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Bose condensation, Cooper pairing and Superfluidity in ultracold atomic gases: Some basic questions

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SOME (VERY) BASIC QUESTIONS CONCERNING BOSE CONDENSATION and SUPERFLUIDITY

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1. What is Bose-Einstein Condensation ("BEC")?

What it is NOT: "$\langle \psi(\mathbf{r}) \rangle \neq 0$"

(never true for any system of conserved particles)

What it is (Penrose and Onsager 1956):

Consider single-particle density matrix

$$\rho(\mathbf{r},\mathbf{r}':t) \equiv \int d\mathbf{r}_2 \dots d\mathbf{r}_N \Psi^*(\mathbf{r}_1\mathbf{r}_2\dots\mathbf{r}_N : t)\Psi(\mathbf{r}_1'\mathbf{r}_2\dots\mathbf{r}_N : t) \quad (\mathbf{r}_1 \equiv \mathbf{r}, \mathbf{r}_1' \equiv \mathbf{r}')$$

$$\equiv \left\langle \psi^\dagger(\mathbf{r})\psi(\mathbf{r}')(t) \right\rangle$$

Since ρ Hermitian, can diagonalize:

$$\rho(\mathbf{r},\mathbf{r}':t) = \sum_i n_i(t)\chi_i^*(\mathbf{r}:t)\chi_i(\mathbf{r}':t)$$

If all $n_i \sim 0\ (1)$, *no BEC*

If for one and only one $i(\equiv 0)$, $n_i = N_o \sim N$, "simple" BEC

If for more than one i $n_i \sim N$, "fragmented" BEC

For case of "simple" BEC only, define order parameter

$$\Psi(r:t) = \sqrt{N_o(t)}\chi_o(\mathbf{r},t) \leftarrow \equiv |\chi_o(rt)| \exp i\varphi(\mathbf{r}t)$$

then

$$\mathbf{v}_S(\mathbf{r}t) \equiv \frac{\hbar}{m}\nabla\varphi(rt)$$

is "superfluid velocity"

$$\rightarrow \text{curl } \mathrm{v}_S = 0. \quad \oint \mathrm{v}_s \cdot dl = nh/m$$

[Contrast:

$$\mathbf{v}_h(\boldsymbol{r}) \equiv \mathbf{j}(\boldsymbol{r})/\rho(\boldsymbol{r})$$

$$\neq \sum_i n_i \nabla\varphi_i(\mathbf{r})$$

$$\Rightarrow \text{curl } \mathrm{v}_h(\boldsymbol{r}) \neq 0]$$

WHY IS BEC SO UBIQUITOUS AND ROBUST?

WHY IS BEC SO ROBUST?

1. No restrictions: compare "simple BEC" in $|0\rangle$ or $|1\rangle$ with "fragmented" (FR) state of $|0\rangle$ and $|1\rangle$ with

   $\varepsilon_o = \varepsilon_1$ single-particle energy

   $\langle \mathrm{KE} \rangle_{\mathrm{SBEC}} = \langle \mathrm{KE} \rangle_{\mathrm{FR}}$, but in general (for contact pot$^{\ell}$. $U_o\delta(\mathbf{r})$)

   $$\langle E_{\mathrm{int}} \rangle = \frac{1}{2} U_o \sum_{ij} n_i n_j (2-\delta_{ij}) \int |\chi_i(r)|^2 |\chi_j(r)|^2 \, dr$$

   $\Rightarrow$ for $U_o > 0$, $\langle E_{\mathrm{int}} \rangle_{GP} < \langle E_{\mathrm{int}} \rangle_{FR}$

2. Nontrivial restriction to 2 states (e.g. decay of flow in annulus: here $|0\rangle$= const. (φ), $|1\rangle$ = exp iφ)

   Compare:

   $$\Psi_{Fock} \equiv (a_0^+)^{n_o} (a_1^+)^{n_1} |vac\rangle, \qquad n_0 + n_1 = N$$

   $$\Psi_{GP} \equiv \left(\alpha a_o^+ + \beta a_1^+\right)^N |vac\rangle, \qquad \begin{cases} |\alpha|^2 = n_o \\ |\beta|^2 = n_1 \end{cases}$$

   Again,

   $\langle KE \rangle_{GP} \cong \langle KE \rangle_{Fock}$, but

   $$\langle \rho(r) \rangle_{Fock} = N\left\{ |\alpha|^2 |\chi_o(r)|^2 + |\beta|^2 |\chi_1(\mathbf{r})|^2 \right\}$$

   $$\langle \rho(r) \rangle_{GP} = \langle \rho(r) \rangle_{Fock} + 2\,\mathrm{Re}\left\{ \alpha^* \beta \int \chi_o^*(\mathbf{r}) \chi_1(\mathbf{r}) d\mathbf{r} \right\}$$

   $\Rightarrow$ if small perturbation V(r) added, can make $\langle \mathrm{E} \rangle_{\mathrm{GP}} < \langle \mathrm{E} \rangle_{\mathrm{Fock}}$ by appropriate choice of $\alpha^*\beta$ ("single-particle" effect)

WHY IS BEC SO ROBUST? (cont.)

2a. Nontrivial restriction to 2 states, but no "single-particle" purturbation: (for contact particle $U_o\delta(\mathbf{r})$)

$$\langle E_{\text{int}}\rangle_{GP}(\Delta\varphi)-\langle E_{\text{int}}\rangle_{Fock}=NU_o\,\text{Re}\left\{Ae^{i\Delta\varphi}+Be^{2i\Delta\varphi}\right\},$$

↑ arg α*β

$$A\equiv 2|\alpha|\bullet|\beta|\bullet\int\left(|\alpha|^2|\chi_o(\mathbf{r})|^2+|\beta|^2|\chi_1(\mathbf{r})|^2\right)\chi_o(r)\chi_1^*(\mathbf{r})d\mathbf{r},$$

$$B\equiv 4|\alpha|^2\bullet|\beta|^2\int\chi_o^2(r)\chi_1^{*2}(\mathbf{r})d\mathbf{r}$$

⇒unless A and B both zero (or path$^{\ell}$ cancellation).

can always choose Δφ to make $\langle E_{\text{int}}\rangle_{GP}(\Delta\varphi)<\langle E_{\text{int}}\rangle_{Fock}$.

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3. Fermi case. (Cooper pairing)

BCS ("simple BEC-like") state with COM momentum **Q** is

$$\Psi_{BCS}=\left(\sum_k c_k^{(Q)}a_{k\uparrow}^+a_{-k+Q,\downarrow}^+\right)^{N/2}|vac\rangle$$

Consider:

$$\Psi_{Fock}=\left(\sum_k c_k^{(o)}a_{k\uparrow}^+a_{-k\downarrow}^+\right)^M\left(\sum_k c_k^{(Q)}a_{k\uparrow}^+a_{-k+\varphi,\downarrow}^+\right)|vac\rangle$$

This is an equal-weight superposition of

$$\Psi_{GP}(\Delta\varphi)=\left(\sum_k\left\{c_k^{(o)}a_{k\uparrow}^+a_{-k\downarrow}^++e^{i\Delta\varphi}c_k{}^{(\varphi)}a_{k\uparrow}^+a_{-k+\varphi,\downarrow}^+\right\}\right)^{N/2}|vac\rangle$$

⇒O.P. $\Psi(\mathbf{r})$ in real space inhomogeneous

⇒by arguments similar to Bose case, always disfavored relative to Ψ_{BCS} with same value of $|\Psi(r)|^2$.

2. Rigorous Theorems on BEC
(interacting system)

1. Existence at T=0
   3D free space, perturbation theory starting from noninteracting gas convergent: Gavoret and Nozieres 1965
   hard-core lattice gas at half filling: Kennedy et al. 1988.

2. Existence at $T \neq 0$
   infinite-range interaction: Toth, Penrose 1992
   short-range interactions: Lieb and Seiringer 2001

3. Nonexistence at $T \neq 0$
   free space, $d \leq 2$: Hohenberg 1967
   many extensions to partially finite geometrics, etc.

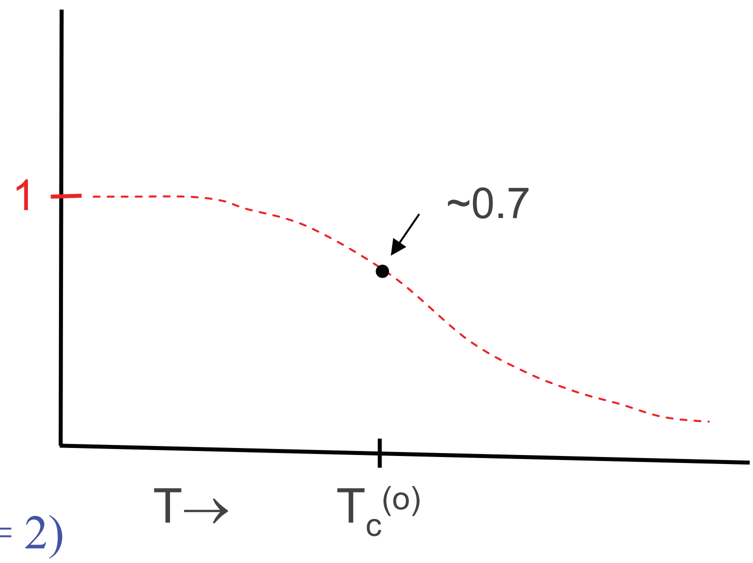
4. Upper Bound on $f \equiv N_o/N$
   Hohenberg's lemma: (general for velocity-independent interactions):

$$\langle n_k \rangle \geq \left(\frac{mk_2T}{\hbar^2 k^2} \right) f - \frac{1}{2}$$

3D free space $\Rightarrow$

$$\left(\frac{f}{(1-f)^{2/3}} \right) \leq \gamma(T_c^{(0)}/T)$$

(Roepstorff (1978): $\gamma = 2$)



RIGOROUS THEOREMS ON BEC, cont.

5. Perturbation theory (nonrigorous!) suggests repulsive interactions increase T_c = specifically, (3D free space)

$$\Delta T_c / T_c^{(o)} = \text{const } (na_S^3)^{1/3}$$

(e.g. Baym et al. 2000)

QUESTION: Can we derive an upper bound on *f* which is tighter than the Hohenberg-derived one, and in particular tends to the free-gas value for interaction ⇒ 0?

ANSWER: Yes, at least for a simple model of interactions. (A.J.L., New Journal of Physics **3**, 23 (2001))

Model: N spinless bosons in vol. Ω, N, Ω→∞, N/Ω → const. ≡ n.

Interaction: $\frac{1}{2}\sum_{ij} V(\boldsymbol{r}_i - \boldsymbol{r}_j), \qquad V(\boldsymbol{r}) \geq 0, \qquad \forall \boldsymbol{r}$

Method:

Consider free energy $F(N)(\equiv -k_B T \, \ell n Tr_N \exp -\hat{H}/kT)$

(i) Derive (*f*-independent) upper limit on F. (F_{max})

(ii) Derive (*f*-dependent) lower limit on F. (F_{min} (*f*))

(iii) Then F_{min} (*f*) ≤ F_{max} ⇒ upper bound on *f*.

(Assume, for simplicity only, that condensation is "simple" and occurs in **k** = 0 state)

RIGOROUS THEOREMS ON BEC, cont.

Step 1: Upper bound on F(N)

From "Hartree-Fock" variational ansatz,

$$\hat{\rho}_N = z^{-1}\exp - \beta\hat{H}_o \equiv \hat{\rho}_N^{(0)}$$

↑ KE only

$$\Rightarrow F(N) \le F_o(N) + \frac{1}{2}\left(NnV_o + \Omega^{-1}\sum_{k\neq k'} V_{\mathbf{k}-\mathbf{k}'}\langle n_k\rangle\langle n_{k'}\rangle\right)$$

↑ "Hartree" ↑ "Fock"

since $V(r) \ge 0, V_k \le V_o, \forall \mathbf{k}$ $\quad V_o \equiv \int V(\mathbf{r})d^3\mathbf{r}$

$$\Rightarrow \quad F(N,\Omega,T) \le F_o(N,\Omega,T) + NnV_o \equiv F_{\max}$$

Step 2: Lower bound on F(N)

Principle: F(N, Ω, T) cannot be less than $F_o(N(1-f), \Omega, T)$, otherwise we could construct a density matrix $\hat{\rho}_{N(1-f)}^{(o,\text{ trial})}$ which does better for the noninteracting gas with $N(1-f)$ particles than the standard one $\hat{\rho}_{N(1-f)}^{(o)}$!

Proof: apply to true density matrix $\hat{\rho}_N$ operator $\hat{Y} \equiv (a_o)^{\hat{N}_o}(\hat{N}_o!)^{-1/2}$, i.e., ...

RIGOROUS THEOREMS ON BEC, cont.

To create trial density matrix for noninteracting gas of N(1–*f*)≡N–N$_o$ particles, start with exact density matrix of N particles and remove all the particles in the condensate, leaving rest unchanged.*

$$\left(\text{Technically: } \hat{\rho}_{trial} \equiv \hat{Y}\hat{\rho}_N\hat{Y}^\dagger\right)$$

- KE unchanged (since $\varepsilon_o \equiv 0$)
- Entropy unchanged ($1 \to 1$ mapping)
- PE, originally, ≥ 0, is identically zero for noninteracting system

$$\Rightarrow F_o^{trial}(N(1-f),\Omega,T) \leq F(N,\Omega,T)$$

But, if $F_o^{trial} < F_o(N(1-f),\Omega,T)$, we have found a better density matrix for N(1–*f*) particles than the "trivial" one $\hat{\rho}_{N(1-f)} \equiv Z^{-1}\exp-\beta\hat{H}_o$!

Thus,

$$F(N,\Omega,T) \geq F_o(N(1-f),\Omega,T) \equiv F_{\min}(f)$$

*Technical complication: $[\hat{\rho}_N, \hat{N}_o] \neq 0$. See paper.

RIGOROUS THEOREMS ON BEC, cont.

We have proved:

(i) $F(N, \Omega, T) \le F_o(N, \Omega, T) + NnV_o$

(ii) $F(N, \Omega, T) \ge F_o(N(1-f), \Omega, T)$

Thus,

$$F_o(N(1-f),\Omega,T) - F_o(N,\Omega,T) \le NnV_o$$

free energy of noninteracting gas

This is an implicit limit on f. To make it explicit, need to bound LHS below by an explicit function of f (messy but straightforward).

Final result: $(T \ge T_c^{(o)})$

Limiting cases:

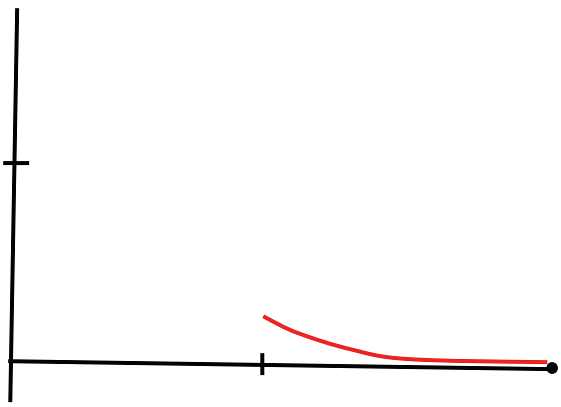
$$T = T_c^{(o)} : f \le \text{const.} \left(\frac{nV_o}{kT_c^{(o)}}\right)^{1/3}$$

(const. $\cong 2 \cdot 2$)

$$\frac{nV_o}{kT_c^{(o)}} \ll 1 - T_c^{(o)}/T \ll 1 :$$

$$f \le \text{ const. } \frac{nV_o}{kT_c}\left(1-\left(\frac{T_c^{(o)}}{T}\right)^{3/2}\right)^{-2}$$

(const. $\cong 3 \cdot 3$)

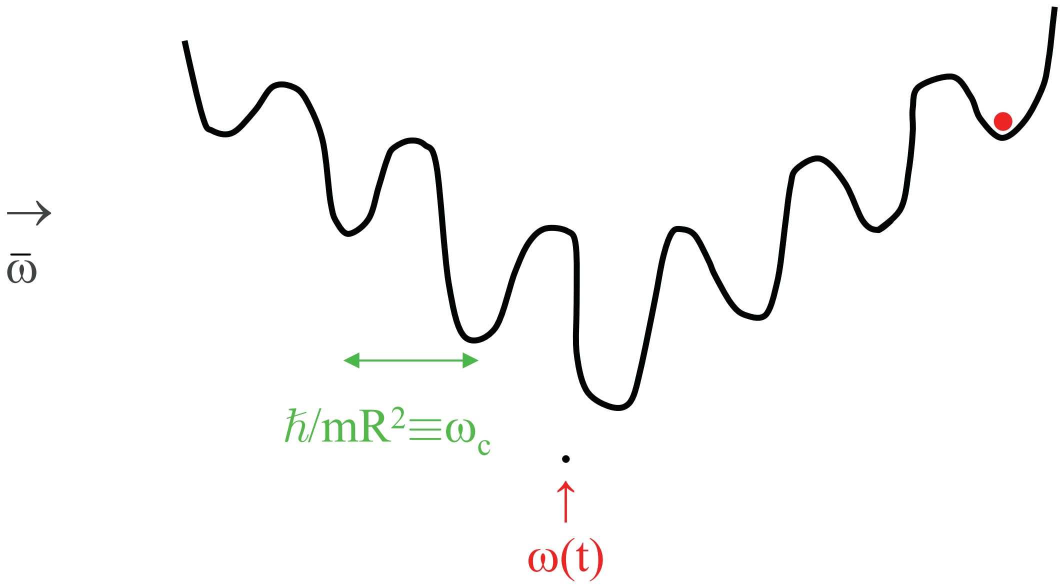


Manifestations of "Superfluidity" (Spinless Bose system)

(relevance: "supersolidity" of solid ^{4}He)

Manifestation		Necessary conditions: BEC	Necessary conditions: Repulsion
NCRI		✓	X
Persistent super-currents		✓	✓
Vortices:	stable	✓	X
	metastable	✓	✓
Josephson effect		✓	X

General form of free energy of BEC system in rotating container:



In solid ^{4}He TO experiments, $\omega_{max}(t)/\omega_c \sim 0{\cdot}8$–$30$

The \$64 K Question: Can argument be (usefully) generalized to Fermi case?

A. Attractive interactions (e.g. BCS-BEC Xover): apparently no nonvacuous result provable.

B. Repulsive interactions ($V(r) \geq 0, \forall r$) (e.g. cuprates, either first-principles or Hubbard):

Step 1: Upper bound on $F(N, \Omega, T)$ (trivial):

$$F(N,\Omega,T) \leq F_{var}(N,\Omega,T)$$

↑ from any var^l ~~wave function~~ density matrix for "true" $\hat{H}$

Step 2: Remove C. pairs. Remaining DM for $N(1-f)$ particles has $F_0 \leq F(N,\Omega,T)$, but must also have

↑ free energy for $V(r)=0, \forall r$

$F_0 \geq F_{true}(N(1-f), \Omega, T; V=0)$, otherwise nonint^d state unstable! Hence — call this $F_{nonint}(N(1-f), \Omega, T)$

$$F_{nonint}(N(1-f), \Omega, T) \leq F_{var}(N, \Omega, T)$$

This result is or is not vacuous, depending on whether $\mu_0(N, \Omega, T)$ is +ve/−ve.

μ_0: chemical pot^l of nonint^d system.

If μ_0 −ve:

If $\mu_0(N,\Omega,T) < 0$, then very crudely

$$F_{nonint}(N(1-f),\Omega,T) \cong F_{nonint}(N,\Omega,T) + |\mu_0| N_0$$

and thus

$$N_0 \lesssim \frac{F_{var}(N,\Omega,T) - F_{nonint}(N,\Omega,T)}{|\mu_0|(N,\Omega,T)}$$

Unfortunately, condition $\mu_0 < 0$ is only met

free gas { for $T \sim T_F$! e.g. in 2D, $\mu_0(T) < 0$ for $T < T_0 = T_F / \ln 2$; in 3D, $T_0/T_F = \left[\frac{4}{3\sqrt{\pi}\,\zeta(3/2)}\right]^{2/3}$ ($\sqrt{\pi}$)

~ 0.95

Only case in which $T_0 \ll T_F$ appears to be when DOS increases sharply above ϵ_F (jump)

Conclusion: in Fermi case, technique mainly useful as check on "wilder" speculations!