Microscopic Derivation of Ginzburg–Landau Theory and the BCS Critical Temperature Shift in a Weak Homogeneous Magnetic Field

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PDE and Mathematical Physics Seminar @ University of Zurich November 04, 2021

Joint work with Christian Hainzl and Marcel Schaub

Funding from the European Union's Horizon 2020 research and innovation programme (Marie Sklodowska-Curie fellowship) and from the SNSF (Ambizione grant) is gratefully acknowledged.

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Superfluidity

Vortex lattice of Fermi gas across the **BEC** - **BCS** crossover.



M. W. Zwierlein, J. R. Abo-Shaeer, A. Schirotzek, C. H. Schunck, W. Ketterle, *Vortices* and superfluidity in a strongly interacting Fermi gas, Nature **435**, 1047–1051 (2005)

Setup: Particles in a constant magnetic field



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Setup: Particles in a constant magnetic field



We consider **attractively** interacting fermionic particles in a weak external magnetic field $|\mathbf{B}| \ll 1$.

Fermionic quasi-free states

- States on the fermionic Fock space obeying the Wick theorem are called quasi-free.
- Such states are uniquely determined by their generalized one-particle density matrix Γ ∈ L (L²(ℝ³) ⊕ L²(ℝ³)), 0 ≤ Γ ≤ 1, which is of the form

$$\mathsf{\Gamma} = egin{pmatrix} \gamma & lpha \ \overline{lpha} & 1 - \overline{\gamma} \end{pmatrix} .$$

This, in particular, implies $0 \le \gamma \le 1$ and $\alpha \alpha^* \le \gamma(1 - \gamma)$. We assume that $\alpha(x, y) = \alpha(y, x) \Rightarrow$ s-wave Cooper pairs (spin-singulett).

• Our states are gauge-periodic w.r.t. $\Lambda_B = \sqrt{2\pi B^{-1}}\mathbb{Z}^3$, that is, for $\lambda \in \Lambda_B$ we have

$$\gamma(x + \lambda, y + \lambda) = e^{-i\frac{\mathbf{B}}{2} \cdot (\lambda \wedge (x - y))} \gamma(x, y),$$

$$\alpha(x + \lambda, y + \lambda) = e^{-i\frac{\mathbf{B}}{2} \cdot (\lambda \wedge (x + y))} \alpha(x, y).$$

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The BCS free energy functional

For gauge-periodic BCS states we define the BCS free energy functional by

$$\mathcal{F}_{\mathbf{B},\mathcal{T}}^{\mathrm{BCS}}(\Gamma) = \mathrm{Tr}\big[\big((-\mathrm{i}\nabla + \mathbf{A})^2 - \mu\big)\gamma\big] - \mathcal{TS}(\Gamma) - \frac{1}{|Q_B|} \int_{Q_B \times \mathbb{R}^3} V(r) |\alpha(X,r)|^2 \mathrm{d}(X,r),$$

where

• $\operatorname{Tr}[A] = \frac{1}{|Q_B|} \operatorname{Tr}_{L^2(Q_B)}[\mathbb{1}(x \in Q_B)A\mathbb{1}(x \in Q_B)]$, that is, we consider energy per unit volume, $(Q_B$ is the unit cell of the lattice Λ_B)

•
$$\mathbf{A}(x) = \frac{1}{2}\mathbf{B} \wedge x$$
 (Vector potential),

- $\mu \in \mathbb{R}, T \ge 0$ (chemical potential, temperature),
- $S(\Gamma) = -\text{Tr}[\Gamma \ln(\Gamma)]$ (Von Neumann entropy),
- r = x y, $X = \frac{x+y}{2}$, and $\alpha(X, r) \equiv \alpha(x, y)$, that is, we express α in relative- and center-of-mass coordinates.

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Normal state, free energy and superconductivity

• The unique minimizer for V = 0 is called **normal state** and reads

$$\Gamma_0 = \begin{pmatrix} \gamma_0 & 0 \\ 0 & 1 - \overline{\gamma}_0 \end{pmatrix} \quad \text{with} \quad \gamma_0 = \frac{1}{e^{((-i\nabla + \mathbf{A}(x))^2 - \mu)/T} + 1}.$$

• The BCS free energy is defined by

$$F^{\mathrm{BCS}}(B,T) = \inf_{\Gamma} \{ \mathcal{F}^{\mathrm{BCS}}_{B,T}(\Gamma) - \mathcal{F}^{\mathrm{BCS}}_{B,T}(\Gamma_0) \}.$$

• The system is said to be superconducting at temperature ${\cal T}$ and magnetic field ${\bf B}$ if

$$F^{\mathrm{BCS}}(B,T) < 0.$$

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Effective models I: Translation-invariant BCS functional

If $\mathbf{B} = 0$ we describe the system by translation-invariant states, that is,

$$\gamma(x,y) = \gamma(x-y)$$
 and $\alpha(x,y) = \alpha(x-y)$.

In this case it has been shown that there exists a **critical temperature** T_c such that the system is superconducting if $T < T_c$ and in its normal state if $T \ge T_c$.

Moreover, T_c can be defined as the **unique value of** T such that the operator

$$K_T - V(x) = rac{-\Delta - \mu}{ anh\left(rac{-\Delta - \mu}{2T}
ight)} - V(x)$$

has 0 as its lowest eigenvalue. The corresponding eigenfunction will be denoted by α_* .

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Critical temperature in translation-invariant case

- **B** = 0,
- Second variation of BCS functional equals K_T - V(x).





Effective models II: The Ginzburg-Landau functional

We call a function $\Psi : \mathbb{R}^3 \to \mathbb{C}$ gauge-periodic if for all $\lambda \in \Lambda_B$ we have

$$\Psi(X + \lambda) = e^{-i\mathbf{B}\cdot(\lambda \wedge X)}\Psi(X).$$

For such functions and parameters $\Lambda_1, \Lambda_2, \Lambda_3 > 0$, $D \in \mathbb{R}$ the **Ginzburg–Landau** functional is defined by

$$\mathcal{E}_{\mathbf{B},D}^{\mathrm{GL}}(\Psi) = \frac{1}{B^2 |Q_B|} \int_{Q_B} \left(\Lambda_1 |(-\mathrm{i} \nabla + 2\mathbf{A}) \Psi(X)|^2 - DB \Lambda_2 |\Psi(X)|^2 + \Lambda_3 |\Psi(X)|^4 \right) \mathrm{d} X.$$

Its minimal value is the Ginzburg-Landau energy

$$E^{\mathrm{GL}}(D) = \inf_{\Psi} \mathcal{E}^{\mathrm{GL}}_{\mathbf{B},D}(\Psi),$$

which, by scaling, does not depend on B.

Selected literature

Translation-invariant BCS functional

- Hainzl, Hamza, Seiringer, Solovej, The BCS functional for general pair interactions, CMP 281, 349 (2008)
- Hainzl, Seiringer, *The Bardeen–Cooper–Schrieffer functional of superconductivity* and its mathematical properties, J. Math. Phys. **57**, 021101 (2016) (review)

BCS functional with external fields, zero magnetic flux through unit cell

- Frank, Hainzl, Seiringer, Solovej, Microscopic derivation of Ginzburg–Landau theory, J. Amer. Math. Soc. 25, 667 (2012)
- Frank, Hainzl, Seiringer, Solovej, *The external field dependence of the BCS critical temperature*, CMP **342**, 189 (2016)

Linearized BCS theory, constant magnetic field

• Frank, Hainzl, Langmann, *The BCS critical temperature in a weak homogeneous magnetic field*, J. Spectr. Theory **9**, 1005 (2019)

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Main result part I: Free energy asymptotics

Assumptions:

- V radial function with $(1+|\cdot|^2)V\in L^\infty(\mathbb{R}^3)$,
- V such that $T_{\rm c} > 0$ in translation-invariant case,
- Zero eigenvalue of $K_{T_c} V(x)$ is simple.

Theorem (D., Hainzl, Schaub)

There are constants C > 0 and $B_0 > 0$ such that for all $0 < B \le B_0$, we have

$$\mathcal{F}^{\mathrm{BCS}}_{\mathbf{B},T_{\mathrm{c}}(1-DB)}=B^{2}\left(E^{\mathrm{GL}}(D)+\mathcal{R}
ight)$$

with

$$-CB^{\frac{1}{12}} \leq \mathcal{R} \leq CB.$$

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Main result part II: Approximate minimizers

Theorem (continued)

For any approximate minimizer Γ of $\mathcal{F}_{B,T}^{\rm BCS}$ at $T=T_{\rm c}(1-DB)$ in the sense that

$$\mathcal{F}^{\mathrm{BCS}}_{\mathbf{B},\mathcal{T}}(\Gamma) - \mathcal{F}^{\mathrm{BCS}}_{\mathbf{B},\mathcal{T}}(\Gamma_0) \leq B^2 \left(E^{\mathrm{GL}}(D) + \rho
ight)$$

holds for some $\rho \geq 0$, we have the decomposition

$$\alpha(X,r) = \alpha_*(r)\Psi(X) + \sigma(X,r)$$

for the **Cooper pair wave function** $\alpha = \Gamma_{12}$. Here, σ satisfies

$$\frac{1}{|Q_B|}\int_{Q_B\times\mathbb{R}^3}|\sigma(X,r)|^2\mathrm{d}(X,r)\leq CB^{11/6},$$

 α_* is the zero energy eigenfunction of $K_{T_c} - V(x)$, and Ψ obeys

$$\mathcal{E}_{\mathbf{B},D}^{\mathrm{GL}}(\Psi) \leq E^{\mathrm{GL}}(D) + \rho + CB^{1/12}.$$

Separation of scales



- Ψ approximate minimizer of $\mathcal{E}_{\mathbf{B},D}^{\mathrm{GL}}$
- $(K_{T_c} V(x)) \alpha_* = 0$

Main result part III: Critical temperature shift

Assumptions: Same as for previous theorem.

Definition: $D_{\rm c} = \Lambda_1 \inf \sigma_{L^2_{\rm mag}(Q_1)} ((-i\nabla + e_3 \wedge X)^2).$

Theorem (D., Hainzl, Schaub)

There are constants C > 0 and $B_0 > 0$ such that for all $0 < B \le B_0$ the following holds:

• Let $0 < T_0 < T_{\rm c}.$ If the temperature satisfies

$$T_0 \leq T \leq T_c (1 - B(D_c + CB^{1/2})),$$

then we have $F^{BCS}(B, T) < 0$.

• If the temperature satisfies

$$T \geq T_{\rm c}(1 - B(D_{
m c} - CB^{1/12})),$$

then we have $\mathcal{F}_{\textbf{B},\mathcal{T}}^{\rm BCS}(\Gamma)-\mathcal{F}_{\textbf{B},\mathcal{T}}^{\rm BCS}(\Gamma_0)>0$ unless $\Gamma=\Gamma_0.$

Phase Diagram



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Phase Diagram



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Proof strategy in a nutshell

• Step 1) Learn to carry out very accurate computation with **trial states** (Gibbs states) of the form

$$\Gamma_{\Delta} = \frac{1}{1 + e^{H_{\Delta}/T}} \text{ with } H_{\Delta} = \begin{pmatrix} (-i\nabla + \mathbf{A})^2 - \mu & \Delta \\ \overline{\Delta} & -(-i\nabla + \mathbf{A})^2 + \mu \end{pmatrix},$$

and $\Delta(X, r) = 2V(r)\alpha_*(r)\Psi(X)$. \Rightarrow Upper bound for free energy and lower bound for critical temperature.

- Step 2) Proof a-priori bound for low energy states close to $T_{\rm c}$.
- Step 3) For given low energy state Γ , construct Gibbs state Γ_{Δ} , estimate $\mathcal{F}^{\rm BCS}_{{\bf B},T}(\Gamma)$ from below in terms of $\mathcal{F}^{\rm BCS}_{{\bf B},T}(\Gamma_{\Delta})$ (this is a highly non-trivial thing to do), and use step 1 to compute $\mathcal{F}^{\rm BCS}_{{\bf B},T}(\Gamma_{\Delta})$. Attention: Regularity from a-priori bounds not good enough for trial state analysis. Solution: Introduce cut-off to obtain more regularity (at the price of additional remainder terms). \Rightarrow Lower bound for free energy and upper bound for critical temperature.

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Proof techniques I: Upper bound

• Main novelty of our trial state analysis is to write

$$\begin{split} -\operatorname{Tr}_0 \left[\ln \left(1 + e^{-H_{\Delta}/T} \right) - \ln \left(1 + e^{-H_0/T} \right) \right] \\ &= \operatorname{Tr}_0 \left[\ln \left(\cosh \left(\frac{H_{\Delta}}{2T} \right) \right) - \ln \left(\cosh \left(\frac{H_0}{2T} \right) \right) \right], \end{split}$$

where

$$\mathcal{H}_{\Delta} = \begin{pmatrix} (-i\nabla + \mathbf{A})^2 - \mu & \Delta \\ \overline{\Delta} & -(-i\nabla + \mathbf{A})^2 + \mu \end{pmatrix},$$

and use a product expansion of $\cosh(x)$.

• Extension of the **phase approximation method**, which has been pioneered in the framework of linearized BCS theory by Frank, Hainzl and Langmann, to our nonlinear setting. The approach makes use of the formula

$$\frac{1}{z-(-\mathrm{i}\nabla+\mathbf{A})^2}(x,y)=e^{\mathrm{i}\frac{\mathbf{B}}{2}\cdot(x\wedge y)}g_B^z(x-y).$$

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Proof techniques II: Lower bound

The main novelty of our work are the following a-priori bounds for low energy states:

Theorem (Structure of low energy states)

For all $D_0, D_1 \ge 0$, there is a constant $B_0 > 0$ such that for all $0 < B_0 \le B$ we have the following statement: If $T - T_c \ge -D_0B$ and if Γ obeys

$$\mathcal{F}^{\mathrm{BCS}}_{\mathbf{B},T}(\Gamma) - \mathcal{F}^{\mathrm{BCS}}_{\mathbf{B},T}(\Gamma_0) \leq D_1 B^2,$$

then there exist $\Psi \in H^1_{\mathrm{mag}}(\mathcal{Q}_B)$ and $\xi \in H^1_{\mathrm{mag}}(\mathcal{Q}_B imes \mathbb{R}^3)$ such that

$$\alpha(X,r) = \Psi(X)\alpha_*(r) + \xi(X,r),$$

where

$$\sup_{0 < B \le B_0} \|\Psi\|^2_{H^1_{\mathrm{mag}}(Q_B)} \le C \quad \text{ and } \quad \|\xi\|^2_{H^1_{\mathrm{mag}}(Q_B \times \mathbb{R}^3)} \le CB^2 \left(\|\Psi\|^2_{H^1_{\mathrm{mag}}(Q_B)} + D_1 \right).$$

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