On the Bogoliubov-de Gennes equations

A. J. Leggett
Department of Physics
University of Illinois at
Urbana-Champaign
U.S.A.

Support: John D. and Catherine T. MacArthur Foundation

ILLINOIS

On the Bogoliubov-de Gennes equations.

Main claims of this talk:

1. For 50 years, almost all theoretical work on inhomogeneous Fermi Superfluids, including work on topological quantum technology in $(p + ip)$ superconductors, has been based on the Bogoliubov-de Gennes (generalized mean-field) method.

2. Consideration of some simple examples shows that results obtained by this method (at least if applied naively) may be wrong.

3. This is because in the cases of interest the response of the Cooper pairs cannot be ignored.

4. The question most relevant to TQT relates to the Berry phase: here again consideration of a simple example strongly suggests that the response of the Cooper pairs cannot be ignored, so that results obtained by (naïve application of) the BdG equations may be qualitatively misleading.

5. If so, this could be a disaster for the whole program of TQT in $(p + ip)$ Fermi superfluids.

The Bogoliubov-de Gennes (generalized mean-field, “BdG”) method.

Original Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{\alpha}\int d\boldsymbol{r}\left\{\boldsymbol{\nabla}\hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r})\cdot\nabla\hat{\psi}_{\alpha}(\boldsymbol{r})\right\} + {}_{\alpha\beta}[U_{\alpha\beta}(\boldsymbol{r})\hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r})\hat{\psi}_{\beta}(\boldsymbol{r})$$

$$+\sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta}(\boldsymbol{r},\boldsymbol{r}')\iint d\boldsymbol{r}\, d\boldsymbol{r}'\,\hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r})\hat{\psi}^{\dagger}_{\beta}(\boldsymbol{r}')\hat{\psi}_{\gamma}(\boldsymbol{r}')\hat{\psi}_{\delta}(\boldsymbol{r})$$

$\left(\hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r}) \equiv \text{fermion creation operator(etc.)}\right)$,

$$V_{\alpha\beta\gamma\delta}(\boldsymbol{r},\boldsymbol{r}') = V^{*}_{\delta\gamma\beta\alpha}(\boldsymbol{r},\boldsymbol{r}')$$

Mean-field approximation:

$$\hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r})\hat{\psi}^{\dagger}_{\beta}(\boldsymbol{r}')\hat{\psi}^{\dagger}_{\gamma}(\boldsymbol{r}')\hat{\psi}^{\dagger}_{\delta}(\boldsymbol{r}) \Rightarrow$$

$$\hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r})\hat{\psi}^{\dagger}_{\beta}(\boldsymbol{r}')\langle\hat{\psi}_{\gamma}(\boldsymbol{r}')\hat{\psi}_{\delta}(\boldsymbol{r})\rangle + \left\langle\hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r})\hat{\psi}^{\dagger}_{\beta}(\boldsymbol{r}')\right\rangle\hat{\psi}^{\dagger}_{\gamma}(\boldsymbol{r}')\hat{\psi}^{\dagger}_{\delta}(\boldsymbol{r})$$

c-number

operators

(+ Hartree + Fock terms)

$\Rightarrow$ MF Hamiltonian:

$$\hat{H}_{MF} = \frac{-\hbar^2}{2m}\sum_{\alpha}\int d\boldsymbol{r}\left\{\boldsymbol{\nabla}\hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r})\cdot\boldsymbol{\nabla}\hat{\psi}_{\alpha}(r)\right\} + \sum_{\alpha\beta} U_{\alpha\beta}(\boldsymbol{r})\hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r})\hat{\psi}_{\beta}(\boldsymbol{r})$$

$$\sum_{\alpha\beta}\iint \boldsymbol{dr}\,\boldsymbol{dr}'\left\{\Delta_{\alpha\beta}(\boldsymbol{r},\boldsymbol{r}')\,\hat{\psi}^{\dagger}_{\alpha}(\boldsymbol{r})\,\hat{\psi}^{\dagger}_{\beta}(\boldsymbol{r}') + H.c.\right\}$$

$$\Delta_{\alpha\beta}(\boldsymbol{r},\boldsymbol{r}') \equiv \sum_{\gamma} V_{\alpha\beta\gamma\delta}(\boldsymbol{r},\boldsymbol{r}')\langle\hat{\psi}_{\gamma}(\boldsymbol{r}')\hat{\psi}_{\delta}(\boldsymbol{r})\rangle$$

$\leftarrow$ must eventually be chosen self-consistently

$\widehat{H}_{MF}$ is bilinear in $\hat{\psi}, \hat{\psi}^{\dagger} \Longrightarrow$ can be diagonalized by writing

$$\hat{\psi}(r) = \sum_i \left\{\hat{\gamma}_i u_i(r) + \hat{\gamma}_i^{\dagger} v_i(r)\right\}$$

$$\widehat{H}_{MF} = \sum_i \mathrm{E}_i \, \hat{\gamma}_i^{\dagger} \gamma_i (+\text{const.})$$

where $u_i(r), v_i(\boldsymbol{r})$ are spinors (in ordinary spin space) satisfying the BdG equations

$$\widehat{H}_o u_\alpha^i(r) + \sum_\beta \int dr' \Delta_{\alpha\beta}(r, r') v_\beta^i(r') = \mathrm{E}_i \, u_\alpha^{\mathrm{i}}(\boldsymbol{r})$$

$$\sum_\beta \int dr' \Delta_{\alpha\beta}(\boldsymbol{r}\boldsymbol{r}') u_\beta^{\mathrm{i}}(r') - \widehat{H}_o^* v_\alpha^{\mathrm{i}}(r) = \mathrm{E}_i \, v_\alpha^{\mathrm{i}}(\boldsymbol{r})$$

where $\widehat{H}_o \equiv \left(\frac{-\hbar^2}{2m} \nabla^2 + \widehat{U}\right)$

In simple BCS case $\Delta_{\alpha\beta}(r, r') = i\sigma_{\alpha\beta}^y \delta(\boldsymbol{r} - \boldsymbol{r}')\Delta(r)$, so reduces to

$$\begin{pmatrix} \widehat{H}_o & \Delta(r) \\ \Delta^*(r) & -\widehat{H}_o^* \end{pmatrix} \begin{pmatrix} u_i(r) \\ v_i(r) \end{pmatrix} = E_i \begin{pmatrix} u_i(r) \\ v_i(r) \end{pmatrix}$$

Some notes on the BdG method:

1. The mean-field Hamiltonian is particle-nonconserving ("spontaneous breaking of U(1) Symmetry")

2. Relation phase of $v(r)$ and $u(r)$ is determined by phase of $\Delta(r)$. But global phase of $\Delta(r)$ is determined by that of "order parameter" $\langle\psi^\dagger(r)\psi^\dagger(r')\rangle$, which is physically meaningless

3. Hence all the physics is invariant under global phase transformation
$u(r) \to u(r), v(r) \to (\exp i\varphi)v(r)$. $[\varphi \neq f(\boldsymbol{r})]$.

4. If $(u_i(r), v_i(r))$ is a solution of BdG equations with eigenvalues E_i then $\left(v_i^*(r), u_i^*(r)\right)$ is a solution with eigenvalues $-E_i$

5. Hence, by (3) with $\varphi = \pi$, we can as well choose the "negative-energy" solution to be $\left(v_i^*(r), u_i^*(r)\right)$
($\Rightarrow$ possibility of Majorana solutions,
$u(r) = v^*(r), E = 0$)

6. The (solutions of the) BdG equations tell us the relation between the (even-number-parity) groundstate and the simplest fermionic (add-points) energy eigenstates. They do not tell us anything directly about the GS (though cf. Stone & Chung, Phys. Rev. B **73**, 014505 (2006).)

Failure of (a naïve interpretation of) the BdG equations: a trivial example:

Consider an even-number-parity BCS superfluid at rst. (so $\boldsymbol{P}_o = 0$)

total momentum

Now create a single fermionic quasiparticle in state **k**:

For this, the appropriate BdG qp creation operator $\gamma_i^\dagger$ turns out to be

$$\gamma_i^\dagger = u_k a_{k\uparrow}^+ + v_k a_{-k\downarrow} \qquad , u_k \equiv \frac{1}{2}\left(1 + \frac{\epsilon_k}{E_k}\right), v_k \equiv \frac{1}{2}\left(1 - \frac{\epsilon_k}{E_k}\right)$$

$$E_k \equiv \left(\epsilon_k^2 + |\Delta_k|^2\right)^{1/2}$$

The total momentum $\boldsymbol{P}_f$ of the (odd-number-parity) many-body state created by γ_i is

standard textbook result

$$\boldsymbol{P}_f = |u_k|^2(\hbar\boldsymbol{k}) - |v_k|^2(-\hbar\boldsymbol{k}) = (|u_k|^2 + |v_k|^2)\hbar\boldsymbol{k} \equiv \hbar\boldsymbol{k}$$

$$\text{so } \Delta\boldsymbol{P}_f \equiv \boldsymbol{P}_f - \boldsymbol{P}_o = \hbar\boldsymbol{k}$$

Now consider the system as viewed from a frame of reference moving with velocity $-\boldsymbol{v}$, so that the condensate COM velocity is $\boldsymbol{v}$. Since the pairing is now between states with wave vector $\boldsymbol{k}$ and $(-\boldsymbol{k} + m\boldsymbol{v}/\hbar)$, intuition suggests (and explicit solution of the B&G equations confirms) that the form of $\gamma_i^\dagger$ is now

$$\gamma_i^\dagger = u_k a^\dagger_{k+\frac{mv}{\hbar},\uparrow} + v_k a_{-k\downarrow} \qquad \leftarrow \text{nb. not } a_{-\left(k+\frac{mv}{\hbar}\right)}!$$

Thus the added momentum is

$$\Delta\boldsymbol{P}'_f = |u_k|^2(\hbar\boldsymbol{k} + m\boldsymbol{v}) - |v_k|^2(-\hbar)\boldsymbol{k}$$
$$= \hbar\boldsymbol{k} + |u_k|^2 m\boldsymbol{v}$$

Recap: BdG $\rightarrow \Delta P'_f = \hbar \boldsymbol{k} + |u_k|^2 m\boldsymbol{v}$

However, by Galilean invariance, for any given condensate number N,

$$\boldsymbol{P'}_o = \boldsymbol{P}_o + Nm\boldsymbol{v}, \boldsymbol{P'}_f = \boldsymbol{P}_f + (N+1)m\boldsymbol{v}.$$

$$\Rightarrow \Delta P'_f \equiv P'_f - P'_o = \Delta \boldsymbol{P'}_f + m\boldsymbol{v} = \hbar \boldsymbol{k} + m\boldsymbol{v}.$$

And this result is independent of N (so involving "spontaneous breaking of U(1) symmetry" in GS doesn't help!)

So: BdG $\Rightarrow \Delta P'_f = \hbar \boldsymbol{k} + |u_k|^2 m\boldsymbol{v}$

GI $\longrightarrow \Delta P'_f = \hbar \boldsymbol{k} + m\boldsymbol{v}$

Galilean invariance

What has gone wrong?

Solution: Conserve particle no.!

When condensate is at rest, correct expression for fermionic correlation operator $\gamma_i^\dagger$ is

$$\gamma_i^\dagger = u_k a_{k\uparrow}^+ + v_k a_{-k\downarrow} \hat{C}_{(v)}^\dagger$$ ←creates ultra Cooper pair (with COM velocity O)

Because condensate at rest has no spin/momentum/spin current …, the addition of $\hat{C}$ has no effect. However:
when condensate is moving

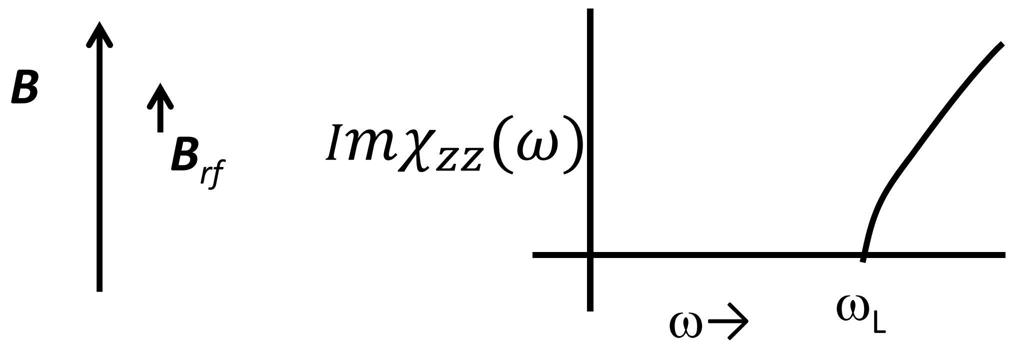
$$\gamma_i^\dagger = u_k a_{\boldsymbol{k}+\frac{mv}{\hbar},\uparrow}^+ + v_k a_{-k,\downarrow} \hat{C}_{(0)}^\dagger$$ ← creates extra Cooper pair (with velocity **v**)

$$\Rightarrow \Delta P'_f = |u_k|^2 (\boldsymbol{k} + m\boldsymbol{v}/\hbar) + |v_k|^2 \{-(-\hbar k) + m\boldsymbol{v}\}$$
$$= (|u_k|^2 + |v_k|^2)(\hbar \boldsymbol{k} + m\boldsymbol{v}) = \hbar \boldsymbol{k} + m\boldsymbol{v}$$

In accordance with GI argument

Failure of BdG/MF: a slightly less trivial example

For a thin slab of (appropriately oriented) ^{3}He-B, calculations based on BdG Equations predict a Majorana fermion state on the surface. A calculation* starting from the fermionic MF Hamiltonian then predicts that in a longitudinal NMR experiment, appreciable spectral weight should appear above the Larmor frequency $\omega_L \equiv \gamma B_o$:



The problem: no dependence on strength of dipole coupling g_D, (except for initial orientation)! But for g_D =0, $\hat{S}_z$ commutes with $\hat{H}$ ⇒

$$\int \omega \, Im\chi_{zz}(\omega)d\omega \sim [\hat{S}_z, [\hat{S}_z, \hat{H}]] = 0$$

$$\Rightarrow Im\chi_{zz}(\omega) \sim \delta(\omega)!$$

For nonzero g_D,

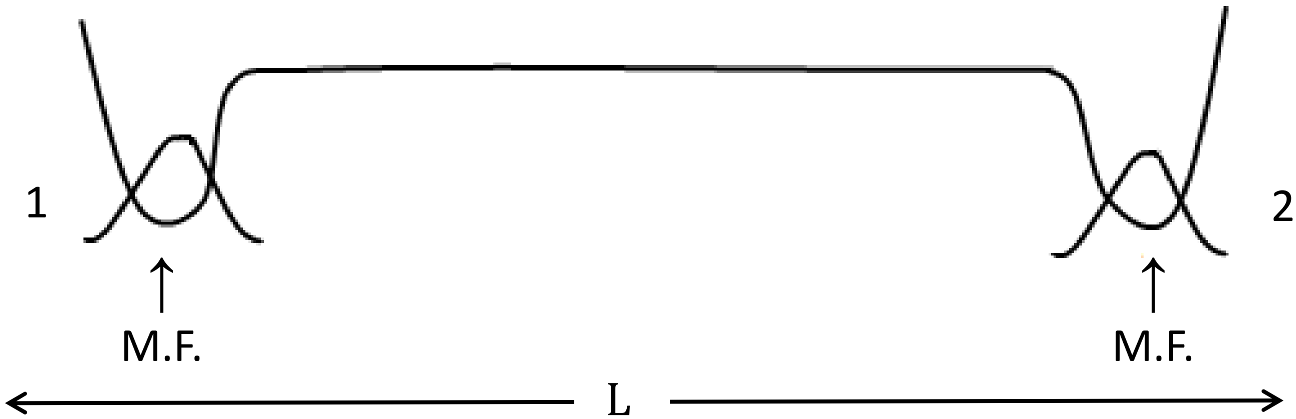
$\int \omega \, Im\chi_{zz}(\omega)d\omega \sim g_D$ ⇒ result cannot be right for $g_D \to 0$

Yet – follows from analysis of MF Hamiltonian!

MORAL: WE CANNOT IGNORE THE COOPER PAIRS!

*M.A. Silaev, Phys. Rev. B **84**, 144508 (2011)

(Conjectured) further failure of MF/BdG approach



Imagine a many-body Hamiltonian (e.g. of a $(p + ip)$ superconductor) which admits single Majorana fermion solutions at two widely separated points. These M.F.'s are "halves" of a single $E = 0$ Dirac-Bogoliubov fermion state. Intuitively, by injecting an electron at 1 one projects on to this single state and hence gets an instantaneous response at 2. Semenoff and Sodano (2008) discuss this problem in detail and conclude that unless we allow for violation of fermion number parity, we must conclude that this situation allows instantaneous teleportation.

Does it? Each Majorana is correctly described, not as usually assumed by

$$\gamma_M^\dagger = \int \{u(r)\hat{\psi}^\dagger(r) + u^*(r)\hat{\psi}(r)\}d\boldsymbol{r} \quad (\equiv \gamma_{\dot{M}})$$

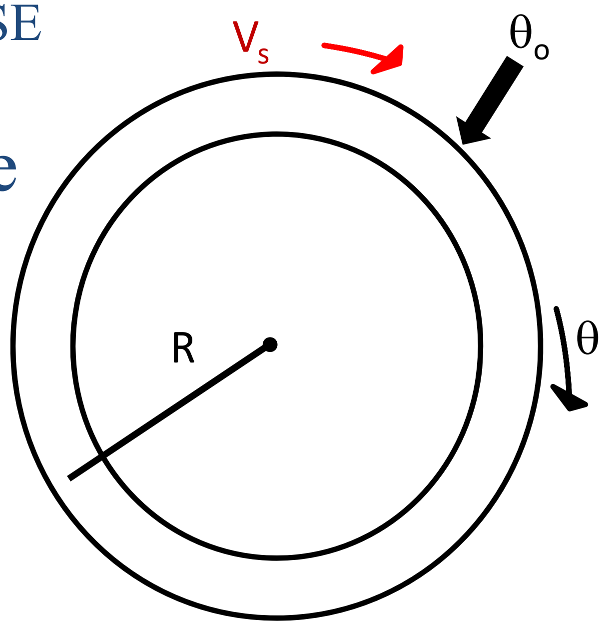
but rather by

$$\gamma_M^\dagger = \int \{u(r)\hat{\psi}^\dagger(r) + u^*(r)\hat{\psi}(r)C^\dagger\}d\boldsymbol{r}$$

Cooper pair creation operator

But it is impossible to apply the "global" operator $C^\dagger$ instantaneously! What the injection will actually do (inter alia) is to create, at 1, a quasihole–plus–extra–Cooper –pair at 1, and the time needed for a response to be felt at 2 is bounded below by L/c when C is the $C.$ pair propagation velocity (usually $\sim v_f$).

A TRIVIAL-LOOKING PROBLEM
INVOLVING THE BERRY PHASE



Consider a neutral s-wave Fermi superfluid in an annular geometry: single quantum of circulation

$$\mathbf{v}_s = \hbar / 2mR$$

$$\left(\oint \boldsymbol{v}_s \cdot \boldsymbol{dl} = h/2m\right).$$

Create Zeeman magnetic field trap:

$$\hat{H}_z = -\mu_B \sigma_z B(r) \equiv V(r)$$

$$V(r) = V_o f(\theta - \theta_o)$$

pair radius

$$v_o \ll \Delta, \text{ range of } f(\theta) \gg \xi/R \text{ but } \ll 1.$$

So effect on condensate $o(\mu_B B_o/\Delta)^2 \ll 1$

GS of 2N+1-particle system presumably has single Bogoliubov quasiparticle trapped in Zeeman trap.

Now, let's move θ_o adiabatically once around annulus:

Question:

What Berry phase is picked up?

Possible conjectures:

(a) π
(b) 0
(c) something else
(d) question ill-defined

Let's do this problem by two different methods:

Method 1 (BdG)

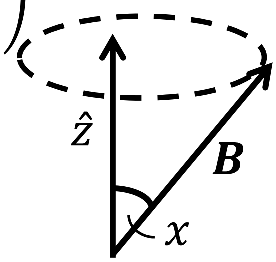
The phase of the superconducting condensate rotates through 2π as we go once around the annulus, so without loss of generality we may take

$$\Delta\,(\theta) = \; |\Delta| \exp i\theta$$

So BdG equations read:

$$\begin{pmatrix} \hat{H}_o & |\Delta| e^{i\theta} \\ |\Delta| e^{-i\theta} & -\hat{H}_o \end{pmatrix} \begin{pmatrix} u(\theta) \\ v(\theta) \end{pmatrix} = E \begin{pmatrix} u(\theta) \\ v(\theta) \end{pmatrix}$$

$$\left(\hat{H}_o \equiv - \frac{\hbar^2}{2mR^2} \frac{\partial^2}{\partial \theta^2} + \mathrm{V}(\theta - \theta_o) - \mu \right)$$



Cf: particle of spin ½ in trap centered at θ_o, with field rotating around z-axis:

$$\begin{pmatrix} \hat{H}_o & \mu B e^{i\theta} \\ \mu B e^{-i\theta} & -\hat{H}_o \end{pmatrix} \begin{pmatrix} \chi_\uparrow\,(\theta) \\ \chi_\downarrow\,(\theta) \end{pmatrix} = E \begin{pmatrix} \chi_\uparrow\,(\theta) \\ \chi_\downarrow\,(\theta) \end{pmatrix}$$

$$(\hat{H}_o = \mu B \cos x)$$

Thus: $|\uparrow> \longrightarrow |p>$ ("particle")

$|\downarrow> \longrightarrow |h>$ ("hole")

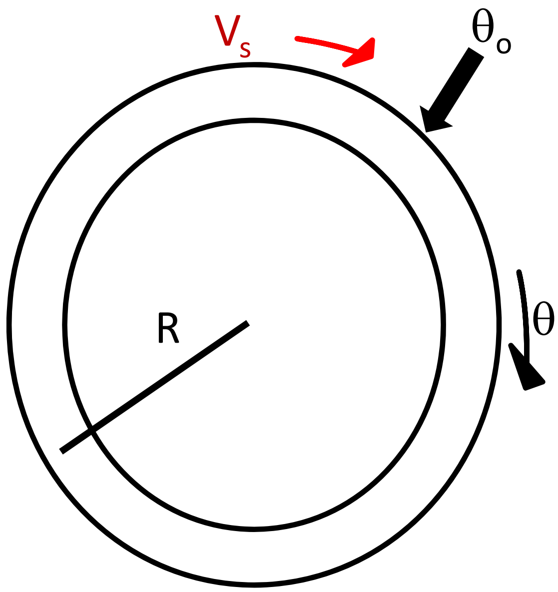
Now in the magnetic case it is a textbook result that Berry phase φ_B is

$$\varphi_B = 2\pi\, cos^2(x/2) \leftarrow \text{"weight" of } |\uparrow> \text{ component}$$

Our (superconducting) case corresponds to weight of $|p> = 1/2$, i.e. to $\chi = \pi/2$, so infer

$$\varphi_B = \pi \text{ (BdG)}$$

Method 2: Microscopic (N-conserving) argument



Ansatz:

2N-particle "ground" state for $\ell_o \neq 0$ is

$$\Psi_{2n} = (\textstyle\sum_\ell \eta_L \; a^+_{\ell\uparrow} a^+_{-\ell+\ell_o})^{N/2}\,|vac\rangle \qquad (\eta_\ell \equiv v_\ell / u_\ell)$$

$$\equiv (\hat{C}^\dagger_{\ell_o})^{N/2}\,|vac\rangle$$

Creates C. pair with any momentum ℓ_o

$f_\ell \sim e^{i\ell\theta}$

In presence of Zeeman trap, 2N+1-particle "ground" state with $l_o \neq 0$ is of general form

$$\Psi_{2N+1} = \textstyle\sum_\ell f_\ell \alpha^+_\ell \Psi_{2N} \qquad \alpha^+_\ell \equiv u_\ell a^+_{\ell\uparrow} - v^*_\ell a_{-\ell+\ell_o\downarrow} \hat{C}^\dagger_{\ell_o}$$

Conserves N!

Then easy to show that

$$\varphi_B \equiv \text{lm} \int_O^{2\pi} \Psi^*(\theta_o) \frac{\partial \Psi}{\partial \theta_O} d\theta_O = 2\pi \textstyle\sum_\ell (\ell |f_\ell|^2.)$$

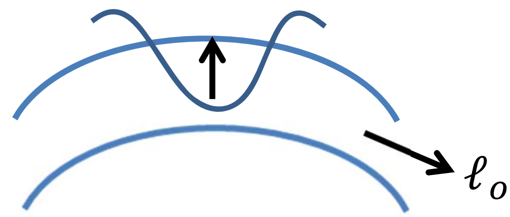
Recap: in particle-conserving calculation,

$$\varphi_B = 2\pi \sum_\ell \ell |f_\ell|^2$$

But recall: In particle-conserving calculation, a Bogoliubov qp with wave vector **k** (ℓ), even in a moving (rotating) condensate, adds (angular) momentum $\hbar\boldsymbol{k}$ $(\hbar\ell)$. Hence difference ΔJ in angular momentum between even-parity and odd-parity groundstate is just $\sum_\ell \ell |f_\ell|^2$.

i.e. involving $a_{\boldsymbol{k}}^\dagger \left(a_\ell^\dagger\right)$

$\Longrightarrow$ $\varphi_B = 2\pi \cdot \Delta J$



The $64K argument: what is ΔJ?

Consider situation as viewed from frame of moving condensate: then condensate is at rest, Zeeman trap is moving at speed $-v_. = -\hbar/2mR$. But since the weights of particle and hole is then added qp or equal, no extra particle density is associated with the trap, hence no ΔJ. However, there is a probability of exactly ½ of the hole component and hence of an extra Cooper pair relative to the even-parity groundstate. When we go back to the last frame, this cancels <u>half</u> the effect of the added single particle and gives $\Delta J = 1/2$.

Hence, apparently,

$\varphi_B = \pi$ (microscopic particle-conserving calculation)

$\Longrightarrow$ particle-conserving calculation agrees with (naïve) BdG approach

↑ : Is there a first-order (in v) connection to ΔJ in the moving frame?