The BEC – BCS crossover: what (if anything) do we fundamentally not understand?*

Anthony J. Leggett

Department of Physics
University of Illinois at Urbana-Champaign
Urbana, IL

Workshop
"Universal themes of Bose-Einstein condensation"
Lorentz Center, Leiden

11 March 2013

*Work supported by the National Science Foundation
under grant no. NSF-DMR-09-06921

Some History

	BOSE-EINSTEIN CONDENSATION ("BEC")	COOPER PAIRING ("BCS")
Originators	Einstein 1925 London 1938	Bardeen et al. 1957
what?	(spinless) bosons	degenerate fermions
applied to	Liquid ^{4}He Dilute Bose alkali gases	Superconductors Liquid ^{3}He Neutron Stars
interactions must be …	nonexistence or repulsive	attractive
"fraction" of condensed particles	~1	$\sim T_c/T_F \ll 1$
main excitations	phonons, $E(k) = \hbar ck$ (bosons)	quasiparticles, $E(k) = \sqrt{(\varepsilon_k - \mu)^2 + \lvert\Delta\rvert^2}$ (fermions)
transition temperature T_c,	$\sim T_{\text{deg}}$ $\sim "T_F"$	$\sim T_{\text{deg}} \exp -1/N_o V_o$ $\sim T_F$
consequences	superfluidity	superfluidity (or superconductivity)
"Crossover" systems:		
electrons + holes in semiconductors	unstable	long-range polarization
dilute Fermi alkali gases	stable	no long-range polarization

A Unifying Concept: Pseudo-BEC (~ODLRO)

(Penrose-Onsager, Yang)

Consider a general system of N indistinguishable particles (bosons or fermions) occupying N-particle states $\Psi_n(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2 \ldots \mathbf{r}_N\sigma_N)$ with probability p_n.

spin may be absent (0)

Define:

(a) Single-particle reduced density matrix (RDM)

$$\rho_1(\mathbf{r}_1\sigma_1, \mathbf{r}_1'\sigma_1') \equiv \sum_{\sigma_2 \ldots \sigma_N} \int d\mathbf{r}_2 \ldots d\mathbf{r}_N \; \bullet$$

$$\sum_n p_n \Psi_n(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2 \ldots \mathbf{r}_N\sigma_N) \Psi_n^*(\mathbf{r}_1'\sigma_1', \mathbf{r}_2\sigma_2 \ldots \mathbf{r}_N\sigma_N)$$

("behavior of single atom arranged over behavior of all the N-1 others")

Can diagonalize:

$$\rho_1(\mathbf{r}_1\sigma, \mathbf{r}_1\sigma') = \sum_i n_i \chi_i(\mathbf{r}_1\sigma_1) \chi_i^*(\mathbf{r}_1'\sigma_1')$$

For bosons (only!), can have $n_0 \sim N \equiv N_0$ (condensate)

(b) 2-particle RDM:

$$\rho_2(r_1\sigma_1, r_2\sigma_2 : r_1'\sigma_1', r_2'\sigma_2') \equiv \sum_{\sigma_3 \ldots \sigma_N} \int dr_3 \ldots dr_N \cdot$$

$$\sum_n p_n \Psi_n(r_1\sigma_1, r_2\sigma_2, r_3\sigma_3 \ldots r_N\sigma_N) \Psi_n^*(r_1'\sigma_1', r_2'\sigma_2', r_3\sigma_3 \ldots r_N\sigma_N)$$

$$= \sum_i n_i \chi_i(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) \chi_i^*(\mathbf{r}_1'\sigma_1', \mathbf{r}_2'\sigma_2')$$

"behavior of single pair arranged over behavior of the N-2 particles"

Pseudo-BEC of fermions:

$$\rho_2(r_1\sigma_1 r_2\sigma_2 : r_1'\sigma_1' r_2'\sigma_2') = \sum_i n_i \chi_i(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2)\chi^*(\mathbf{r}_1'\sigma_1'\mathbf{r}_2'\sigma_2')$$

$$\left(\sum_i n_i = N(N-1)\right)$$

Thermal equilibrium in translation-invariant system:

3 classes of eigenfunctions $\chi_i(r_i\sigma_i r_2\sigma_2)$:

(1) $\chi_i \sim$ const. for $|\mathbf{r}_1 - \mathbf{r}_2| \to \infty$ — unbound — $o(N^2)$

(2) $\chi_i \to 0$ for $|r_1 - r_2| \to \infty$, — bound, — N_b

$\chi(\mathbf{R}) \sim \exp i\mathbf{K}\cdot R,\ \mathbf{K} \neq 0$ — noncondensate

$\uparrow$

$\dfrac{r_1 + r_2}{2}$

(3) $\chi_i \to 0$ for $|r_1 - r_2| \to \infty$, $\chi(\mathbf{R}) \sim$ const. $\Big\} \equiv \chi_0$ — bound, condensate — N_0

$N_b + N_0 \le o(N)$

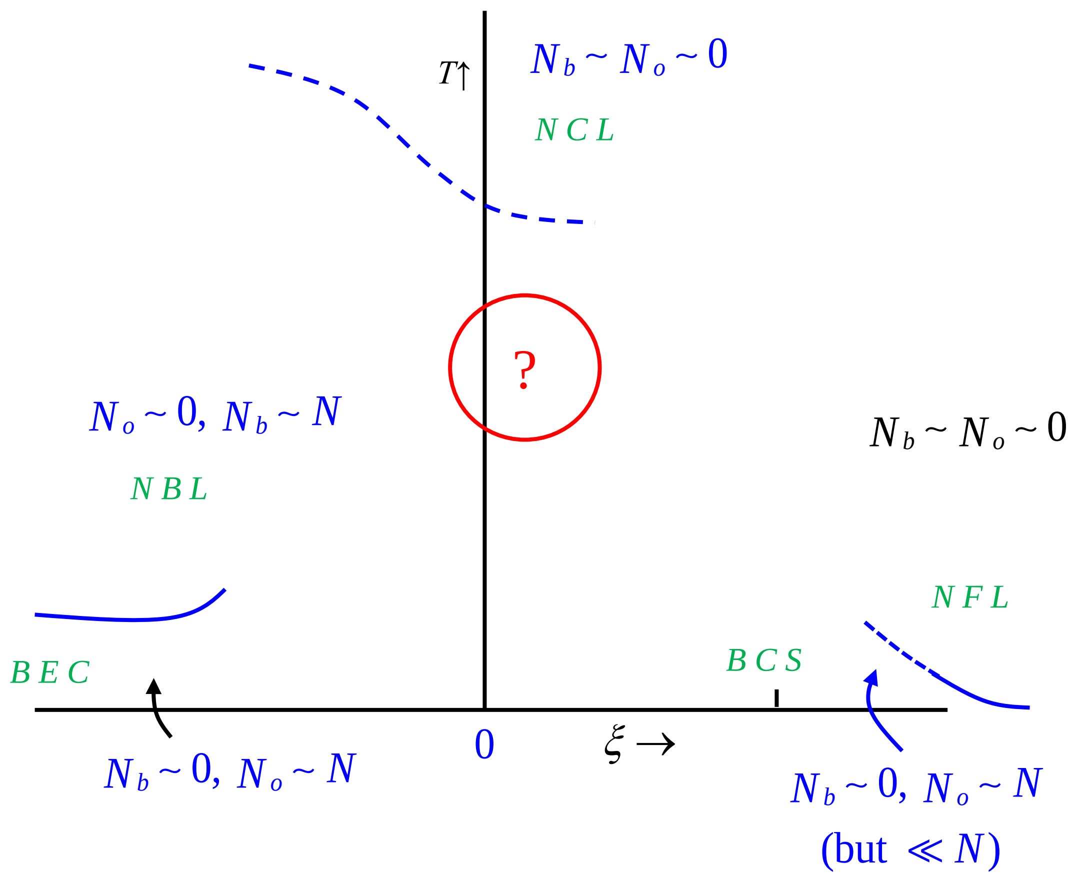
"Condensate function" $\equiv N_0/N,\ N_0 =$ eigenvalue assoc. with χ_0.

Can classify χ_i's by spin and relative orbital angular momentum ℓ

Special case: dilute ultracold 2-species Fermi gas with attraction s-wave state (specified by a_s)

General expectation: phase diagram specified completely by T and dimensionless parameter:

$$\xi \equiv -1/k_f a_s$$



Separation of "atomic" and "many-body" effects

Consider av. A of any short-range 2-particle property described by $f(r_{12})$ where $f(r) \to 0$ for $r \gg r_o$ (range of 2-particle potential) (exx: potential en. V(r), closed-channel fraction …). Then $\ell \neq 0$ eigenfunctions do not contribute. So

$$A = \sum_{i \in s \wedge}^{n_i} \iint dr_1 dr_2 \, f(r_1 - r_2 : \sigma_1 \sigma_2) \left| \chi_i (r_1 r_2 : \sigma_1 \sigma_2) \right|^2$$

Crucial observation (Tan 2005):

in range $r_o \ll r \ll k_F^{-1}$, all the s-wave χ_i are of the form

$$\chi_i(r) = C_i(\xi, T) \left(\frac{1}{r} - \frac{1}{a_s} \right)$$

(with $C_i \sim L^{-1/2}$ for unbound eigenf. and $\sim \ell^{-1/2}$ for bound ones)

↗ microscopic length

More generally, for r $\ll k_F^{-1}$ (but possibly $\lesssim r_o$).

$$\chi_i(r) = C_i(\xi, T) \times \psi_{at}(r) \leftarrow \text{2-particle } \in = 0 \text{ w.f.}$$

Thus,

$$A = N k_F h(\xi, T) \cdot \underbrace{\int_0^\infty dr f(r) \left| \psi_{at}(r) \right|^2}_{\text{atomic}}$$

$$\underbrace{h(\xi, T) \equiv \sum_{i \in s} (n_i / N k_F) \left| C_i(\xi, T) \right|^2}_{\text{many-body}} \quad (\equiv \text{ const.} \times \text{"contact"})$$

⇒ ratios of (2-body) microscopic quantities entirely det. by atomic physics, absolute value by many-body physics.

All this is quite general …

The problem: N fermions, equal nos. ↑ and ↓,

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2$$

$$N_{tot} = (k_F^3 / 3\pi^2)$$

subject to b.c.

$\Psi_N \sim$ const. $(1 - a_s/r_{ij})$ for antiparallel-spin particles *i*, *j* *for*

$r_o \ll r_{ij} \ll n^{-1/3}$

(in dilute limit, parallel-spin particles noninteracting)

All (equilibrium) props. must be functions only of $\xi \equiv -1/k_F a_S$

"Naïve" Ansatz (Eagles 1969, AJL 1980, Randeria et al. 1985, Stajic et al. 2005 . . .):

$$\Psi_N = \mathcal{N} \cdot \mathcal{A} \cdot \{\varphi(r_1 - r_2 : \sigma_1\sigma_2)\varphi(r_3 - r_4 : \sigma_3\sigma_4)\ldots\varphi(r_{N-1} - r_N : \sigma_{N-1}\sigma_N)\}$$

$\langle \Psi_N | \hat{H} | \Psi_N \rangle =:$

1. Pairing terms ← fully taken into account
2. Fock terms ← vanish in dilute limit
3. Hartree terms ← ??

equivalently: each term of $\Psi_N^{(\text{naïve})}$ satisfies b.c. for paired particles only, e.g. 1st term satisfies it for 1, 2 but not (e.g.) for 1, 3.

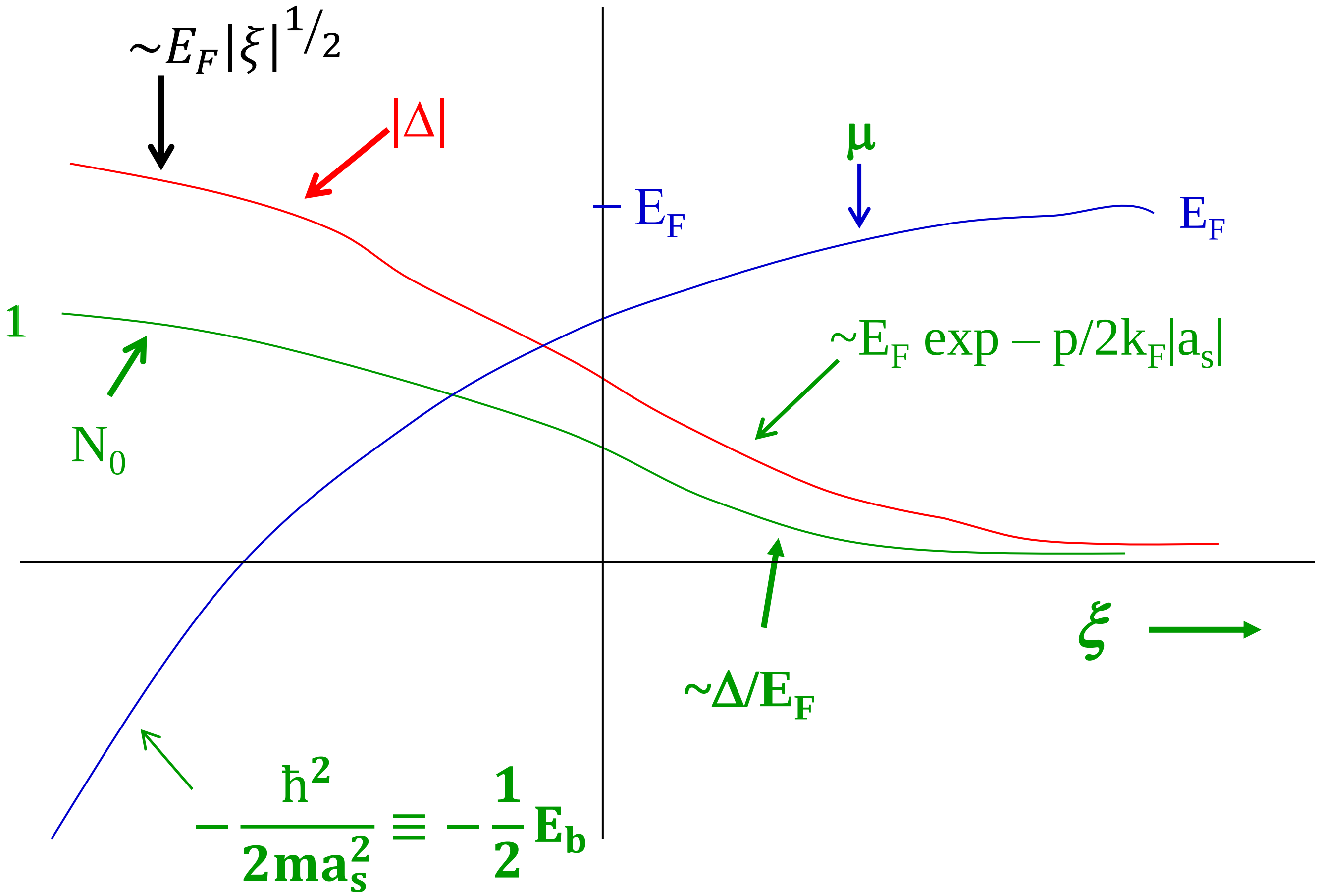
Output of naïve ansatz:

$\mu(\xi), \Delta(\xi)$

Hence also $(E/N)(\xi)$.

(calc^n analytic except for 2 |D numerical integrals)

↑: *not obvious a priori that naïve ansatz is even qualitatively right!*



$\left(\xi \equiv {}^{-1}/_{k_F a_s}\right)$

No (T=0) phase transition!

Excitation energy of quasiparticle with momentum $\underline{k}$

(normal-state energy $\xi_k \equiv \hbar^2 k^2/2m$):

$$E_K = \sqrt{(\xi_k - \mu)^2 + |\Delta|^2}$$

$$\mu > 0: \min E_k = |\Delta|$$

$$\mu < 0: \min E_k = \sqrt{|\mu|^2 + |\Delta|^2}$$

Why is the "naïve ansatz" so (comparatively) good?

- correct qualitatively (e.g. no phase transition as $f(\xi)$)

- not so bad quantitatively (e.g. predicts Bertsch parameter ~ 0.59: variational estimates ~ 0.4)

Clue by analogy: low-T props. of normal metals close to Fermi gas model.

Solution: Landan Fermi-liquid theory!

Landan's "adiabatic" argument:

$$|O'\rangle = \hat{U}(\infty)|O\rangle, \qquad \alpha_p^+|O\rangle' = \hat{U}(\infty)\alpha_p^+|O\rangle \qquad \hat{U}(t) = \exp i\int_{-\infty}^{t} \lambda(t')dt' \cdot \hat{V}/t_r$$

$|O'\rangle$ ↑ GS; $|O\rangle$ ↑ GS of Fermi gas; $\alpha_p^+|O\rangle'$ ↑ qp; $\alpha_p^+|O\rangle$ ↑ real-particle

$$\left(\lambda(-\infty) = 0,\ \lambda(+\infty) = 1\right)$$

i.e. low-lying excitations (qp states) in 1-1 correspondence with excited states of Fermi gas. (Very detailed discussion + justification: Nozières, Theory of Interacting Fermi Systems)

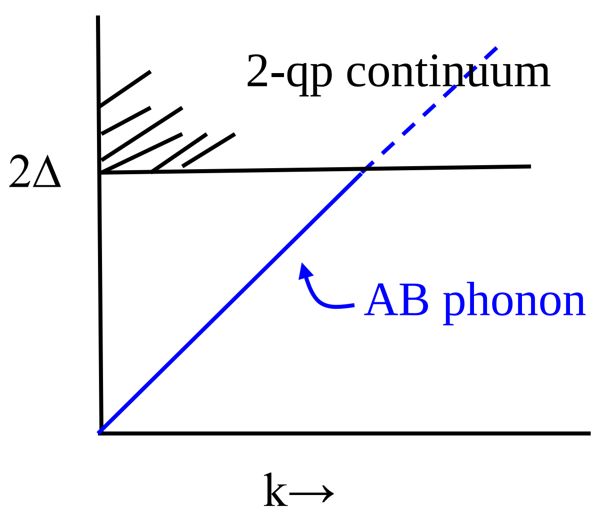
Can we do something similar for low-lying excitations of UC Fermi gas?

e.g. start close to BCS, end ($\xi \to +\infty$), i.e. $0 < \lambda(-\infty) \ll 1$.

GS is BCS state, excited states are
(a) Bogoliubov quasiparticles
(b) AB phonons. Should evolve adiabatically …

: at BCS end, AB phonons not well-defined for $k \gtrsim \xi_p^{-1} \to 0$

↑ pair radius



⇒ region of validity of "Landan-like" theory vanishes? (may need nontrivial extension of Nozières argument).

BEC-BCS crossover: The $\ell \neq 0$ case

Qualitative differences from s-wave case:

1. (2-body prob): In s-wave case, general E=0 solution outside potential is

$$\Psi(\boldsymbol{r}) = 1 - a_s / r$$

and in particular, at unitarity, $\Psi(\boldsymbol{r}) \sim r^{-1}$ $\Rightarrow$ in many-body cases expect strong 3, 4 . . . -body interaction effects.

In $\ell \neq 0$ case,

$$\Psi(\boldsymbol{r}) \sim + \frac{c_2}{r^{\ell+1}}$$

suggests unitary limit may be (almost) trivial in lim $r_o \ll a\, n^{-1/3}$!

2. Standard BCS-type ansatz gives topological phase transition at $\mu = 0$.

BEC-BCS crossover: The $\ell \neq 0$ case (cont.)

3. The angular momentum problem:

In BEC of tightly bound $\ell \neq 0$ diatomic modules, overwhelmingly plausible that

$$\boldsymbol{L} = \frac{N}{2}\hbar\hat{\underset{\sim}{\ell}}$$

What is situation in BCS limit?

Most "obvious" number-conserving ansatz:

$$\Psi \sim \left(\sum_k c_k a_k^+ a_{-k}^+ \right)^{N/2}, \qquad c_k \equiv \upsilon_k / u_k$$

with (e.g.) $c_k \sim \exp i\varphi_k$. This has $\boldsymbol{L} = \frac{N}{2}\hbar\hat{\boldsymbol{\ell}}$ just as in BEC limit, irrespective of magn. of |Δ|.

Problem: macroscopic discontinuity at transition to normal state $(\boldsymbol{L} = 0)$!

This may not be worrying, because as $|\Delta| \to 0$ there is a char. length (the pair radius $\xi_r \sim \hbar v_F / |\Delta|$) which $\to \infty$.
(so that for any finite container radius R transition is smooth)

↑: What about limit $T \to T_c$? Here $\xi_p \sim \hbar v_F / k_B T_c$ does not diverge

Alternative MBWF of (p + ip) Fermi superfluid

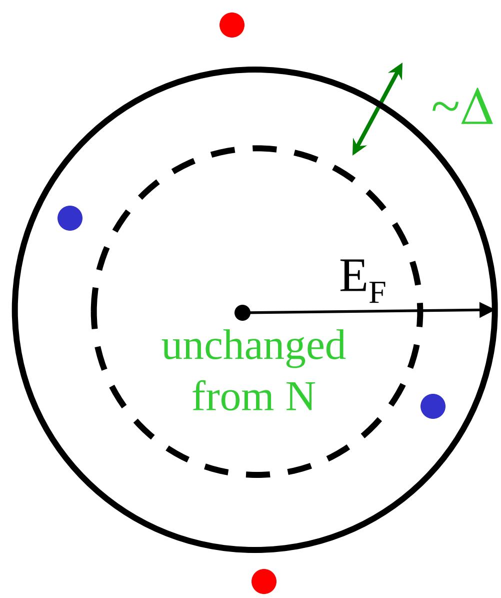
Recap: standard ansatz is (for say ↑↑)

$$\Psi \sim \left(\sum_k c_k a_k^+ a_{-k}^+ \right)^{N/2} |\,\text{vac}\rangle, c_k \sim \exp i\varphi_k$$

i.e. all pairs of states in Fermi sea have angular momentum ħ.

Alternative ansatz:

first shot:



$$\Psi(N_p, N_h)$$

$$\sim \left(\sum_{k>k_F} c_k a_k^+ a_{-k}^+ \right)^{N_p/2},$$

$$\left(\sum_{k<k_F} d_k a_{-k} a_k \right)^{N_h/2} |\,\text{vac}\rangle$$

⚠: keeps pp→pp and hh→hh, but not (e.g.) pp→hh.

Remedy:

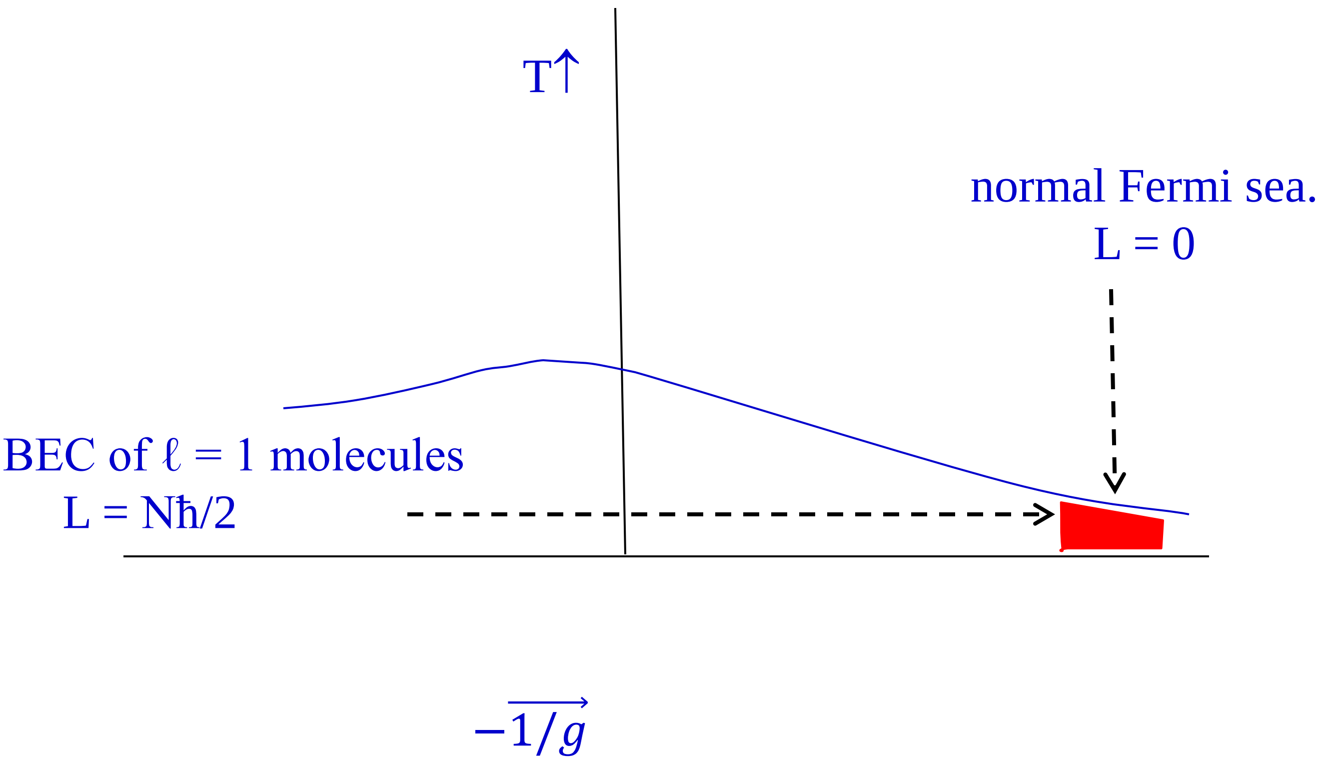
$$\Psi \sim \sum_{N_p, N_K} Q_{N_p N_k} \Psi(N_p, N_k),$$

$$Q \text{ slowly varying as } f(N_p, N_k)$$

degenerate with standard ansatz to 0($N^{-1/2}$), but

$$L \sim (N\hbar/2) \cdot (\Delta / E_F)^2$$

IS GS OF (p + ip) FERMI SUPERFLUID UNIQUE?



Can we settle this question experimentally?

(and does alternative description have any implications for topological phase transition?)