Is superconductivity a quantum or a classical phenomenon?

Emil Yuzbashyan



124th Statistical Mechanics Conference Rutgers University, Department of Mathematics May 7 – 9, 2023 Textbooks: Superconductivity is a macroscopic quantum phenomenon

But... the theory of superconductivity is a mean-field theory

Mean-field approximation + Ehrenferst theorem imply the theory is classical (will show this explicitly for superconductivity)

Superconductivity is a purely classical phenomenon in contradiction to textbooks!

BCS theory of superconductivity



BCS mean-field approximation

Heisenberg equations of motion for the BCS Hamiltonian:

Heisenberg equations of motion
For the BCS Hamiltonian:
$$\frac{d\hat{s}_j}{dt} = i[\hat{H}, \hat{s}_j] = 2(\varepsilon_j z - g\hat{\ell}_{\perp}) \times \hat{s}_j$$
$$\hat{\ell}_{\perp} = \hat{\ell}_x \hat{x} + \hat{\ell}_y \hat{y}, \quad \hat{\ell} = \sum_{j=1}^N \hat{s}_j$$

k=1

j,k

BCS Hamiltonian in terms of Anderson's pseudospins: $\hat{H} = \sum 2\varepsilon_k \hat{s}_k^z - g \sum \hat{s}_j^+ \hat{s}_k^-$

j=1

BCS mean-field approximation

Heisenberg equations of motion for the BCS Hamiltonian:

Teisenberg equations of motion
for the BCS Hamiltonian:
$$\frac{d\hat{s}_j}{dt} = i[\hat{H}, \hat{s}_j] = 2(\varepsilon_j z - g\hat{\ell}_{\perp}) \times \hat{s}_j$$
$$\hat{\ell}_{\perp} = \hat{\ell}_x \hat{x} + \hat{\ell}_y \hat{y}, \quad \hat{\ell} = \sum_{j=1}^N \hat{s}_j$$

BCS mean-field approximation: $\hat{\ell} \rightarrow \langle \hat{\ell} \rangle \equiv L \implies \frac{d\hat{s}_j}{dt} = 2(\varepsilon_j z - L_\perp) \times \hat{s}_j$

j=1

Spins decouple. Each spin- $\frac{1}{2}$ moves in its own "magnetic field" field \Rightarrow the system wavefunction is a product state $\Psi_{\rm mf}(t) = \prod (u_k |\downarrow\rangle + v_k |\uparrow\rangle)$

BCS mean-field approximation

Heisenberg equations of motion for the BCS Hamiltonian:

Teisenberg equations of motion
for the BCS Hamiltonian:
$$\frac{d\hat{s}_j}{dt} = i[\hat{H}, \hat{s}_j] = 2(\varepsilon_j z - g\hat{\ell}_{\perp}) \times \hat{s}_j$$
$$\hat{\ell}_{\perp} = \hat{\ell}_x \hat{x} + \hat{\ell}_y \hat{y}, \quad \hat{\ell} = \sum_{j=1}^N \hat{s}_j$$

BCS mean-field approximation: $\hat{\ell} \rightarrow \langle \hat{\ell} \rangle \equiv L \implies \frac{d\hat{s}_j}{dt} = 2(\varepsilon_j z - L_\perp) \times \hat{s}_j$

j=1

Take the quantum mechanical average with respect to system wavefunction

$$\frac{d\langle \hat{\boldsymbol{s}}_j \rangle}{dt} = 2(\varepsilon_j \boldsymbol{z} - \boldsymbol{L}_\perp) \times \langle \hat{\boldsymbol{s}}_j \rangle$$

These are Hamilton's equations for a classical angular momentum Hamiltonian

$$H = \sum_{k} 2\varepsilon_k S_k^z - g \sum_{k,j} S_k^+ S_j^-$$
 where $S_j = \langle \hat{s}_j \rangle$ $L = \sum_j S_j$

Status of the BCS mean-field in equilibrium

BCS mean field is exact for the ground state and low lying excited states in the thermodynamic limit $N\to\infty$

□ Physical argument: Mean field is exact for models with infinite-range interactions. Specifically, since $\hat{\ell}$ is a sum of N spin $-\frac{1}{2}$, its quantum fluctuations are negligible as long as $\langle \hat{\ell} \rangle$ is macroscopically large. For the low-energy states $\langle \hat{\ell} \rangle \sim N$, but for highly excited states (macroscopic # of excitations) $\langle \hat{\ell} \rangle \sim 1$ and mean field breaks down.

□ Rigorous proof: Richardson proved that mean field is exact for low-energy states starting from Bethe's Ansatz solution of the BCS model [Richardson, J. Math. Phys. (1977)].

All observable equilibrium properties of superconductors (excitation spectrum, Josephson effect, topological properties etc.) are low energy and can be obtained from this classical spin Hamiltonian.

We conclude that equilibrium superconductivity is a purely classical phenomenon!

In the past 15 years, <u>far from equilibrium</u> superconductivity has been observed in cold Fermi gases, cavity QED, and THz pumped superconducting films triggering a flood of theory papers (about a paper a week nowadays)

All these papers do mean-field. But <u>far from equilibrium</u> highly excited states contribute to the dynamics for which mean field is invalid. **Does mean field break down <u>far from</u>** <u>equilibrium</u> or is it still valid?

We're interested in unitary evolution with the BCS Hamiltonian. A natural way to initiate such an evolution, e.g., in ultracold atomic fermions, is to drive the system by making the superconducting coupling vary in time: g = g(t)

Then, we need to solve for the dynamics of a time-dependent BCS Hamiltonian:

$$\hat{H}(t) = \sum_{k} 2\varepsilon_k \hat{s}_k^z - g(t) \sum_{j,k} \hat{s}_j^+ \hat{s}_k^-$$

What do we need to do to determine if mean field is exact?

1) Solve the non-stationary Schrödinger equation for the quantum time-dependent BCS Hamiltonian in the thermodynamic limit $N \to \infty$ exactly

$$\frac{\partial \Psi(t)}{\partial t} = \hat{H} \Psi(t)$$

- 2) Solve Hamilton's equations for the classical version of the BCS Hamiltonian in $N \to \infty$ limit exactly and obtain $\Psi_{\rm mf}(t) = \prod_k (u_k |\downarrow\rangle + v_k |\uparrow\rangle)$ using $S_k = \langle \hat{s}_k \rangle$ $\frac{dS_k}{dt} = \{H, S_k\}$
- 3) Compare exact quantum $\Psi(t)$ and exact mean-field $\Psi_{mf}(t)$ wavefunctions

Unfortunately, solving for the time evolution of a macroscopically large number of interacting quantum particles or spins with a time-dependent Hamiltonian is essentially impossible both numerically and analytically even for an integrable model 😒 😒

But...the BCS Hamiltonian turns out to be special! Its integrals of motion are the Gaudin magnets:

$$\hat{H}_k = 2B\hat{s}_k^z - \sum_{j \neq k} \frac{\hat{s}_k \cdot \hat{s}_j}{\varepsilon_k - \varepsilon_j}$$

$$2B = \frac{1}{g} \Rightarrow \quad \hat{H} = \sum_{k} 2\varepsilon_k \hat{s}_k^z - \frac{1}{2B} \sum_{j,k} \hat{s}_j^+ \hat{s}_k^- \qquad [\hat{H}_k, \hat{H}_j] = [\hat{H}_k, \hat{H}] = 0$$

Gaudin magnets describe *N*-point correlation function $\Psi(\varepsilon_1, \ldots, \varepsilon_N, B)$ in SU(2) Wess-Zumino-Witten CFT through *N* compatible equations of evolution type

Knizhnik-Zamolodchikov equations:
$$i \nu \frac{\partial \Psi}{\partial \varepsilon_k} = \hat{H}_k \Psi$$

Knizhnik & Zamolodchikov, Nucl. Phys. B (1984)

Moreover, it turns out that the evolution of the correlation function with respect to *B* is governed by the BCS Hamiltonian $\bigcirc \bigcirc \bigcirc \bigcirc$ [Yuzbashyan, Ann. Phys. (2018)]

$$i\nu\frac{\partial\Psi}{\partial B} = \hat{H}\Psi$$

(1)
$$i\nu \frac{\partial \Psi}{\partial B} = \hat{H}\Psi, \qquad \hat{H} = \sum_{k} 2\varepsilon_k \hat{s}_k^z - \frac{1}{2B} \sum_{j,k} \hat{s}_j^+ \hat{s}_k^-$$

Let $B = \nu t$. Eq. (1) becomes the non-stationary Schrödinger equation for the BCS Hamiltonian with superconducting interaction strength inversely proportional to time

$$g(t) = \frac{1}{2\nu t}$$

This is the time dependence that is native to ultracold atomic Fermi gases. BCS interaction strength is inversely proportional to the detuning from the Feshbach resonance (deviation of the external magnetic field from the resonance)

$$g(\mathsf{B}_{\mathrm{ext}}) \propto rac{1}{\mathsf{B}_{\mathrm{ext}}-\mathsf{B}_{0}}$$

(1)
$$i\nu \frac{\partial \Psi}{\partial B} = \hat{H}\Psi, \qquad \hat{H} = \sum_{k} 2\varepsilon_k \hat{s}_k^z - \frac{1}{2B} \sum_{j,k} \hat{s}_j^+ \hat{s}_k^-$$

Let $B = \nu t$. Eq. (1) becomes the non-stationary Schrödinger equation for the BCS Hamiltonian with superconducting interaction strength inversely proportional to time

$$g(t) = \frac{1}{2\nu t}$$

A natural problem is to start in the ground state at $t = 0^+$ (infinite interaction strength),

$$\Psi(t=0^+) = \left| S_{\text{tot}} = \frac{N}{2}, S_{\text{tot}}^z \right\rangle,$$

Evolve to $t = +\infty$ and determine the asymptotic wavefunction $\Psi(t \to +\infty) = ???$

We will use this many-body Landau-Zener-type problem to test the accuracy of the meanfield approximation far from equilibrium

Exact quantum and exact classical solutions

General formal solution of Knizhnik-Zamolodchikov equations in terms of an *M*-fold contour integral over off-shell BA states weighted by exponentiated Yang-Yang action [Babujian, J. Phys. A (1993); Babujian & Kitaev, J. Math. Phys. (1998); Fioretto, Caux & Gritsev, New J. Phys. (2014)]

Solution of the non-stationary Schrödinger equation for the BCS Hamiltonian with $g(t) \propto \frac{1}{t}$ Yuzbashyan, Ann. Phys. (2018)

At $t \to +\infty$ the integral localizes to the stationary points of the Yang-Yang action (Bethe roots). Sum over stationary points and take the thermodynamic limit $N \to \infty$. Do this for spins of magnitude $s = \frac{1}{2}$ (quantum solution) and for $s \to \infty$ (classical solution) and compare [Zabalo, Wu, Pixley & Yuzbashyan, Phys. Rev. B (2022)].

1) Exact quantum solution:

$$\Psi(t \to +\infty) = C \sum_{\{\alpha\}} e^{i\Lambda_{\{\alpha\}}} \prod_{\alpha} \left[e^{-2it\varepsilon_{\alpha}} e^{-\frac{\pi\alpha}{\nu}} e^{-i\theta_{\alpha}} \right] |\{\alpha\}\rangle \equiv |M\rangle_{\infty}$$

 $|\{\alpha\}\rangle$ – the state where energy levels $\{\alpha\} = \{\alpha_1, \alpha_2, \dots, \alpha_M\}$ are doubly occupied and the remaining levels are empty, M – number of Cooper pairs

$$\theta_{\alpha} = \frac{1}{\nu} \sum_{j \neq \alpha} \ln |\varepsilon_j - \varepsilon_{\alpha}|, \quad \Lambda_{\{\alpha\}} = \frac{1}{\nu} \sum_{\beta \neq \alpha} \ln |\varepsilon_{\beta} - \varepsilon_{\alpha}|$$

This is the exact answer for any N single-particle levels $\varepsilon_1, \ldots, \varepsilon_N$ and arbitrary number M of fermion pairs

2) Exact classical (mean-field) solution:

$$\Psi_{\rm mf}(t \to +\infty) = \prod_{k=1}^{N} \left(u_k + v_k \hat{c}_{k\uparrow}^{\dagger} \hat{c}_{k\downarrow}^{\dagger} \right) |0\rangle$$

$$u_{k} = \frac{e^{\frac{\zeta_{k} - i\varphi_{k}}{2}}}{\sqrt{2\cosh\zeta_{k}}}, \quad v_{k} = \frac{e^{-2i\varepsilon_{k}t}e^{\frac{-\zeta_{k} + i\varphi_{k}}{2}}}{\sqrt{2\cosh\zeta_{k}}}, \quad \varphi_{k} = -\frac{1}{\nu}\sum_{j\neq k}\tanh\zeta_{j}\ln|\varepsilon_{j} - \varepsilon_{k}|, \quad \zeta_{k} = \frac{\pi(k-\mu)}{\nu}$$
$$\mu = \frac{N+1}{2} + \frac{N}{2\pi\eta}\ln\left\{\frac{\sinh\left[\frac{\pi\eta M}{N}\right]}{\sinh\left[\pi\eta - \frac{\pi\eta M}{N}\right]}\right\} \qquad \eta = \frac{N}{\nu}$$

Similar probabilities, but the total particle # is not fixed and phases are different

$$\hat{H}(t \to +\infty) = \sum_{k=1}^{N} \varepsilon_k \hat{n}_k \qquad \qquad \Psi(t \to +\infty) = \sum_{\{n_k\}} C_{\{n_k\}} e^{-iE(\{n_k\})t} |\{n_k\}\rangle$$

$$P_{0 \to \{n_k\}} = |C_{\{n_k\}}|^2$$
 - LZ transition probabilities

In our case, for both quantum & classical solutions: $P_{0 \to \{n_k\}} = \mathcal{N}e^{-\frac{\pi}{\nu}(k-\mu)n_k}$

Independence of LZ transition probabilities of the parameters of the model (ε_k) is a characteristic feature of time-dependent integrability

The asymptotic state is nonthermal but conforms to emergent Generalized Gibbs Ensemble

$$\hat{
ho}_{\rm GGE} = e^{-\sum_k \beta_k \hat{n}_k}$$
 with $\beta_k = \frac{\pi}{\nu} (k - \mu)$ (Only N parameters vs. 2^N)

3) Mean field is <u>exact</u> for local observables in the thermodynamic limit!

Consider the most general product of n operators with nonzero expectation value:

$$\hat{O} = \hat{o}_{k_1} \dots \hat{o}_{k_n}$$
 $k_1, \dots, k_n - n$ distinct energy levels

 \hat{O}_k is pair creation $\hat{s}_k^+ = \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\downarrow}^\dagger$ or annihilation $\hat{s}_k^- = \hat{c}_{k\downarrow} \hat{c}_{k\uparrow}$ or level occupancy \hat{n}_k operator We say that \hat{O} is local if and only if $\frac{n}{N} \to 0$ when $N \to \infty$

Averages of local operators in the exact asymptotic state coincide with their expectation values in the mean-field wavefunction in the thermodynamic limit:

$$\langle M+l|\hat{O}|M\rangle_{\infty} = \langle \hat{O}\rangle_{\mathrm{mf}} = \langle \hat{o}_{k_1}\rangle_{\mathrm{mf}} \dots \langle \hat{o}_{k_n}\rangle_{\mathrm{mf}}$$

Corrections to mean field are of order $\frac{n}{N}$

Moreover, we know all local asymptotic averages explicitly $\langle \hat{c}_{k\uparrow}^{\dagger} \hat{c}_{k\downarrow}^{\dagger} \rangle_{mf} = u_k v_k^*,$ $\langle \hat{c}_{k\downarrow} \hat{c}_{k\uparrow} \rangle_{mf} = u_k^* v_k,$ $\langle \hat{n}_k \rangle_{mf} = 2|v_k|^2.$

Classical description (mean field) <u>breaks down</u> for global measures both <u>in</u> and out of equilibrium

Example #1: Entanglement. The mean-field wavefunction is unentangled (a product state), while the exact ground state and asymptotic wavefunctions are entangled

$$\Psi_{\rm mf} = \prod \left(u_k + v_k \hat{c}_{k\uparrow}^{\dagger} \hat{c}_{k\downarrow}^{\dagger} \right) |0\rangle \implies \text{Entanglement entropy } \mathbf{S}_{\rm ent} = 0$$



In contrast, in exact quantum dynamics starting from the unentangled mean-field ground state, the entropy monotonically grows as

$$S_{ent} = \sqrt{1 + \frac{\tau^2}{4}} \operatorname{coth}^{-1} \left[\sqrt{1 + \frac{\tau^2}{4}} \right] + \ln \frac{\tau}{4}, \quad \tau = \eta \ln \frac{t}{t_0}$$

and saturates at $\tau \sim \sqrt{N}$ at ${\rm S}_{\rm ent} \sim \ln N$

In exact ground state $S_{\rm ent} \sim \ln N$

Classical description (mean field) <u>breaks down</u> for global measures both <u>in</u> and out of equilibrium

Example #2: Loschmidt echo (return amplitude): $\mathcal{Z}(t) = \langle \Psi_i | e^{-i\hat{H}t} | \Psi_i \rangle$

Classical (mean-field) analysis: Numerous singularities (DQPTs) in $\mathcal{Z}(t)$ for quench dynamics of s-wave BCS superconductors and none for p-wave. Rylands, Yuzbashyan, Gurarie, Zabalo, Galitski, Ann. Phys. (2021).

Quantum analysis: no singularities for s-wave and periodic singularities for the topological p-wave superconductor, for the evolution starting from a quantum critical point separating the topological and non-topological phases. Gaur, Gurarie, Yuzbashyan, <u>arXiv:2207.08131</u>

Reason: mean field fails because it determines the bulk of the time-dependent system wavefunction, while the Loschmidt is determined by the exponentially small tails of the wavefunction

- Conclusion (beyond superconductivity): Mean-field theories are able to capture the order parameter and other local observables, but the entanglement and many-particle structure of the quantum state are out of reach both in and out of equilibrium.
- The success of mean-field theories to date thus secretly relied on the order parameter being a "classical" object (local operator in our case).



Aidan Zabalo



Angkun Wu



Jed Pixley

Zabalo, Wu, Pixley & Yuzbashyan, Phys. Rev. B 106, 104513 (2022).