The Mean-Field Method in the Theory of Superconductivity: A Wolf in Sheep's Clothing?

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1. Spontaneously broken U(1) symmetry: the weakly interacting Bose gas

2. Spontaneously broken U(1) symmetry: BCS theory of superconductivity

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4. The Bogoliubov-de Gennes equations: general case

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6. What could be wrong with all this? A couple of (rather trivial) illustrations.

7. A simple but worrying thought-experiment.

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Spontaneously Broken U(1) Symmetry: The General Idea

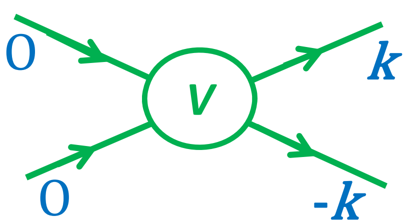
1. Dilute Bose gas with weak repulsion (Bogoliubov, 1947)

$$\hat{H} = \sum_k \underset{\uparrow \atop \hbar^2 k^2/2m}{\varepsilon_k} a_k^+ a_k + \hat{V} \qquad [\hat{H}, \underset{\uparrow \atop \text{Total particle number}}{\hat{N}}] = [\hat{H}, \underset{\uparrow \atop \text{Total momentum}}{\hat{P}}] = 0$$

To zero[th] order in $\hat{V}$, groundstate of *N* particles is that of free Bose gas, *i.e.* (apart from normalization)

$$\Psi_o^{(N)} = (a_o^+)^N |\text{vac}\rangle \qquad \left(\equiv (a_o^+ a_o^+)^{N/2} |\text{vac}\rangle\right)$$

Most important scattering processes:



$$\begin{pmatrix} + \text{ inverse} \\ \text{process} \end{pmatrix}, \ \textit{i.e.} \ \underbrace{V_k a_k^+ a_{-k}^+ a_o a_o (+H.c.)}_{\hat{V}_{\text{pair}}}$$

The simplest ansatz for *N*-particle GSWF incorporating these processes: (apart from normalization)

$$\Psi_o^{(N)} = \left(a_o^+ a_o^+ - \sum_k c_k a_k^+ a_{-k}^+\right)^{N/2} |\text{vac}\rangle \leftarrow \text{particle-conserving!}$$

Coefficients c_k can be found by minimizing $\widehat{H}$ including $\widehat{V}$ pair terms*. However, calculations rather messy…

Bogoliubov: in "reduced" Hamiltonian

$$\widehat{H}_{red} \equiv \sum_k \varepsilon_k a_k^+ a_k + \left\{ \sum_k V_k a_k^+ a_{-k}^+ a_o a_o + \mathrm{H.c.} \right\}$$

treat quantity $a_o a_o$ (or actually a_o) as c-number $\left(a_o \to \sqrt{N_o} \quad \text{so} \quad a_o a_o \to N_o \right)$;

then

$$\widehat{H}_{Bog} = \sum_k \{ \varepsilon_k a_k^+ a_k + N_o V_k (a_k^+ a_{-k}^+ + \mathrm{H.c.}) \}$$

(but see below…)

*see e.g. AJL, Revs. Mod. Phys. 73, 307 (2001), section VIII.

What are the implications of treating $a_o a_o$ as a c-number? Implies a nonzero expectation value

$$\langle\Psi|a_o a_o|\Psi\rangle \cong N_o \qquad (\equiv \langle a_o^+ a_o\rangle)$$

This is not true for the (particle-conserving) wave function

$$\Psi_o^{(N)} \equiv \left(a_o^+ a_o^+ - \sum_k c_k a_k^+ a_{-k}^+\right)^{N/2} |\mathrm{vac}\rangle \qquad (\langle a_o a_o\rangle \equiv O)$$

but is true e.g. for

$$\Psi_o^{Bog} \equiv \exp\left\{\lambda\left(a_o^+ a_o^+ - \sum_k c_k a_k^+ a_{-k}^+\right)\right\} \equiv \sum_{N=\mathrm{even}} \lambda^N \Psi_o^{(N)}/N!$$

(neglect details about normalization, etc.)

What fixes $\langle N\rangle(\sim\lambda)$? If we just minimize $\hat{H}_{Bog}$ as it stands this automatically gives $\lambda\sim\langle N\rangle\sim 0$! Hence must add chemical potential term, *i.e.* minimize

$$\hat{H}'_{Bog} \equiv \hat{H}_{Bog} - \mu\hat{N} \qquad (\textit{i.e.}\ \varepsilon_k \rightarrow \varepsilon_k - \mu)$$

and adjust μ so that $\langle N\rangle(\mu) = N$ $\Leftarrow$ actual number of particles

This procedure is standard in conventional statistical mechanics (macrocanonical $\Rightarrow$ ground canonical), but then resultant state is a mixture of different *N*. Now by contrast we have a quantum superposition of states of different *N*.

Let's define an operator $\hat{\varphi}$ which is canonically conjugate to $\widehat{N}$, so that its eigenfunctions $|\varphi\rangle$are related to those of $\widehat{N}$ by

$$|\varphi\rangle = \sum_N \big(\exp(iN\varphi)\big)|N\rangle. \quad |N\rangle = \int d\varphi \exp - iN\varphi \quad |\varphi\rangle$$

Since original $\widehat{H}$ (not $\widehat{H}_{Bog}$!) satisfies $\langle N|\widehat{H}|N'\rangle \sim \delta_{NN'}$, it is invariant under "rotation" of φ ("U(1)symmetry") . However Ψ_o^{Bog} picks out a definite value (0) of φ:

"Spontaneously broken U(1) symmetry"

THE MEAN-FIELD (BOGOLIUBOV) METHOD: QUASIPARTICLES:

"Mean-field" Hamiltonian $\hat{H}_{MF} \equiv \hat{H}'_{Bog}$, *i.e.*

$$\hat{H}_{MF} \equiv \sum_k \{(\epsilon_k - \mu) a_k^+ a_k + N_o V_k (a_k^+ a_{-k}^+ + \mathrm{H.c.})\}$$

with standard Bose C.R.'s

$$[a_k, a_{k'}] = [a_k^+ a_{k'}^+] = 0, \qquad [a_k, a_{k'}^+] = \delta_{kk'}$$

This can be diagonalized by Bogoliubov transformation

$$\alpha_k^+ = u_k a_k^+ + v_k a_{-k} \text{ (etc.)}, \; |u_k|^2 - |v_k|^2 = 1$$

which preserves Bose C.R.'s.:

$$\hat{H}_{MF} \equiv \sum_k E_k \alpha_k^+ \alpha_k + \text{const.}$$

where (after μ is fixed to give $\langle N \rangle = N$ and V_k *set* $\cong V_O$)

$$E_k = (\varepsilon_k(\varepsilon_k + 2NV_O))^{1/2} \Leftarrow \text{Bogoliubov spectrum}$$

Note: All these results, including formula for E_k, can be obtained by particle-conserving method based on ansatz $\Psi_O^{(N)}$. However, in that method we have

$$\alpha_k^+ = \underset{+1}{u_k a_k^+} + v_k \underbrace{(a_o^+ a_o^+ / N_o)}_{+2} \underset{-1}{a_{-k}}$$

$\Leftarrow$ particle-conserving! $(N \to N+1)$

By contrast, in Bogoliubov method

$u_k a_k^+$ adds a particle $(N \to N+1)$

$v_k a_{-k}$ subtracts a particle $(N \to N-1)$

So qp state is not an eigenstate of N. (but neither is groundstate…)

[Density fluctuation in number-conserving formalism:

$$\hat{\rho}_k = \alpha_k^+ a_o = u_k a_k^+ a_o + v_k (a_o^+ a_o^+ / N_o) a_{-k} a_o$$

$$= u_k a_k^+ a_o + v_k a_{-k} a_o^+]$$

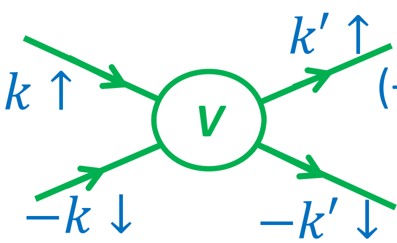
[Generalization of Bogoliubov method to inhomogeneous situations]

Spontaneously Broken U(1) Symmetry: The General Idea (cont.)

2. Superconductors (BCS 1957)

$$\hat{H} = \sum_{k\sigma} \varepsilon_k a_{k\sigma}^{+} a_{k\sigma} + \hat{V} \qquad [\hat{H}, \hat{N}] = [\hat{H}, \hat{P}] = 0$$

Most important scattering process:



(+ inverse process),

i.e.

$$\underbrace{V_{kk'} a_{k'\uparrow}^{+} a_{-k'\downarrow} a_{-k\downarrow} a_{k\uparrow} (+\mathrm{H.c.})}_{\hat{V}_{\text{pair}}}$$

Simplest ansatz for N-particle GSWF incorporating these processes (apart from normalization)

even (N)

$$\Psi_0^{(N)} = \left(\sum_k c_k a_{k\uparrow}^{+} a_{-k\downarrow}^{+} \right)^{N/2} |\mathrm{vac}\rangle \Leftarrow \text{particle-conserving!}$$

with coefficients found by minimizing $\hat{H}$ including $\hat{V}_{\text{pair}}$ terms*.

*See e.g. AJL, Quantum Liquids, section V.

Again, calculations messy…

BCS: in "reduced" Hamiltonian

$$\hat{H}_{red} = \sum_{k\sigma} \epsilon_k a^+_{k\sigma} a_{k\sigma} + \sum_{kk\prime} (V_{kk\prime} a^+_{k\uparrow} a^+_{-k\downarrow} a_{-k\prime\downarrow} a_{k\prime\uparrow} + \mathrm{H.c.})$$

treat the quantity

$$\hat{\Delta}_k \equiv \sum_{k\prime} V_{kk\prime} a_{-k\prime\downarrow} a_{k\prime\uparrow}$$

as c-number. Then (adding chemical potential term as in Bose case)

$$\hat{H}_{MF} = \sum_{k\sigma} (\epsilon_k - \mu) a^+_{k\sigma} a_{k\sigma} + \sum_{k} (\Delta_k a^+_{k\uparrow} a^+_{-k\downarrow} + \mathrm{H.c.})$$

$$\Delta_k \equiv \sum_{k\prime} V_{kk\prime} \langle a_{-k\prime\downarrow} a_{k\prime\uparrow} \rangle$$

Again, this makes sense only if U(1) symmetry spontaneously broken, e.g.

$$\Psi_{BCS} = \exp\left(\sum_k c_k a^+_{k\uparrow} a^+_{-k\downarrow} \right) |\mathrm{vac}\rangle \left(\equiv \prod_k (u_k |oo\rangle_k + v_k \,|11\rangle_k \right)$$

The Mean-Field (BCS) Method: Quasiparticles

As above, mean-field Hamiltonian is

$$\hat{H}_{MF} = \sum_{k\sigma}(\epsilon_k - \mu)a^+_{k\sigma}a_{k\sigma} + \sum_k (\Delta_k a_{k\uparrow}a^+_{-k\downarrow} + \mathrm{H.c.})$$

with standard Fermi ACR's

$$\{a_{k\sigma}, a_{k'\sigma'}\} = \{a^+_{k\sigma}, a^+_{k'\sigma'}\} = O, \{a_{k\sigma}, a^+_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'}$$

This can be diagonalized by Bogoliubov (-Valatin) transformation

$$\alpha^+_{k\sigma} = u_k a^+_{k\sigma} + \sigma v_k a_{-k-\sigma} \text{ (etc.)}, \;\; |u_k|^2 + |v_k|^2 = 1$$

which preserves Fermi ACR's:

$$\hat{H}_{MF} = \sum_{k\sigma} E_k \alpha^+_{k\sigma}\alpha_{k\sigma} \qquad E_k \equiv \left(\varepsilon_k^2 + |\Delta_k|^2\right)^{1/2}$$

Note: All these results can be obtained by particle-conserving method based on ansatz $\Psi_o^{(N)}$. However, in that method we have

$$\underset{+1}{\alpha_{k\sigma}^{+} = u_k a_{k\sigma}^{+}} + \sigma v_k \underset{-1}{a_{-k,-\sigma}} \underset{+2}{c^{\dagger}}$$

$\Leftarrow$ particle-conserving! $(N \rightarrow N+1)$

where $C^{\dagger}$ is normalized Cooper-pair creation operator:

$$C^{\dagger} \equiv \underbrace{n}_{\text{normalization}} \cdot \left(\sum_k c_k a_{k\uparrow}^{+} a_{-k\downarrow}^{+} \right)$$

By contrast, in BCS method

$u_k a_{k\sigma}^{+}$ adds an electron $(N \rightarrow N+1)$

$\sigma v_k a_{-k,-\sigma}^{+}$ subtracts an electron $(N \rightarrow N-1)$

so qp state is not an eigenstate of N (but neither is GS …)

[In recent literature on TI's, etc., $\widehat{H}_{MF}$ often described as "noninteracting-electron" Hamiltonian (!)]

The Mean-Field Method for Spatially Inhomogeneous Problems: The Bogoliubov-De Gennes Equations

If the single-particle potential and/or the pairing interaction varies in space, the construction of a GSWF which generalizes $\Psi_O^{(N)}$, while possible in principle*, is usually unfeasible in practice. However, the mean-field method is simply generalized (de Gennes 1964):

Consider for illustration the simple Hamiltonian

(obtained by setting $V(\boldsymbol{r}-\boldsymbol{r}') = g\delta(\boldsymbol{r}-\boldsymbol{r}')$ and using $[\psi_\sigma(\boldsymbol{r})]^2 \equiv O$)

single-particle potential

$$\widehat{H} = \int d\boldsymbol{r} \sum_\sigma \left\{ \frac{\hbar^2}{2m} \left(\boldsymbol{\nabla} \hat{\psi}_\sigma^\dagger(\boldsymbol{r}) \cdot \boldsymbol{\nabla} \hat{\psi}_\sigma(r) \right) + (\mathrm{U}(\boldsymbol{r}) - \mu) \hat{\psi}_\sigma^\dagger(r) \hat{\psi}_\sigma(r) \right\}$$
$$+ g \int dr\, \hat{\psi}_\uparrow^\dagger(r) \hat{\psi}_\downarrow^\dagger(r) \hat{\psi}_\downarrow(r) \hat{\psi}_\uparrow(r)$$

The mean-field approximation: take the quantity

$$\widehat{\Delta}(\boldsymbol{r}) \equiv \boldsymbol{g} \hat{\psi}_\downarrow(\boldsymbol{r}) \hat{\psi}_\uparrow(\boldsymbol{r})$$

to be a c-number. Thus (↑: caution re factors of 2 etc!)

*Stone & Chung, Phys. Rev. B **73**, 014505 (2006)

$$\hat{H}_{MF} = \hat{H}_O + g\int dr\,\{\Delta(r)\hat{\psi}_\uparrow^\dagger(r)\hat{\psi}_\downarrow(r) + \mathrm{H.c.}\}$$

$$\hat{H}_o \equiv \int d\boldsymbol{r}\sum_\sigma \left\{\frac{\hbar^2}{2m}\left(\boldsymbol{\nabla}\psi_\sigma^\dagger(r)\cdot\boldsymbol{\nabla}\psi_\sigma(r)\right) + (\cup\,(\boldsymbol{r}) - \mu)\psi_\sigma^\dagger(r)\psi_\sigma(r)\right\}$$

with standard Fermi ACR's

$$\{\hat{\psi}_\sigma(r), \hat{\psi}_{\sigma'}^\dagger(r')\} = \delta(\boldsymbol{r}-\boldsymbol{r}')\delta_{\sigma\sigma'} \text{ (etc.)}$$

Since H_{MF} is a quadratic form in $\hat{\psi}_\sigma^\dagger(r), \psi_\sigma(\boldsymbol{r})$, it can be diagonalized by introducing operators γ_i^+ defined by

$$\hat{\gamma}_{i\sigma}^+ = \int d\boldsymbol{r}\,\{u_i(r)\hat{\psi}_\sigma^\dagger(r) + \sigma v_i(r)\hat{\psi}_{-\sigma}(\boldsymbol{r})\}$$ ⇐ particle-nonconserving!

not H.c's

which will satisfy Fermi ACR'S provided the $u_i(r), v_i(r)$ satisfy

$$\int dr\{(u_i(r), u_j(r)) + (v_i(r), v_j(r))\} = \delta_{ij}$$

a condition in fact guaranteed by the BdG equations (below). Thus

$$\hat{H}_{MF} = \sum_{i\sigma} E_i\gamma_{i\sigma}^+\gamma_{i\sigma} + \text{const.}$$

The eigenfunctions $\begin{pmatrix} u_i \\ v_i \end{pmatrix}$ and eigenvalues E_i of the mean-field Hamiltonian satisfy the Bogoliubov-de Gennes (BDG) equations:

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

This guarantees

(a) orthonormality of spinors $\begin{pmatrix} u_i \\ v_i \end{pmatrix}$ (c.f. above)

(b) if $\begin{pmatrix} u_i(r) \\ v_i(r) \end{pmatrix}$ is a solution with energy E_i, then $\begin{pmatrix} v_i^*(r) \\ u_i^*(r) \end{pmatrix}$ is also a solution with energy $-E_i$: hence now be able to find solutions with $E_i = 0$, provided $u_i(r) = v_i^*(r)$ ("pseudo-Majorana")

Mean-field method in more general case:

$$\hat{H} = \sum_{\sigma\sigma'} \int d\boldsymbol{r} \left\{ \delta_{\sigma\sigma'} \frac{\hbar^2}{2m} \boldsymbol{\nabla}\hat{\psi}_\sigma^\dagger(r) \cdot \boldsymbol{\nabla}\hat{\psi}_{\sigma'}(r) \right.$$

$$+(\mathrm{U}_{\boldsymbol{\sigma\sigma'}}(\boldsymbol{r}) - \mu\delta_{\sigma\sigma'})\hat{\psi}_\sigma^\dagger(\boldsymbol{r})\hat{\psi}_{\sigma'}(\boldsymbol{r})$$

$$\left. +\frac{1}{2} \sum_{\alpha\beta\gamma\delta} \iint d\boldsymbol{r}d\boldsymbol{r}'\, V_{\alpha\beta\gamma\delta}(r,r')\psi_\alpha(r)\hat{\psi}_\beta^\dagger(r')\hat{\psi}_\gamma(r)\hat{\psi}_\delta(r) \right\}$$

Define

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

and treat it as a c-number. Then

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

Now the BdG equations will in general be 4x4. But note that in the special case of a single spin species ($\alpha, \beta, \gamma, \delta \equiv 1,$ *e.g.* spin-polarized ultracold Fermi alkali gas) we have

$$\gamma_i^\dagger \equiv \int dr\{u(r)\psi^\dagger(r) + v(r)\psi(r)\}$$

H.c's

so in particular $E_i = 0,\ u(r) = v^*(r)$ modes (if any) may be true Majoranas.

The "Topological Insulator – Topological Superconductor" Analogy

Consider a "superconductor" with only one spin species, and assume for the moment spatially homogeneous conditions. Then we can take spatial Fourier transforms and get

$$\hat{H}_{MF} = \sum_k \underbrace{\xi_k}_{\equiv(\varepsilon_k-\mu)} a_k^+ a_k + (\Delta_k a_k^+ a_{-k}^+ + \mathrm{H.c.})\} \; (\Delta_{-k} \equiv -\Delta_k)$$

The eigenfunctions of $\hat{H}_{MF}$ are of form

$$\psi_k \begin{pmatrix} u_k \\ v_k \end{pmatrix} \equiv (u_k a_k^+ + v_k a_{-k})|\mathrm{GS}\rangle$$

Creates particle in state **k**

Creates hole in state -**k**

Thus, if we define a 2D Hilbert space corresponding to "pseudo spin"

$$|\uparrow\rangle \equiv |\text{particle in state } \boldsymbol{k}\rangle$$

$$|\downarrow\rangle \equiv |\text{hole in state } -\boldsymbol{k}\rangle$$

then $\hat{H}_{MF}$ can be written (after subtraction of a constant term from the KE) in the "Nambu" form

$$\hat{H}_{MF} \sum_k \{\xi_k \hat{\sigma}_{zk} + \underbrace{\Delta_{xk}}_{\equiv Re\Delta_k} \hat{\sigma}_{zk} + \underbrace{\Delta_{yk}}_{\equiv Im\Delta_k} \hat{\sigma}_{yk}\} \equiv \sum_k \{\xi_k \hat{\sigma}_{zk} + \boldsymbol{\Delta}_k \cdot \hat{\boldsymbol{\sigma}}_{\perp k}\}$$

Now compare this with a simple 2-band solid with nonzero interband coupling. For this case define (for say real spin ↑) pseudospin states

$$|\uparrow\rangle \equiv |\text{particle in state } \boldsymbol{k} \text{ in band } 1\rangle$$

$$|\downarrow\rangle \equiv |\text{particle in state } \boldsymbol{k} \text{ in band } 2\rangle$$

$$\xi_k \equiv (\varepsilon_k(1) - \varepsilon_k(2))$$

$$\left.\begin{matrix}\Delta_{xk}\\ \Delta_{yk}\end{matrix}\right\} = \left\{\begin{matrix}Re\\ Im\end{matrix}\right. \text{ part of interband matrix element}$$

Then $\hat{H}_{2\text{-}band}$ is formally identical to $\hat{H}_{MF}$!

(↑: physical interpretation is completely different!)

TOPOLOGICAL SUPERCONDUCTORS, cont.

A particularly interesting case is when the system is 2D and

$$\Delta_k = \text{const.}\left(k_x + ik_y\right), \quad \xi_k \text{ changes sign at } |\boldsymbol{k}| = k_o.$$

(e.g. due to spin-orbit coupling

In the 2-band case this corresponds to a topological insulator.* If we now allow k_o to be a $f(\boldsymbol{r})$ and to cross zero on some contour (e.g. the physical boundary of the system) it is easy to show (Volkov & Pankratov 1985) that a localized mode appears on this contour and disperses across the bulk band gap, with zero energy for $\boldsymbol{k} \perp$ contour. For a (real geometrical) "hole" in the T⊥, $\boldsymbol{k}$ is always ⊥ contour so E=0. This mode is a quantum superposition of $|\uparrow\rangle$ and $|\downarrow\rangle$ (*i.e.* $|1\rangle$ and $|2\rangle$) with equal weights (and, in the usual representation, a $\pi/2$ phase shift between them).

Now consider the superconducting analog – a p-wave superconductor with "*p* + *ip*" pairing $\left(\Delta_k = \text{const.}\left(k_x + ik_y\right)\right)$. By analogy we expect boundary modes, and more interestingly, at vortices ("holes") a single E=0 mode with equal weight for the $|\uparrow\rangle$ and $|\downarrow\rangle$ components. But $|\uparrow\rangle$ now represents a particle and $|\downarrow\rangle$ a hole, so

the E=0 state has exactly equal weight for particle & hole components.

*cf. Bernevig et al. 2006

By an appropriate choice of global phases we can set $u(r) = v^*(r)$, so particle is its own antiparticle ("Majorana fermion").

Actually, M.F.'s always come in pairs (2 MF's = 1 Bogoliubov qp), so any pair of vortices may carry either no MF's ("$|0\rangle$") or 2 ("$|1\rangle$").

Ivanov (2001): if 2 vortices exchanged, $|1\rangle$ picks up Berry phase of $\pi/2$ relative to $|0\rangle$. Argument relies heavily on use of BdG equations.

This result is fundamental to the idea of topological quantum computing using $p + ip$ Fermi superfluids (*e.g* UC alkali gases, ^{3}*He-A*, Sr_2RuO_4 . . .).

So: What could be wrong with all this?

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

Consider an even-number-parity BCS superfluid at rest. (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

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

$$E_k \equiv \left(\epsilon_k^2 + |\Delta_k|^2\right)^{1/2} \text{ (so } |u_k|^2 + |v_k|^2 = 1\text{)}$$

The total momentum $\boldsymbol{P}_\mathrm{f}$ 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 $\boldsymbol{k} + m\boldsymbol{v}/\hbar$ 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

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

Thus the added momentum is

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

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

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

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

$$\gamma_i^\dagger = u_k a_{k\uparrow}^+ + v_k a_{-k\downarrow}\hat{C}_{(0)}^\dagger$$ ← creates extra Cooper pair (with COM velocity 0)

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

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

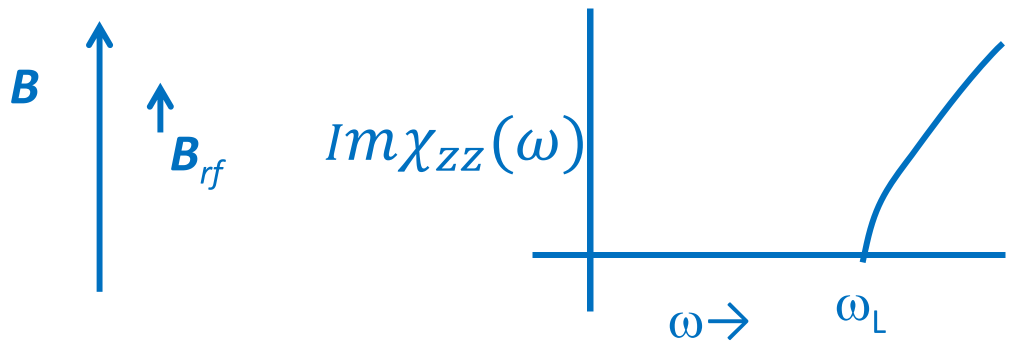
$$\Rightarrow \Delta P'_f = \left(\Delta P'_f\right)_{BdG} + 2m|v_k|^2 = \hbar\boldsymbol{k} + m\boldsymbol{v}$$

in accordance with GI argument

Moral: addition of fermionic particle $u_k a_{\boldsymbol{k}}^+ + ...$ produces total extra momentum $\hbar\boldsymbol{k}$, regardless of whether condensate is moving.

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 $\widehat{H}$ $\Rightarrow$

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

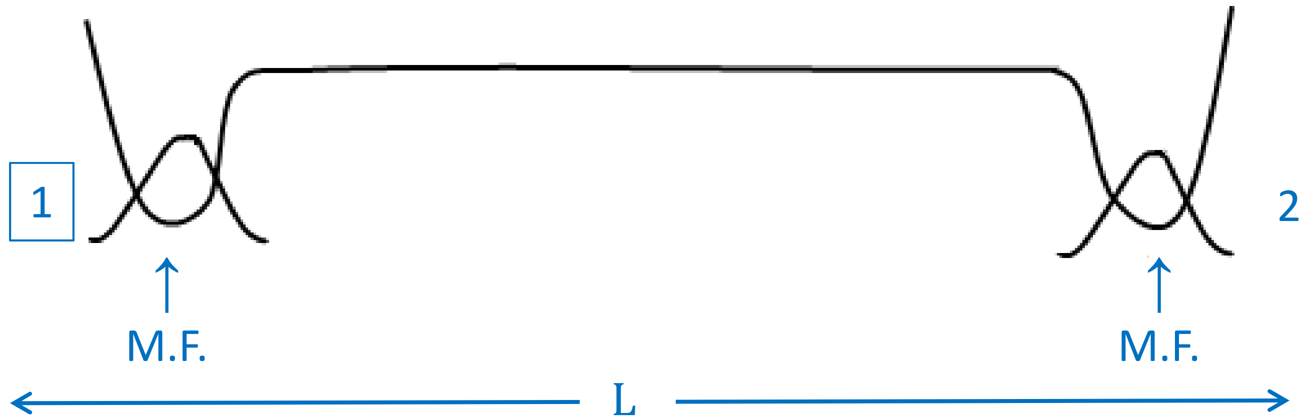
$$\Rightarrow Im\chi_{zz}(\omega) \sim \delta(\omega)!$$

For nonzero g_D,
$\int \omega \, Im\chi_{zz}(\omega) d\omega \sim g_D$ $\Rightarrow$ result cannot be right for $g_D \rightarrow 0$
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 $\sim v_f$).

The $64K question:

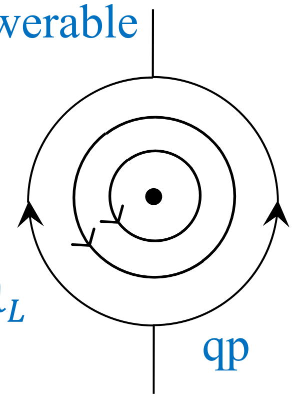
What is the Berry phase (φ_B) accumulated by a Bogoliubov quasiparticle circling the core of an Abrikosov vortex?

(Note: (a) this is in principle an experimentally answerable question:

(b) at large distances ($r \gg \lambda_L$),

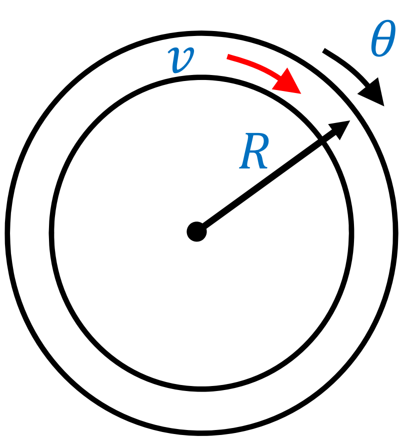
simple AB effect $\Rightarrow$ $\varphi_B = \pi$

However, we are interested in $\xi \ll r \ll \lambda_L$



$\Rightarrow$ replace by problem of neutral liquid in torus

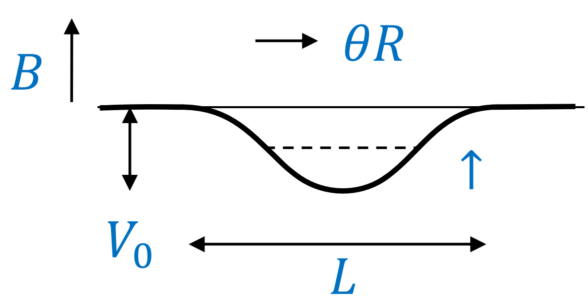
Setup of problem:



A. Neutral superfluid ($2N$ fermions) with s-wave pairing circulating with minimum nonzero velocity:

$$v = \frac{\hbar}{2mR} \qquad \left(k = \frac{h}{2m}\right)$$

note: Δ/ϵ_F may be ~1



B. Create Zeeman trap:

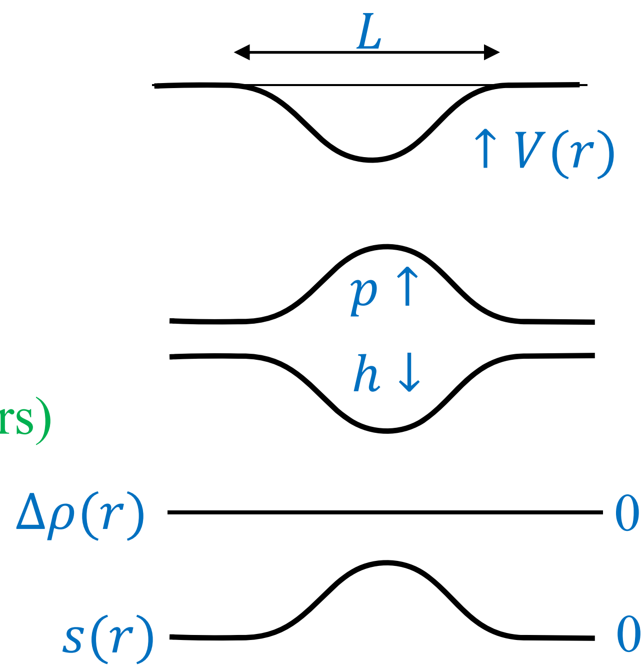
$$V(r) = -\sigma_z B(\theta R)$$

with $\xi \ll L \ll 2\pi R$, $V_0 \ll \Delta$
$V_0 L^2 \geq 1$ (so single $\uparrow$-spin fermion in free space would be bound)

C. Add single extra fermion with spin ↑.

What happens?

For superfluid at rest, Bog. qp presumably sits in Zeeman trap: since for $L \gg \xi$ qp is equal admixture of p ↑ and h ↓, (+ extra C. pairs) no extra mass density associated with trap. (Also, by TR symmetry, no mass current anywhere in system.)



If superfluid moving, presumably above is still true to zeroth order in v

D. Now imagine moving Zeeman trap adiabatically around torus ($v_{\text{trap}} \ll v, c$ ...). Then $\tau_{\text{trap}} \gg \hbar/\Delta E$ ($\Leftarrow$ any excitation energy of system) $\Rightarrow$ Berry phase well-defined.

($64K) question:

WHAT BERRY PHASE IS ACCUMULATED?

note: if superfluid at rest, φ_B is fairly obliviously 0

1st METHOD OF SOLUTION (BdG):

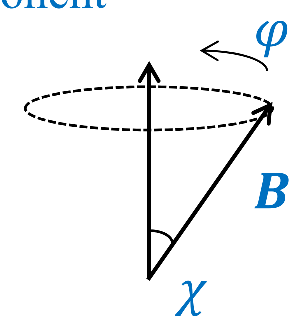
$$\hat{H}_{\text{BdG}} = \begin{pmatrix} \hat{H}_{o\uparrow} & \Delta(r) \\ \Delta^*(r) & -\hat{H}^*_{o\downarrow} \end{pmatrix} \begin{pmatrix} u\,(r) \\ v\,(r) \end{pmatrix} \begin{matrix} \leftarrow \text{particle component} \\ \leftarrow \text{hole component} \end{matrix}$$

with $\Delta(r) = |\Delta_0| \exp i\theta$

Compare this with standard textbook problem of spin ½ in "rotating" magnetic field:

$$\hat{H}_{\text{MF}} = \begin{pmatrix} B_z & B(r) \\ B^*(r) & -B_z \end{pmatrix} \quad \begin{matrix} \leftarrow \text{spin-}\uparrow \text{ component} \\ \leftarrow \text{spin-}\downarrow \text{ component} \end{matrix}$$

$$B(r) = |B_0| \exp i\varphi$$



In textbook problem, known result is

$$\varphi_B = 2\pi \cos^2 \chi /2$$

and in particular for $\chi = \pi/2$ (equal weight of $\uparrow$ and $\downarrow$ spin components), $\varphi_B = \pi$ ("4π symmetry of fermions", verified in neutron interferometry experiments)

Hence, by analogy (or direct calculation!) in BdG problem, since "particle" and "hole" components have equal weight, conclude

$$\boxed{\varphi_B = \pi} \qquad \text{BdG calculation}$$

2^{ND} Method Of Solution (Particle-Conserving Calculation):

Two general theorems:

1. (provided ($2N$+1) GS is any superposition of single fermion excited states, i.e., condensate not affected by Zeeman trap to order $\boldsymbol{v}$):

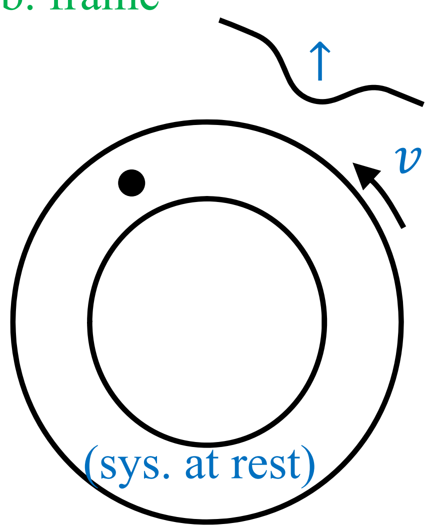
$$\varphi_B = 2\pi \cdot \Delta \mathrm{J}_0$$

difference in (angular momentum/ $\hbar$) in GS of $2N$+1 and $2N$ system (in lab. frame)

2. Galilean invariance $\Rightarrow \Delta J_v - \Delta J_0 = \frac{1}{2}$

ΔJ in rest frame of superfluid

ΔJ in lab. frame



As a result, can state with confidence

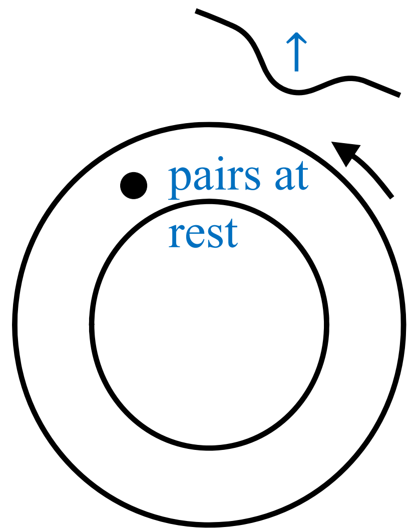
$$\varphi_B = \pi(1 - 2\Delta \mathrm{J}_v)$$

So: if with superfluid at rest and trap rotating, angular momentum J_v is nonzero*, BdG must be wrong

QN: WHAT IS J_v?

(QUESTION UNEXPECTEDLY FULL OF TRAPS! DO WE NEED TO RE-INVENT THE WHEEL?)

* Since unarguably $J_{2N,v} = 0$



Pairs at rest, walls (traps) rotating

WHAT IS $\boldsymbol{J}$?

[note: for free particle, certainly ½ !]

Qp state must generically be of form

$$|\Psi_{qp}\rangle = \sum_p f_p(u_p a^+_{p\uparrow} + u_p a_{-p\downarrow}\hat{C}^\dagger)|2N\rangle$$

$$\equiv \int u(r)\hat{\psi}^\dagger(r) + v(r)\hat{\psi}(r)C^\dagger)\,|2N\rangle$$

ARGTS. FOR $\boldsymbol{J} = 0 \;\; (\varphi_B = \pi)$:

1. For "low-energy" Bog. qp., $\int |u(r)|^2 dr = \int |v(r)|^2 dr = \dfrac{1}{2}$

   $\Rightarrow$ no mass density deviation

   $\Rightarrow$ no mass transport

   $\Rightarrow \boldsymbol{J} = 0$

2. In lab. Frame, no time-dependence

   $\Rightarrow \mathrm{div}\boldsymbol{J} = 0 = \mathrm{div}\,\Delta J$

   $\Rightarrow \Delta J(r)$ far from trap = $\Delta J/L$

   but far from trap $u = v = 0$, so only contribution to $\Delta\boldsymbol{J}$ is from C. pairs: this is $= \frac{1}{2}(2m\boldsymbol{v}) = m\boldsymbol{v}$

   $\Rightarrow \Delta J_0 = 1/2 \Rightarrow \Delta J_{\mathrm{v}} \equiv \boldsymbol{J} = 0$

ARGUMENT FOR $\boldsymbol{J} \neq 0$ $\quad (\varphi_B \neq \pi)$:

Apply adiabatic perturbation theory, then (quite generally, for any state $|0\rangle$) notation of trap generates perturbation

$$V_{no}^{eff} = i\hbar \left(\frac{\partial \hat{H}}{\partial t}\right)_{no} \frac{1}{E_n - E_o} = i\hbar \boldsymbol{v} \frac{\langle n|\hat{\boldsymbol{Q}}|0\rangle}{E_n - E_o}$$

where $\hat{Q} \equiv -\sum_i \hat{\sigma}_{zi} \left.\frac{\partial V(r)}{\partial \boldsymbol{r}}\right|_{r=r_i}$

Hence provided $\langle \boldsymbol{J} \rangle_o = 0$, value of $\boldsymbol{J}$ induced by rotation of trap is

$$\boldsymbol{J} = A\boldsymbol{v} \quad , \quad A \equiv i\hbar \sum_n \frac{\langle 0|\hat{\boldsymbol{J}}|n\rangle\langle n|\hat{\boldsymbol{Q}}|0\rangle}{(E_n - E_0)^2}$$

Now if $|0\rangle$ is the $2N$-particle GS, both $|0\rangle$ and $|n\rangle$ can be chosen to be eigenstates of $\hat{T} \Rightarrow A = 0$ by symmetry.

"pseudo" time reversal $(\sigma \to -\sigma, B \to B)$

However, if $|0\rangle$ is the GS of the $(2N+1)-$ particle system (with **S**=1), this is not true! $\Rightarrow$ no symmetry principle requires A to be nonzero.

Indeed, since $\left[\hat{\boldsymbol{J}}, \hat{H}_{bulk}\right] = 0$,

$$\frac{d\hat{\boldsymbol{J}}}{dt} = i\hbar\left[\hat{J}, \hat{H}_{trap}\right] = -\mathrm{i}\hbar \sum_i \hat{\sigma}_{zi} \left.\frac{\partial V}{\partial r}\right|_{rzri} = -i\hbar\hat{\boldsymbol{Q}}$$

so $\langle n|Q|0\rangle = \frac{1}{i\hbar}(E_n - E_0)\langle n|\boldsymbol{J}|0\rangle$ and so

$$A = \sum_n \left\{\frac{|\langle 0|\boldsymbol{J}|n\rangle|^2}{E_n - E_o}\right\} \equiv \chi_{JJ}(q \to 0, \omega \to 0)$$

↑: Since $A = 0$ for $2N-$ particle GS, must take $\boldsymbol{J}$ to be

$\lim\limits_{q\to 0} \boldsymbol{J}_q$, $\boldsymbol{q} \perp \boldsymbol{J}$ (Meissner effect!). But for extra quasiparticle,

"$J_{long} = J_{transv}$"? If so then from *f*-sum rule $\Rightarrow \boldsymbol{J} = m\boldsymbol{v} \Rightarrow \varphi_B = 0$

Wait for the next thrilling installment . . .

Conclusions

What are implications for TQC program?

1. $\nu = 5/2$ QHE: no implications

2. (p + ip) Fermi superfluids (e.g. Sr_2RuO_4)
   Literature may be right.

3. But urgent to (dis)-confirm using physical (particle-conserving) many-body wave functions

4. More generally:

CMP $\not\rightarrow$ QI !