The Mean-Field Method in the Theory of Superconductivity:

Is it Adequate for Quantum-Information Purposes?

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joint work with Yiruo Lin
(see also poster, this workshop)

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Main theses of this talk:

1. For 50 years, almost all theoretical work on inhomogenous Fermi superfluids, including work on "topological superconductors" has been based on the solution of the BdG (mean-field) Hamiltonian, which in turn is justified by appeal to the idea of "spontaneously broken U(1) gauge symmetry" (SBGS)

2. There is no physical justification for the idea of SBGS, and hence none for the use of the BdG Hamiltonian (at least without considerable caution).

3. Moreover, simple examples show that it can lead to physically incorrect conclusions.

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

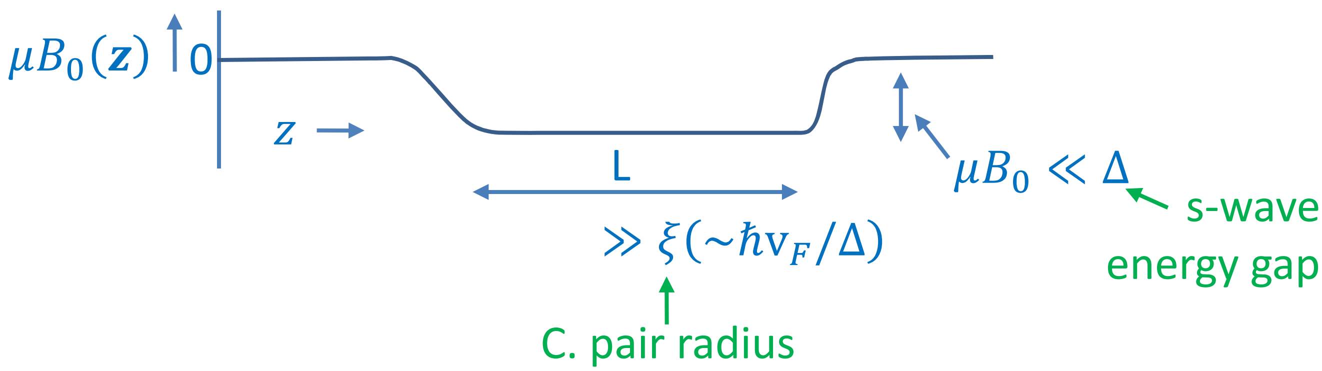
5. This consideration drastically affects arguments about the effects of braiding of Majorana fermions, etc. (see poster): it may also affect arguments about their undetectability by local probes.

6. If so, this could be a disaster for the whole program of using topological superconductors such as Sr_2RuO_4 for topological quantum computing. (Or, it might help...)

(much of this (1) – (4)) could have been said in 1958! Was it?)

A simply posed question:

Consider neutral spin–1/2 Fermi superfluid in s-wave state in presence of Zeeman potential*: (quasi-1D, i.e. tube of cross-section $\lesssim$ (pair radius)^2)



In limit $\mu B_0 \ll \Delta$, even-number-parity ground state (S=0) is presumably insensitive to trap to order $\mu B_0/\Delta$. Consider now odd-parity ground state (S= 1/2). According to standard BdG-type ideas, a single Bogoliubov quasiparticle sits in the Zeeman trap, with equal $\int |u(r)|^2\, dr = \int |v(r)|^2\, dr$, i.e. equal "particle" and "hole" components.

We all agree that the trap localizes a total spin of 1/2.

$64K question: Does it also localize an extra "particle number", and if so what is it?

*Y. R. Lin and AJL, JETP **119**, 1034 (2014)

“Spontaneously broken gauge symmetry”

Claim: An isolated superconductor with an even number of particles need not be in an eigenstate of total particle number N, rather it may be described by the particle-nonconserving (PNC) wave function

$$\Psi_{\mathrm{PNC}}^{(\mathrm{even})} = \sum_{N} C_N \Psi_{2N} \qquad , C_N \sim \exp iN\varphi$$

so that $\langle \hat{\psi}\hat{\psi} \rangle \sim \sum_N C_{N+1}^* C_N \sim$ const. $\exp i\varphi \neq 0$. Then it is consistent to construct odd-parity states by the BdG prescription: e.g. for spin $\uparrow$.

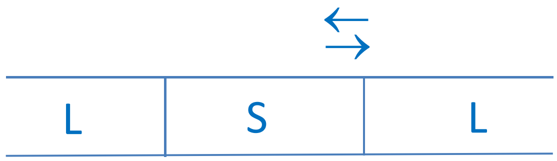
$$\Psi_{\mathrm{PNC}}^{(\mathrm{odd})} = \int \{u(r)\hat{\psi}_\uparrow^\dagger(r) + v(r)\hat{\psi}_\downarrow(r)\} dr \left| \Psi_{\mathrm{PNC}}^{(\mathrm{even})} \right\rangle$$

where the spinors $\big(u(r), v(r)\big)$ are normalized eigenfunctions of the particle-nonconserving mean-field (BdG) Hamiltonian. In (e.g.) a $p + ip$ (“topological”) superfluid the solutions have interesting properties (e.g. Majoranas).

Question: Why should we believe all this?

(“... the Danube is not blue...”)

Ans. no. (1): Particle no. is not conserved (e.g. leads)



However: total particle no. (S + L) is still conserved. Reduced density matrix $\rho_{NN'}$ of S is obtained by tracing over L, so while diagonal elements ρ_{NN} are nonzero for more than one N, still have $\rho_{NN'}$=0 for $N \neq N'$. No go!

Ans. no. (2): (Anderson, 1958)

Write $\Psi_{\mathrm{PNC}}^{(\mathrm{even})} \sim \Psi(\varphi)$, then

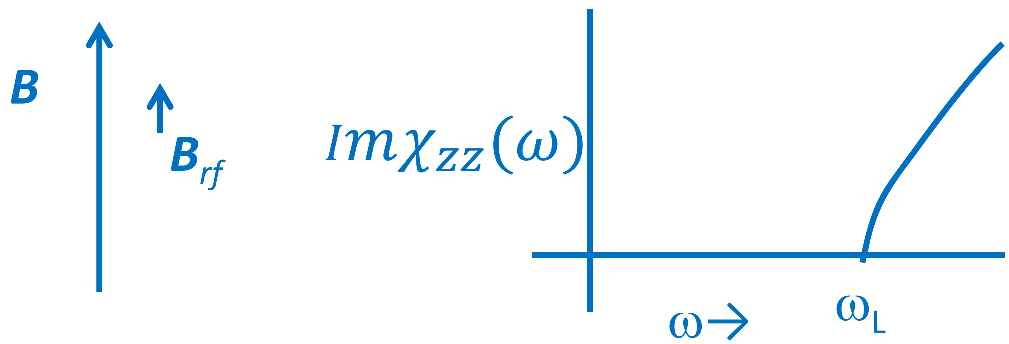
$$\frac{1}{2\pi}\int_0^{2\pi} \Psi(\varphi) \exp iN_0\varphi d\varphi = \Psi_{PC}(N_0)$$

↑ particle-conserving w.f. for $2N_0$ particles

Fine for even-parity states, but what about odd-parity ones? Problem is relation of odd-parity states to even-parity ones.

Failure of BdG/MF: a rather obvious 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 $\hat{H}$ $\Rightarrow$

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

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

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!

and indeed calculation† taking them properly into account removes the effect.

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

†E. Taylor et al., Phys. Rev. B **91**, 134505 (2015)

Failure of BdG/MF: a futher trivial (but apparently not well-known) example:

Consider an even-number-parity BCS superfluid at rest (so $P_0 = 0$)

↑ 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

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

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

The total momentum P_f of the (odd-number-parity) many-body state created by γ_i is

standard textbook result ↓

$$P_f = |u_k|^2(\hbar k) - |v_k|^2(-\hbar k) = (|u_k|^2 + |v_k|^2)\hbar k \equiv \hbar k$$

$$so \Delta P_f \equiv P_f - P_o = \hbar k$$

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

$$\gamma_f^\dagger = u_k a_{\mathrm{k+mv/\hbar}\,,\uparrow}^\dagger + v_k a_{\mathrm{-k\downarrow+mv/\hbar}} \leftarrow nb.not\ \ a_{-(\mathrm{k\downarrow+mv/\hbar})}!$$

Thus the added momentum is

$$\Delta P'_f = |u_k|^2(\hbar k + mv) - |v_k|^2(-\hbar k + mv) = \hbar k + (|u_k|^2 - |v_k|^2)mv$$

Recap: $BdG \rightarrow \Delta P_f^{'} = \hbar k + (|u_k|^2 - |v_k|^2)mv$

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

$$P_0' = P_o + Nmv, P_f' = P_f + (N+1)mv$$
$$\Rightarrow \Delta P_f' \equiv P_f' - P_0' = \Delta P_f + mv = \hbar k + mv$$

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

So:

$$BdG \Rightarrow \Delta P'_f = \hbar k + (|u_k|^2 - |v_k|^2)mv$$
$$GI \rightarrow \Delta P'_f = \hbar k + mv$$

Galilean invarance

What has gone wrong?
Solution: Conserve particle no.!

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

$$\gamma_i^\dagger = u_k a_{k\uparrow}^\dagger + v_{-k\downarrow} a \hat{C}_{(0)}^\dagger$$

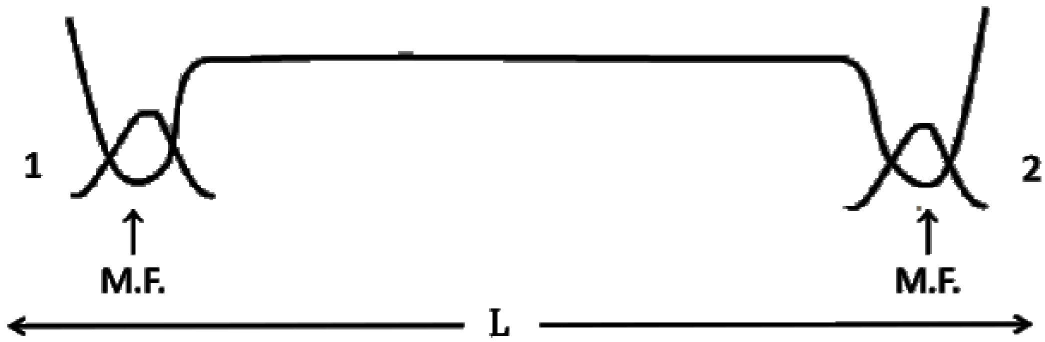
←creates extra Cooper pair (with COM velocity 0)

Because condensate at rest has no spin/momentum/spin current …, the addition of $\hat{C}_{(0)}^\dagger$ has no effect. However: when condensate is moving

$$\gamma_f^\dagger = u_k a_{k+mv/\hbar,\uparrow}^\dagger + v_k a_{-k\downarrow+mv/\hbar} \hat{C}_{(v)}^\dagger$$
$$\Delta P'_f = |u_k|^2(\hbar k + mv) - |v_k|^2(-\hbar k + mv) + |v_k|^2 2mv$$
$$= (|u_k|^2 + |v_k|^2)(\hbar k + mv) = \hbar k + mv$$

in accordance with GI argument

(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 Majoranas is correctly described, not as usually assumed by

$$\gamma_M^\dagger = \int \{u(r)\widehat{\psi}^\dagger(r) + u^*\hat{\psi}(r)\}dr\,(\equiv \gamma_M)$$

by rather by

$$\gamma_M^\dagger = \int \left\{u(r)\widehat{\psi}^\dagger(r) + u^*\hat{\psi}(r)\hat{C}^\dagger\right\} dr$$

But it is impossible to apply the "global" operator $\hat{C}^\dagger$ instantane-ously! 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 where c is the C. pair propagation velocity (usually ~v_f)

Further consequences of taking particle number conservation seriously:

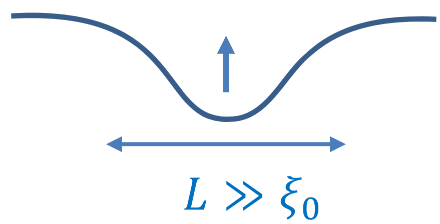
(1) Braiding of Majoranas: see poster (YRL & AJL)

(2) A possible extra effect:

is the added Cooper pair "the same" as the original N ones?

e.g. back to "toy" (Zeeman-trap) problem:

In 2N-particle GS.



$$\Psi_{2N} = \left(\hat{\Omega}_0^\dagger\right)^N |\text{vac}\rangle \qquad (*)$$

$$\hat{\Omega}_0^\dagger = \sum_k c_k a_{k\uparrow}^+ a_{-k\downarrow}^+$$

$$\Psi_{2N+1} = \int dz \left\{ u(z)\hat{\psi}^\dagger(z) + v(z)\hat{\psi}(z)\hat{C}^\dagger \right\} \Psi_{2N}\rangle$$

where

$$\hat{C}^\dagger \equiv \sum_q \lambda_q \Omega_q^\dagger \ , \qquad \Omega_q^\dagger \equiv \sum_k c_k a_{k+q/2\uparrow}^+ a_{-k+q/2\downarrow}^+$$

Crucial question: are the λ_q such as to localize all/part of the extra C. pair in trap? To determine this, need to ascertain energies gained or lost by doing so.

↑: However, at this point we notice an apparently not well-known fact about the 2N-particle BCS GS (*): For a neutral Fermi superfluid with finite compressibility, it violates the sum rules! (and the need to fix this turns out to be essential in the calculations).

Digression: Sum rules and the BCS groundstate.

If we evaluate the pair correlation function $S(q) \equiv \langle \rho_q \rho_{-q} \rangle$ for the BCS groundstate, the pairing contribution is

$$\sum_k \Delta^*_{k+q/2} \Delta_{k-q/2} / (4E_{k+q/2} E_{k-q/2}).$$

(and this is not cancelled by the Fock term). Hence for a neutral Fermi superfluid in this approximation

$S_{BCS}(q \to 0) \sim \sum_k |\Delta_k|^2 / |E_k^2 \nrightarrow 0$ as $q \to 0$. (Already observed by Anderson in 1958).

However, in terms of the density-density response function $\chi(q\omega)$ we have (up to factors of π, etc.)

$$S(q) = \int_0^\infty Im\chi\,(q\omega) d\omega$$

but also

$$\int_0^\infty \frac{Im\chi(q\omega) d\omega}{\omega} = \chi_0$$ ⟵ static compressibility

$$\int_0^\infty \omega Im\chi(q\omega) d\omega = nq^2/m \qquad (\hbar = 1)$$

and hence by CS inequality

↑ Cauchy-Schwarz

particle density

$$S(q) \leq \left(\frac{nq^2\chi_0}{m}\right)^{1/2}$$

or since $\chi_0 = n/mc^2$ ← speed of sound

$$= \frac{1}{\sqrt{3}} V_F$$

$$S(q) \leq nq/mc$$

Thus since $S_{BCS}(q) \sim n\,\Delta/\epsilon_F \sim n/mc\xi$, for $q\xi \lesssim 1$ BCS groundstate violates sum rules.

What has gone wrong? Need to build into GSWF zero-point fluctuations of long-wavelength AB modes:

↑ Anderson-Bogoliubov

$$\Psi_{2N} \sim (\exp - \sum_q \Lambda_q\, \hat{\rho}_q \hat{\rho}_{-q})|\Psi_{BCS}\rangle$$

(long-distance part of Jastrow function).

Actually, inclusion of ZP AB fluctuations in some ways makes life simpler. Example: Calculation of the (total) energy associated with the finite-q pair creation operator acting on Ψ_{2N}.

$$\Omega_q^+ \equiv \sum_k c_k a^+_{k+q/2\uparrow} a^+_{k-q2\downarrow}$$

For $q\xi \ll 1$ we have approximately

$$\Omega_q^+ = (\text{const.})[\rho_q, \Omega_0^\dagger]$$

i.e. intuitively, Ω_q^+ adds an "ordinary" C. pair, then creates a density fluctuation on top of it. With the fluctuations included in the GS (but only then!) we find that $\Omega_q^+|2N\rangle$ is an energy eigenstate of the $2N+2$- particle system with energy $\hbar\omega(q)$.

$$\left(\omega_q = cq = \sqrt{\frac{1}{3}v_F} \cdot q\right)$$

The difficult part is the calculation of $\langle V \rangle$, the extra energy associated with (partial or total) localization of the extra Cooper pair in the presence of a BQP. ← Bogoliubov quasiparticle

However, we note that in the 1D case, independently of the details, if $\langle V \rangle$ is negative definite and independent of the total system size, it will always be energetically advantageous to (completely) localize the extra CP (though possibly only over an exponentially large distance). Thus, for our "toy" problem, can conclude

extra particle no. associated with trap = 1

A naive estimate of $\langle V \rangle$: original gap Δ_0 came from interaction with n particles per unit volume. Extra CP is distributed over volume of $V = L^d$, so equivalent to extra density L^{-d}. Hence, extra contribution to gap is

$$\delta\Delta(r) \sim \Delta_0 \left(L^{-d}/n\right) \sim \Delta_0 N^{-1}$$

← total no. of particles in trap region.

Is this right? If so, can exclude complete localization in $d \geq 2$. However, what about partial localization? (impossible in Schrödinger problem, but...)

work in progress!