp}\rho\ln\rho$ are functionals of the normal and anomalous distribution functions only, $\rho = \rho(\hat f)$ and $S = S(\hat f)$. Note that $\hat f$ is isomorphic under the canonical transformation that diagonalizes both ρ and $\hat f$. As a result, one can show that

$$\frac{\delta S(\hat f)}{\delta f_{\mathbf{p}_2\mathbf{p}_1}} = A_{\mathbf{p}_1\mathbf{p}_2}, \quad \frac{\delta S(\hat f)}{\delta g_{\mathbf{p}_2\mathbf{p}_1}} = \frac{1}{2} B_{\mathbf{p}_1\mathbf{p}_2}, \quad \frac{\delta S(\hat f)}{\delta g^\dagger_{\mathbf{p}_2\mathbf{p}_1}} = \frac{1}{2} B^\dagger_{\mathbf{p}_1\mathbf{p}_2}.$$

The equilibrium values of $\hat f$ and $\hat b$ are determined by maximizing the entropy at fixed energy $E(\hat f, \hat b) = \operatorname{Sp}\rho H$ and particle number $N(\hat f, \hat b) = \operatorname{Sp}\rho N$ with the corresponding Lagrange multipliers interpreted as the inverse temperature β and the chemical potential μ. The solution of the variational problem reads,

$$\hat f = [\exp(\beta\hat\xi) - 1]^{-1}, \qquad \hat\eta - \mu\hat b = 0, \tag{3}$$

where

$$\hat\xi = \begin{pmatrix} \varepsilon - \mu & \Delta \\ -\Delta^* & -\tilde\varepsilon + \mu \end{pmatrix}, \quad \hat\eta = \begin{pmatrix} \eta \\ \eta^* \end{pmatrix} \tag{4}$$

and

$$\varepsilon_{\mathbf{pp}'} = \frac{\delta E(\hat f, \hat b)}{\delta f_{\mathbf{p}'\mathbf{p}}}, \quad \Delta_{\mathbf{pp}'} = 2\frac{\delta E(\hat f, \hat b)}{\delta g_{\mathbf{p}'\mathbf{p}}}, \quad \eta_{\mathbf{p}} = \frac{\delta E(\hat f, \hat b)}{\delta b^*_{\mathbf{p}}}.. \tag{5}$$

For uniform state, $f_{\mathbf{pp}'} = f_{\mathbf{p}}\delta_{\mathbf{pp}'}$, $g_{\mathbf{pp}'} = g_{\mathbf{p}}\delta_{\mathbf{p},-\mathbf{p}'}$, $b_{\mathbf{p}} = b_0\delta_{\mathbf{p},0}$ and $n_0 = b_0^* b_0/V$ is the condensate density.

The self-consistency equations for the Hamiltonian with a pairwise contact interaction

For the Hamiltonian with pairwise contact interaction $U = \frac{4\pi\hbar^2}{m}a > 0$ (repulsive forces), we obtain from (3)–(5) three equations, supplemented by an equation for the total particle number n:

$$\xi_{\mathbf{p}} = \frac{p^2}{2m} - \mu + 2nU, \quad \Delta = n_0 U - \Delta U I, \quad [\Delta + 2(n - n_0)U - \mu]\sqrt{n_0} = 0, \tag{6}$$

$$n = n_0 + \frac{1}{2V}\sum_{\mathbf{p}}\left(\frac{\xi_{\mathbf{p}}}{E_{\mathbf{p}}}(1 + 2\nu_{\mathbf{p}}) - 1\right), \tag{7}$$

where the quasiparticle distribution function $\nu_{\mathbf{p}}$ and quasiparticle energy $E_{\mathbf{p}}$ are given by

$$E_{\mathbf{p}} = \sqrt{\xi^2_{\mathbf{p}} - |\Delta_{\mathbf{p}}|^2}, \quad \nu_{\mathbf{p}} = [\exp(\beta E_{\mathbf{p}}) - 1]^{-1}.$$

The second equation in (6) contains a divergent term I (at high momenta) given by

$$I = \frac{1}{2V}\sum_{\mathbf{p}}\frac{1}{E_{\mathbf{p}}}(1 + 2\nu_{\mathbf{p}}).$$

I. Popov gapless approximation (PA) neglects the divergent term. Therefore, we have

$$\xi^{\text{PA}}_{\mathbf{p}} = \frac{p^2}{2m} + n_0 U, \quad \Delta^{\text{PA}} = n_0 U, \quad \mu^{\text{PA}} = n_0 U + 2(n - n_0)U,$$

$$E^{\text{PA}}_{\mathbf{p}} = \sqrt{\frac{p^2}{2m}\left(\frac{p^2}{2m} + 2n_0 U\right)}.$$

The temperature dependence $n_0(T)$ is provided by (7). The expression for pressure takes the form

$$P^{\text{PA}} = \frac{1}{2V}\sum_{\mathbf{p}}(\xi_{\mathbf{p}} - E_{\mathbf{p}}) + n^2 U - \frac{n_0^2 U}{2} + \frac{k_B T}{V}\sum_{\mathbf{p}}\ln(1 + \nu_{\mathbf{p}}).$$

II. Solution with self-eliminating divergence (SSED):

$$\Delta^{\text{SSED}} = \lim_{I\to\infty}\frac{n_0 U}{1 + UI} = \lim_{I\to\infty}\frac{n_0}{I} = 0, \quad \mu^{\text{SSED}} = 2(n - n_0)U, \quad E^{\text{SSED}}_{\mathbf{p}} = \xi^{\text{SSED}}_{\mathbf{p}} = \frac{p^2}{2m} + 2n_0 U,$$

$$n = n_0 + \frac{1}{V}\sum_{\mathbf{p}}\nu^{\text{SSED}}_{\mathbf{p}}, \quad \nu^{\text{SSED}}_{\mathbf{p}} = \left[\exp\left(\beta\xi^{\text{SSED}}_{\mathbf{p}}\right) - 1\right]^{-1}.$$

The energy gap lies in the range $E_0 \in (0, 2n_0 U]$. Its maximum value, $E_0 = 2n_0 U$, is reached for the SSED. The zero energy gap arises only within the Popov gapless approximation, which does not represent a self-consistent solution of the coupled equations corresponding to the Hartree–Fock–Bogoliubov framework.

Let us find the anomalous correlation function $g_{\mathbf{p}}$ that determines the number of paired particles,

$$\frac{1}{V}\left|\sum_{\mathbf{p}} g_{\mathbf{p}}\right| = \frac{1}{V}\left|\sum_{\mathbf{p}}\frac{\Delta_{\mathbf{p}}}{2E_{\mathbf{p}}}(1 + 2\nu_{\mathbf{p}})\right| = \lim_{I\to\infty}\frac{n_0}{I}\cdot I = n_0.$$

This implies that all correlated particles are in the condensate. The corresponding pressure reads

$$P^{\text{SSED}} = (n^2 - n_0^2)U + \frac{k_B T}{V}\sum_{\mathbf{p}}\ln(1 + \nu_{\mathbf{p}}).$$

At absolute zero temperature ($T = 0$), both condensate depletion ($n = n_0$) and pressure vanish.

Normal state (NS) is obtained by setting $\sqrt{n_0} = 0$ (see the third equation in (6)):

$$\Delta^{\text{NS}} = 0, \qquad E^{\text{NS}}_{\mathbf{p}} = \xi^{\text{NS}}_{\mathbf{p}} = \frac{p^2}{2m} - \mu + 2nU,$$

$$n = \frac{1}{V}\sum_{\mathbf{p}}\nu^{\text{NS}}_{\mathbf{p}}, \quad \nu^{\text{NS}}_{\mathbf{p}} = \left[\exp\left(\beta\xi^{\text{NS}}_{\mathbf{p}}\right) - 1\right]^{-1}.$$

This solution ensures the conservation law for the total particle number by appropriately adjusting the chemical potential μ. The pressure in the normal state is written as

$$P^{\text{NS}} = n^2 U + \frac{k_B T}{V}\sum_{\mathbf{p}}\ln(1 + \nu_{\mathbf{p}}).$$

Physical observables

The turning point in the retrograde behavior of physical observables below defines the transition temperature of the interacting Bose gas.

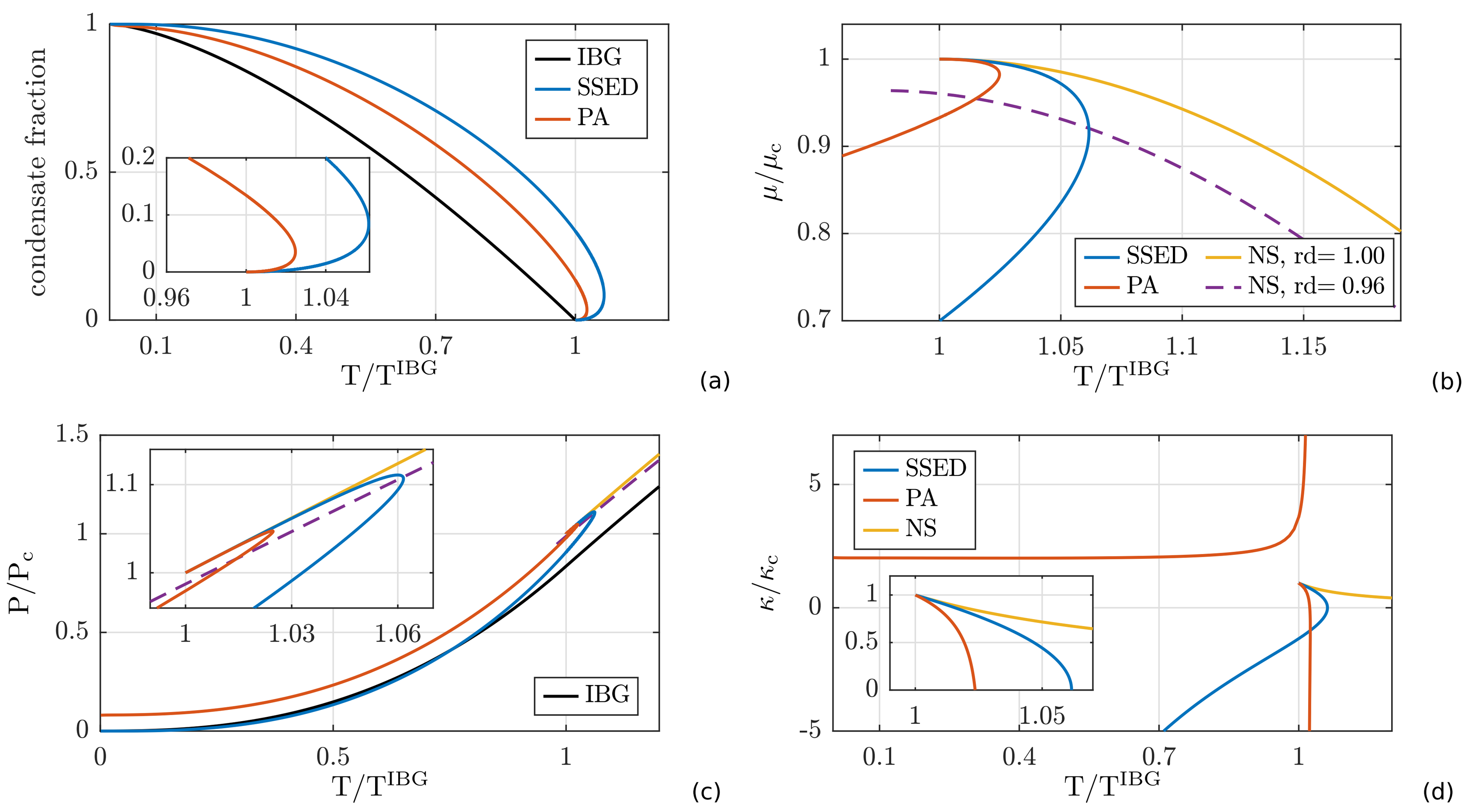

Figure 1: *Temperature dependencies of: (a) condensate fraction n_0/n, (b) chemical potential, (c) pressure, (d) isothermic compressibility — for the total density of degenerate state $n^{deg} = 1.6\cdot 10^{14}$ cm^{-3}, the scattering length $a = 4.9$ nm, $\mu_c = \mu^{NS}(T = T^{IBG}) = 2nU$, $P_c = P^{NS}(T = T^{IBG}) = n^2 U + \zeta(5/2)/\zeta(3/2) n k_B T^{IBG}$ and $\kappa_c = 1/(n\mu_c)$. The solid curves refer to: ideal Bose gas (IBG), solution with self-eliminating divergence (SSED), Popov approximation (PA) and normal state (NS) — for total density $n = n^{deg}$, i.e. relative density rd$= n/n^{deg} = 1$. The dashed curve refers to the normal state for rd$= 0.96$. Magnified sections of the foregoing curves with retrograde behaviour are shown in the insets.*

Summary

- In the case of contact interaction, we have found a solution with self-eliminating divergence to the self-consistency equations within HFB approach.
- This solution implies that at $T = 0$, there is no quantum depletion, all correlated particles are in the condensate and pressure exactly vanishes.
- We have numerically analyzed the temperature dependence of main thermodynamic quantities for the obtained solution and compared them with those predicted by the Popov approximation.
- We have observed a first-order phase transition from the normal to the paired condensate state.
- We have predicted an increase in the transition temperature compared to that of an ideal gas.
- We have observed the negative compressibility below the critical temperature for SSED. At the same time, the system of equations does not allow for the existence of a pure single-particle condensate. Thus, neither pure single-particle nor pure pair condensates exist; only a mixture of both is possible.

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