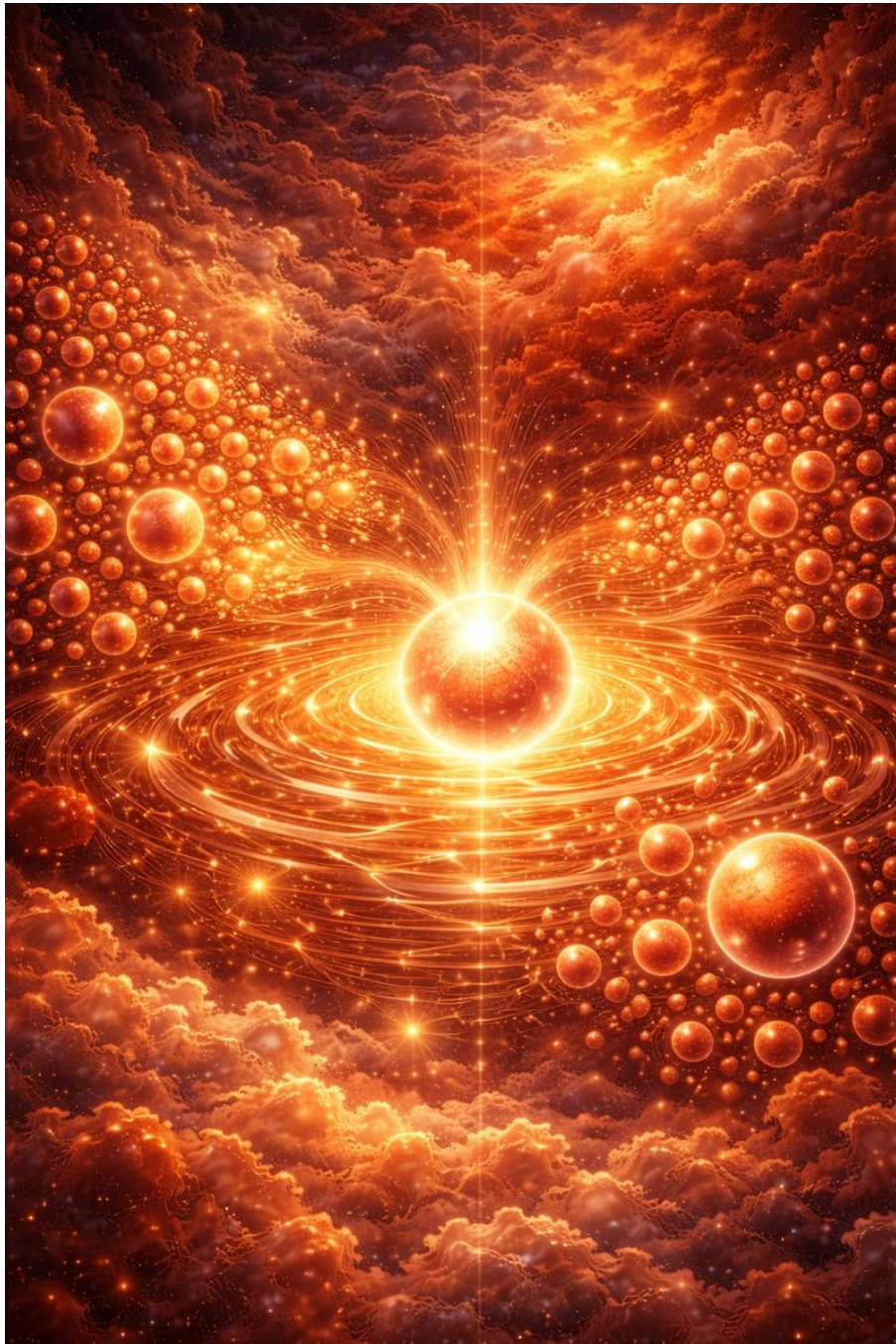


Bose–Einstein Condensation

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1 BEC in a Free Boson Gas

1.1 Bose distribution from a statistical-mechanics viewpoint

Setup and thermodynamic variables. We consider a three-dimensional gas of non-interacting bosons in a volume V . Single-particle eigenmodes are plane waves labeled by wave vector \mathbf{k} , with free-particle dispersion

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}, \quad (1)$$

where m is the particle mass.

Grand-canonical distribution and the role of μ . In the grand-canonical ensemble at temperature T , the thermal average occupation¹ of a single-particle mode \mathbf{k} is

$$n_{\mathbf{k}} = \frac{1}{\exp((\epsilon_{\mathbf{k}} - \mu)/(k_B T)) - 1}, \quad (2)$$

where k_B is Boltzmann's constant and μ is the chemical potential. Here μ is *not* a microscopic interaction energy (there is no interaction); rather, it is a Lagrange multiplier that enforces the correct average particle number in the grand-canonical description.

Particle-number constraint and thermodynamic limit. The total particle number is obtained by summing over all modes,

$$N = \sum_{\mathbf{k}} n_{\mathbf{k}}. \quad (3)$$

At fixed density $n \equiv N/V$, in the thermodynamic limit $N \rightarrow \infty$, $V \rightarrow \infty$ with n fixed, the sum becomes an integral over momentum space,

$$n = \frac{1}{(2\pi)^3} \int d^3k \frac{1}{\exp((\epsilon_{\mathbf{k}} - \mu)/(k_B T)) - 1}. \quad (4)$$

The problem is then: for each T , determine $\mu(T)$ such that (4) holds.

Chemical potential in the Bose distribution: why $\mu \leq 0$ and how μ changes with T

Why must $\mu \leq \epsilon_{\min}$, hence $\mu \leq 0$ for a free gas?. For the Bose distribution (2) to be well-defined (finite and non-negative) for all modes, the denominator must be positive:

$$\exp((\epsilon_{\mathbf{k}} - \mu)/(k_B T)) - 1 > 0 \iff \epsilon_{\mathbf{k}} - \mu > 0 \text{ for all } \mathbf{k}. \quad (5)$$

For a free gas the lowest single-particle energy is $\epsilon_{\min} = \epsilon_{\mathbf{k}=0} = 0$ (choosing the energy zero at the band minimum), therefore one must have $\mu \leq 0$. If one tries $\mu > 0$, then at $\mathbf{k} = 0$ the denominator becomes $\exp(-\mu/(k_B T)) - 1 < 0$, leading to an unphysical negative occupation.

Why does μ increase as T decreases (at fixed density)?. At fixed density n , lowering T suppresses thermal occupation of excited states. For each fixed \mathbf{k} , the function $n_{\mathbf{k}}$ in (2) is monotone increasing in μ ; hence the total density in (4) is also monotone increasing in μ . Therefore, to keep n fixed while decreasing T , the chemical potential must increase (become less negative), approaching its upper bound 0.

A key thermodynamic-limit point. As long as $\mu < 0$, every fixed mode has $n_{\mathbf{k}} = O(1)$ while the total particle number scales as $N = O(V)$. Thus, any *single* mode carries a vanishing fraction

¹Note that here $n_{\mathbf{k}}$ is actually the density in the phase space (\mathbf{r}, \mathbf{k}) . If additional potential is not considered, $n(\mathbf{r})$ is uniform, so we take $n(\mathbf{r}) = n$ for short. For the inhomogeneous case, refer to Thomas-Fermi Distribution.

of particles: $n_k/N \rightarrow 0$. This statement fails precisely when one mode becomes *macroscopically occupied*, which is the defining feature of Bose–Einstein condensation in a free gas.

1.2 The emergence of BEC

Critical temperature from the saturation of μ . The central question is whether there exists a temperature T_c at which μ reaches its maximal allowed value 0. If such a T_c exists, it is determined by the number constraint evaluated at $\mu = 0$:

$$n = \frac{1}{(2\pi)^3} \int d^3k \frac{1}{\exp(\epsilon_k/(k_B T)) - 1} \quad (\mu = 0). \quad (6)$$

Using spherical coordinates $d^3k = 4\pi k^2 dk$ and $\epsilon_k = \hbar^2 k^2/(2m)$, we obtain

$$n = \frac{1}{2\pi^2} \int_0^\infty dk \frac{k^2}{\exp(\hbar^2 k^2/(2mk_B T)) - 1}. \quad (7)$$

Introduce the dimensionless variable

$$z = \frac{\hbar^2 k^2}{2mk_B T}, \quad k = \sqrt{\frac{2mk_B T}{\hbar^2}} z^{1/2}, \quad dk = \sqrt{\frac{2mk_B T}{\hbar^2}} \frac{1}{2} z^{-1/2} dz, \quad (8)$$

so that $k^2 dk = \left(\frac{2mk_B T}{\hbar^2}\right)^{3/2} \frac{1}{2} z^{1/2} dz$. Then

$$n = \frac{1}{4\pi^2} \left(\frac{2mk_B T}{\hbar^2}\right)^{3/2} \int_0^\infty dz \frac{z^{1/2}}{e^z - 1}. \quad (9)$$

Using

$$\frac{1}{e^z - 1} = \sum_{\ell=1}^\infty e^{-\ell z} \quad (z > 0), \quad (10)$$

and the Gamma-function identity $\int_0^\infty dz z^{s-1} e^{-\ell z} = \Gamma(s) \ell^{-s}$ with $s = 3/2$, we find

$$\int_0^\infty dz \frac{z^{1/2}}{e^z - 1} = \frac{\sqrt{\pi}}{2} \zeta(3/2), \quad (11)$$

where ζ is the Riemann zeta function. Plugging this into (9) gives

$$n = \zeta(3/2) \left(\frac{mk_B T}{2\pi\hbar^2}\right)^{3/2}. \quad (12)$$

Setting $T = T_c$ yields the critical temperature

$$T_c = \frac{2\pi\hbar^2}{mk_B} \left(\frac{n}{\zeta(3/2)}\right)^{2/3}. \quad (13)$$

■ Physical interpretation: thermal wavelength \sim inter-particle spacing.

Define the thermal de Broglie wavelength

$$\lambda_T \equiv \sqrt{\frac{2\pi\hbar^2}{mk_B T}}. \quad (14)$$

Then

$$n = \frac{\zeta(3/2)}{\lambda_T^3} \implies n\lambda_{T_c}^3 = \zeta(3/2) \approx 2.612. \quad (15)$$

Thus, at the transition the wave-packet size λ_T becomes comparable to the mean inter-particle distance $d \sim n^{-1/3}$, i.e.,

$$\lambda_{T_c} \sim d \iff k_B T_c \sim \frac{\hbar^2}{md^2}. \quad (16)$$

Macroscopic occupation below T_c . Below T_c , the chemical potential cannot increase above 0, hence it stays pinned at $\mu = 0$. At $\mu = 0$, excited states can hold only a finite particle density

$$n_{\text{ex}}(T) = \frac{1}{(2\pi)^3} \int d^3k \frac{1}{e^{\epsilon_k/(k_B T)} - 1} = \zeta(3/2) \left(\frac{mk_B T}{2\pi\hbar^2} \right)^{3/2} = \frac{\zeta(3/2)}{\lambda_T^3}. \quad (17)$$

For fixed total density n , the remaining particles must accumulate in the lowest-energy mode $k = 0$. Thus, for $T < T_c$,

$$N = N_0 + \frac{V}{(2\pi)^3} \int d^3k \frac{1}{e^{\epsilon_k/(k_B T)} - 1} \quad (\mu = 0), \quad (18)$$

and the condensate fraction is

$$\frac{N_0}{N} = 1 - \frac{n_{\text{ex}}(T)}{n} = 1 - \left(\frac{T}{T_c} \right)^{3/2}. \quad (19)$$

Important conclusion. In a free 3D Bose gas, BEC is the *saturation* of the excited-state population at $\mu = 0$: below T_c , excited states can no longer accommodate all particles at fixed density, forcing a macroscopic occupation $N_0 = O(N)$ of the single mode $k = 0$.

1.3 Extending the notion of BEC to interacting systems

Structural lesson from the free gas.

The free-gas discussion teaches a robust structural criterion:

- above T_c , every single-particle mode carries a negligible fraction $N_i/N \rightarrow 0$;
- below T_c , at least one mode carries a finite fraction $N_0/N \not\rightarrow 0$ (macroscopic occupation).

This criterion suggests a path to generalization, because it is phrased in terms of scaling with system size rather than in terms of a specific momentum label.

Why interactions force a new definition. In a generic interacting many-body system, “counting particles in the eigenmodes of the full Hamiltonian” is not meaningful as a one-body statement, and even momentum need not be a good quantum number (e.g., trapped or inhomogeneous systems). Thus, to generalize BEC beyond a free gas, one needs an operational, basis-independent definition.

Penrose–Onsager idea. The key idea is to define condensation through the spectral structure of the *one-body reduced density matrix*, which is defined directly from the many-body state and exists irrespective of interactions. Macroscopic occupation becomes a statement about the scaling of the largest eigenvalue of that reduced density matrix, and the corresponding eigenfunction plays the role of the condensate orbital.

2 General Definition of BEC: one-body density matrix and ODLRO

2.1 Definition of the one-body density matrix

■ **Second-quantized definition.** In second quantization, the one-body density matrix (one-body reduced density matrix) is defined as the equal-time two-point function

$$\rho(\mathbf{r}, \mathbf{r}') \equiv \langle \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}') \rangle, \quad (20)$$

where $\hat{\Psi}(\mathbf{r})$ annihilates a boson at position \mathbf{r} and $\hat{\Psi}^\dagger(\mathbf{r})$ creates one. Operationally, $\rho(\mathbf{r}, \mathbf{r}')$ is the (state-averaged) amplitude for removing a particle at \mathbf{r}' and inserting it at \mathbf{r} , hence it directly measures single-particle coherence in space.

■ **First-quantized representation: how $\hat{\Psi}(\mathbf{r})$ acts in coordinate space.** Let $|\Psi_N\rangle$ be a normalized N -boson state, and define its symmetric first-quantized wave function by

$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) \equiv \langle \mathbf{r}_1, \dots, \mathbf{r}_N | \Psi_N \rangle. \quad (21)$$

Define the coordinate basis states via field operators,

$$|\mathbf{r}_1, \dots, \mathbf{r}_N\rangle \equiv \frac{1}{\sqrt{N!}} \hat{\Psi}^\dagger(\mathbf{r}_1) \dots \hat{\Psi}^\dagger(\mathbf{r}_N) |0\rangle. \quad (22)$$

Similarly, the $(N-1)$ -particle coordinate basis states are

$$|\mathbf{r}_2, \dots, \mathbf{r}_N\rangle \equiv \frac{1}{\sqrt{(N-1)!}} \hat{\Psi}^\dagger(\mathbf{r}_2) \dots \hat{\Psi}^\dagger(\mathbf{r}_N) |0\rangle. \quad (23)$$

Using these definitions, one finds the fundamental identity

$$\langle \mathbf{r}_2, \dots, \mathbf{r}_N | \hat{\Psi}(\mathbf{r}) | \Psi_N \rangle = \sqrt{N} \Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N), \quad (24)$$

i.e., $\hat{\Psi}(\mathbf{r})$ removes one coordinate from the symmetric N -body wave function, with the factor \sqrt{N} fixed by normalization.

Deriving the standard integral formula for $\rho(\mathbf{r}, \mathbf{r}')$. Insert a resolution of identity on the $(N-1)$ -particle Hilbert space,

$$\mathbb{I}_{N-1} = \int d^3\mathbf{r}_2 \dots d^3\mathbf{r}_N |\mathbf{r}_2, \dots, \mathbf{r}_N\rangle \langle \mathbf{r}_2, \dots, \mathbf{r}_N|. \quad (25)$$

Then, using (24),

$$\begin{aligned} \rho(\mathbf{r}, \mathbf{r}') &= \langle \Psi_N | \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}') | \Psi_N \rangle \\ &= N \int d^3\mathbf{r}_2 \dots d^3\mathbf{r}_N \Psi^*(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \Psi(\mathbf{r}', \mathbf{r}_2, \dots, \mathbf{r}_N). \end{aligned} \quad (26)$$

This makes the “reduction” explicit: $\rho(\mathbf{r}, \mathbf{r}')$ is the partial trace of the full N -body density operator over $N-1$ coordinates, represented as an integral kernel.

Density-matrix formalism: “matrix” vs “kernel” and one-body observables

In finite dimensions one writes a density matrix as ϱ_{ij} in a basis $\{|i\rangle\}$. In the continuum, the same object is represented by its coordinate-space kernel $\varrho(\mathbf{r}, \mathbf{r}') = \langle \mathbf{r} | \hat{\varrho} | \mathbf{r}' \rangle$, i.e., an “infinite matrix” with continuous indices.

Why ρ determines all one-body expectation values. If a one-body observable has the second-quantized form

$$\hat{O} = \int d^3r d^3r' O(\mathbf{r}, \mathbf{r}') \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}'), \quad (27)$$

then its expectation value is

$$\langle \hat{O} \rangle = \int d^3r d^3r' O(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}, \mathbf{r}'). \quad (28)$$

This is the continuum analogue of $\langle O \rangle = \text{Tr}(\hat{\rho} \hat{O})$.

The one-body density matrix $\rho(\mathbf{r}, \mathbf{r}')$ is not merely a definition: it is the *complete* object controlling all one-body physics (densities, currents, momentum distribution, and interference), because every one-body expectation value reduces to a contraction with ρ .

2.2 Eigen-decomposition of the one-body density matrix

Operator viewpoint. View $\rho(\mathbf{r}, \mathbf{r}')$ as the integral kernel of a linear operator $\hat{\rho}$ acting on single-particle wave functions:

$$(\hat{\rho}\psi)(\mathbf{r}) = \int d^3r' \rho(\mathbf{r}, \mathbf{r}') \psi(\mathbf{r}'). \quad (29)$$

For physically relevant states, $\hat{\rho}$ is Hermitian, positive semidefinite, and trace-class with $\text{Tr} \hat{\rho} = N$.

Spectral decomposition and natural orbitals. These properties imply an orthonormal eigenbasis $\{\psi_i\}$ with nonnegative eigenvalues $\{N_i\}$ summing to N :

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_i N_i \psi_i^*(\mathbf{r}) \psi_i(\mathbf{r}'), \quad N_i \geq 0, \quad \sum_i N_i = N. \quad (30)$$

The $\psi_i(\mathbf{r})$ are called *natural orbitals*, and the N_i are their *occupation numbers* extracted from the many-body state itself.

Mathematical principle behind the spectral decomposition

Under mild conditions, $\hat{\rho}$ is a positive, self-adjoint, trace-class operator on the one-particle Hilbert space. Trace-class implies compactness; compact self-adjoint operators admit a discrete spectrum (possibly accumulating only at zero) with an orthonormal eigenbasis. Positivity implies $N_i \geq 0$, and $\text{Tr} \hat{\rho} = N$ gives $\sum_i N_i = N$. Thus (30) is as canonical as diagonalizing a Hermitian matrix, with \mathbf{r} and \mathbf{r}' playing the role of continuous indices.

2.3 ODLRO and types of BEC

Penrose–Onsager criterion. In the thermodynamic limit, classify phases by how the eigenvalues in (30) scale with N :

- **Normal phase:** for every i , $\lim_{N \rightarrow \infty} N_i/N = 0$.
- **Simple BEC:** there exists exactly one eigenvalue N_0 such that $\lim_{N \rightarrow \infty} N_0/N \neq 0$.
- **Fragmented BEC:** more than one eigenvalue has a finite fraction, i.e., $\lim_{N \rightarrow \infty} N_i/N \neq 0$ for multiple i .

Connection to off-diagonal long-range order (ODLRO). If a simple condensate exists, then the leading contribution to $\rho(\mathbf{r}, \mathbf{r}')$ is

$$\rho(\mathbf{r}, \mathbf{r}') \approx N_0 \psi_0^*(\mathbf{r}) \psi_0(\mathbf{r}'). \quad (31)$$

If ψ_0 is extended (as in a homogeneous system), this term does not decay with $|\mathbf{r} - \mathbf{r}'|$, implying long-range single-particle coherence. This long-distance persistence of off-diagonal correlations is what is meant by ODLRO.

2.4 Higher-order density matrices and “pair condensation”

Two-body density matrix. To diagnose condensation of composite objects, define higher-order reduced density matrices. For example, the two-body density matrix is

$$\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = \langle \hat{\Psi}^\dagger(\mathbf{r}_1) \hat{\Psi}^\dagger(\mathbf{r}_2) \hat{\Psi}(\mathbf{r}'_1) \hat{\Psi}(\mathbf{r}'_2) \rangle. \quad (32)$$

Meaning of a macroscopic eigenvalue of $\rho^{(2)}$. If $\rho^{(2)}$ has an eigenvalue that scales macroscopically with system size (with the appropriate thermodynamic scaling for pairs), one speaks of “pair condensation”: a macroscopic number of pairs occupy a single two-body orbital. The logical structure mirrors the one-body case: form the reduced density operator for the object of interest, diagonalize it, and examine eigenvalue scaling.

2.5 Brief experimental criteria

Time-of-flight (TOF) as a practical probe. In ultracold-atom experiments, a common signature of BEC is the appearance of a sharp, slowly expanding component in TOF imaging. The basic idea is that, after suddenly turning off the trap, atoms expand approximately ballistically so that the long-time density profile reflects the initial momentum distribution. A condensate corresponds to macroscopic occupation of a single mode (in a homogeneous system, near $k = 0$), producing a pronounced peak in the measured distribution. Finite-size and interaction effects during early expansion can complicate the details, but the organizing principle remains: BEC manifests as a dramatic reorganization consistent with a macroscopically occupied mode.

3 Condensate wave function vs the true many-body state

3.1 The condensate wave function

Definition from the dominant natural orbital. In a simple BEC, the one-body density matrix is dominated by a single eigenvalue $N_0 = O(N)$ and its eigenfunction $\psi_0(\mathbf{r})$. It is natural to define the *condensate wave function* as

$$\Phi(\mathbf{r}) \equiv \sqrt{N_0} \psi_0(\mathbf{r}). \quad (33)$$

Then (31) can be written as $\rho(\mathbf{r}, \mathbf{r}') \approx \Phi^*(\mathbf{r}) \Phi(\mathbf{r}')$, which highlights that $\Phi(\mathbf{r})$ encodes the long-range one-body coherence.

The condensate wave function $\Phi(\mathbf{r})$ is a *one-particle-level descriptor* extracted from the many-body state via $\rho(\mathbf{r}, \mathbf{r}')$; it is not the full many-body wave function. Distinct many-body states can share the same ρ (hence the same Φ) while differing in higher-order correlations.

3.2 Two useful microscopic pictures

Option I: number-conserving Hartree product state. A microscopic realization of a simple condensate is the symmetric product state

$$\Psi(r_1, \dots, r_N) = \prod_{i=1}^N \psi(r_i), \quad \int d^3r |\psi(r)|^2 = 1. \quad (34)$$

Substituting (34) into the first-quantized formula (26) gives

$$\rho(r, r') = N \psi^*(r) \psi(r'), \quad (35)$$

which is rank one with $N_0 = N$ and $\psi_0 = \psi$.

Option II: coherent-state description (useful for fluctuations). A single-mode coherent state $|\alpha\rangle$ is defined by

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \quad |\alpha\rangle = e^{-|\alpha|^2/2} \exp(\alpha \hat{a}^\dagger) |0\rangle. \quad (36)$$

For a spatially varying condensate one uses a field coherent state

$$|\Psi_{\text{coh}}\rangle = \exp\left(-\frac{1}{2} \int d^3r |\Phi(r)|^2\right) \exp\left(\int d^3r \Phi(r) \hat{\Psi}^\dagger(r)\right) |0\rangle, \quad (37)$$

which satisfies

$$\hat{\Psi}(r) |\Psi_{\text{coh}}\rangle = \Phi(r) |\Psi_{\text{coh}}\rangle. \quad (38)$$

Consequently,

$$\rho(r, r') = \langle \hat{\Psi}^\dagger(r) \hat{\Psi}(r') \rangle = \Phi^*(r) \Phi(r'), \quad (39)$$

displaying the rank-one ODLRO structure.

Coherent states: why they are useful in many-body physics

A coherent state does not have a fixed particle number, i.e., it explicitly breaks the global $U(1)$ symmetry associated with number conservation. However, if the condensate occupation $N_0 \gg 1$, relative number fluctuations scale as $\Delta N_0/N_0 \sim 1/\sqrt{N_0}$, which becomes negligible in the thermodynamic limit. This makes coherent states extremely effective as a computational language: one treats $\Phi(r)$ as a classical background field and expands

$$\hat{\Psi}(r) = \Phi(r) + \delta\hat{\psi}(r), \quad (40)$$

which is the conceptual starting point of Bogoliubov theory for quasiparticles and quantum depletion.

3.3 Remarks

■ **Ansatz choosing: what each picture emphasizes.** The Hartree product (34) and the coherent state (37) are not competing “truths”. The Hartree picture is number-conserving and connects naturally to mean-field energy functionals and variational derivations. The coherent-state picture is tailor-made for fluctuation theory: it converts the condensate into a classical field and makes linearization around it straightforward.

■ **Symmetry breaking vs ODLRO (what is the real diagnostic?).** A number-conserving eigenstate satisfies $\langle \hat{\Psi}(r) \rangle = 0$ because $\hat{\Psi}$ changes particle number by one. Nevertheless, BEC can still exist: the symmetry-respecting diagnostic is ODLRO in $\rho(r, r')$, equivalently a macroscopic eigenvalue N_0 in (30). In the thermodynamic limit, the system becomes extremely sensitive to global phase choices; one may use phase-labeled (symmetry-breaking) states for practical calculations, while restoring number conservation when needed.