EBERHARD KARLS UNIVERSITÄT TÜBINGEN

# Mathematical aspects of the BCS theory of superconductivity

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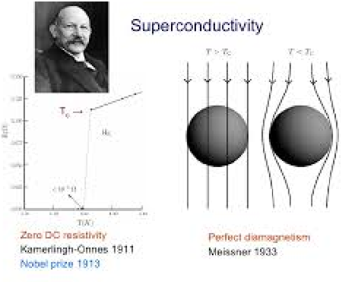
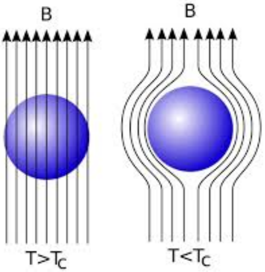
# History

- 1911 Discovery of Superconductivity, by Kammerling Onnes.




- 1933 Meissner-Ochsenfeld-effect

- 1935 London brothers give first phenomenological explanation, $\Delta B = \frac{1}{\lambda} B$.




- 1950 phenomenological theory of Ginzburg-Landau. Schrödinger-type equation

$$(-i\nabla + A)^2\psi(x) - a\psi(x) + b|\psi(x)|^2\psi(x) = 0$$

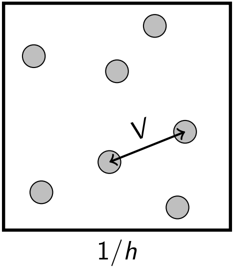
.

- 1957 First microscopic explanation by Bardeen-Cooper-Schrieffer (BCS)

- 1959 Gorkov argued that the Ginzburg-Landau theory can be derives from BCS theory close to the critical temperature. (Mathematical proof by "Frank-H-Seiringer-Solovej").
- Till 1986 there were theories telling that superconductivity is impossible over 30K. Then Bednorz and Müller found material with 35K transition

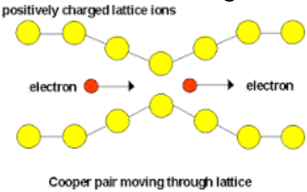
temperature. Later up to 130K

# System




- Gas of neutral spin-$\frac{1}{2}$ particles interacting via a two-body potential $V(x-y)$. $V$ can be tuned in the lab.

- Electrons in a metal interacting via effective rank-1 potential $V(x,y)$ mediated by phonons.



# BCS-Functional

**BCS free energy functional**: Temperature $T \geq 0$

$$\mathcal{F}(\Gamma) = \mathrm{Tr}\,[(\mathfrak{h} - \mu)\gamma] - T\,S(\Gamma) + \int_{\mathbb{R}^3 \times \mathcal{C}} V(x-y)|\alpha(x,y)|^2\,dx\,dy\,.$$

$$\mathfrak{h} = (-i\nabla + h\mathbf{A}(hx))^2 + h^2 W(hx)$$

The BCS-states are $2 \times 2$ matrix-operators

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \overline{\alpha} & 1 - \overline{\gamma} \end{pmatrix}$$

$$0 \leq \Gamma \leq 1.$$

- $\gamma = \gamma(x,y) = \langle a_y^\dagger a_x \rangle$
- $\alpha = \alpha(x,y) = \langle a_y a_x \rangle$
- $\mu$ ist **chemical potential** $\simeq$ density of particles

$$S(\Gamma) = -\mathrm{Tr}\,[\Gamma \ln \Gamma] = -\frac{1}{2}\mathrm{Tr}\,[\Gamma \ln \Gamma + (1-\Gamma)\ln(1-\Gamma)]$$

[BLS] Bach, Lieb & Solovej, *J. Statist. Phys.* **76** (1994), p. 3–89.

# Cooper pairs

System is superconductive, superfluid if $\alpha \neq 0$ in the ground state of $\mathcal{F}$.

$$\boxed{\alpha(x, y)}$$

expectation of Cooper-pairs

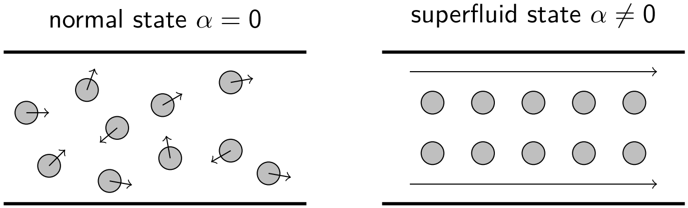
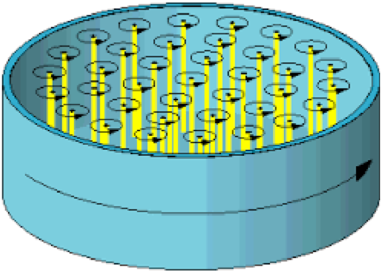
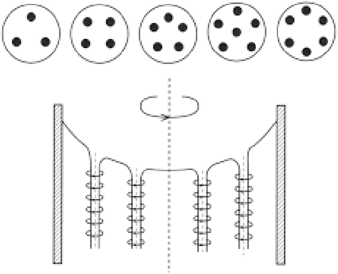



Figure: $\alpha \neq 0$ implies macroscopic coherence of the particles in the system

# Bose-Einstein condensation of pairs

$$\Psi(x_1,...,x_N) \simeq \mathcal{A}(\alpha(x_1,x_2) \wedge \alpha(x_3,x_4) ... \wedge \alpha(x_{N-1},x_N))$$





# The translation invariant case: $A, W = 0$

In the case of

$$\gamma = \gamma(x-y), \qquad \alpha = \alpha(x-y),$$

the BCS-functional reads

$$\mathcal{F}_{\mathrm{BCS}}(\Gamma) = \int (p^2-\mu)\widehat{\gamma}(p)\,dp + \int V(x)|\alpha(x)|^2\,dx \\ - T\int \mathrm{tr}_{\mathbb{C}^2}\widehat{\Gamma}(p)\log\widehat{\Gamma}(p)\,dp$$

times $1/h^3$.

If $V = 0$, minimizer is **normal state**

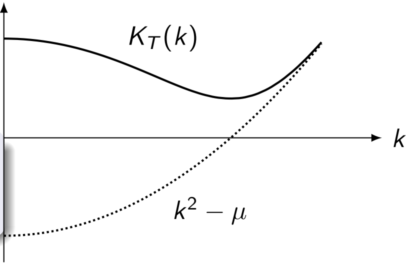
$$\Gamma_n = \begin{pmatrix} \gamma_n & 0 \\ 0 & 1-\overline{\gamma_n} \end{pmatrix}, \quad \gamma_n = \frac{1}{1+e^{(p^2-\mu)/T}}$$

**Key question:** suppose $V \neq 0$. Is $\alpha \neq 0$ for minimizers?

# Linear criterion

**Answer [HHSS]**:

$$K_T = \frac{-\Delta - \mu}{\tanh((-\Delta-\mu)/2T)}$$




Then $\alpha \neq 0$ **if and only if**

$K_T + V$ has a **negative** eigenvalue.

**Critical temperature:** from **monotonicity** in $T$, there exists $0 \leq T_c < \infty$ such that **minimizers** of $\mathcal{F}_{\mathrm{BCS}}$ have

$$\alpha = 0 \quad \text{for all } T \geq T_c$$
$$\alpha \neq 0 \quad \text{for all } T < T_c$$

Note that $T_c > 0$ if the linear operator

$|-\Delta - \mu| + V$ has a **negative** eigenvalue.

[HHSS] C. Hainzl, E. Hamza, R. Seiringer, J.P. Solovej, Commun. Math. Phys. **281**, 349–367 **(2008)**.

# Unique critical temperature

$$T_c: \qquad (K_{T_c} + V)\alpha_* = 0, \quad K_T(p) = \frac{p^2 - \mu}{\tanh \frac{p^2 - \mu}{2T}} \geq 2T$$

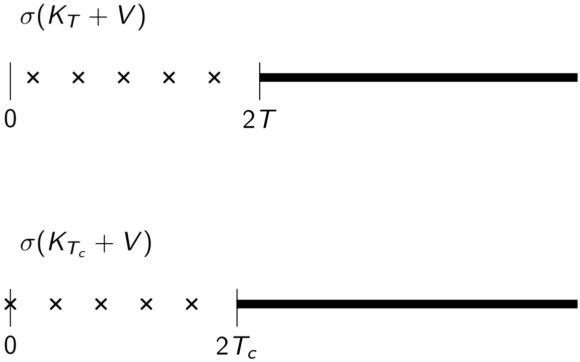



Figure: Spectrum of $K_T + V$

# Eigenvalues

The system is **superconductive/superfluid** for some $T > 0$ iff $|p^2 - \mu| + V$ has a negative eigenvalue.

The fact that the resolvent is not integrable at $p^2 = \mu$ has as a consequence that small negative parts of $V$ can lead to negative bound states.

$$\frac{1}{|p^2 - \mu|} = \frac{1}{||p| - \sqrt{\mu}||\,|p| + \sqrt{\mu}|}.$$

# Spectral theory

## Theorem ([FHNS,HS1])

*Let* $M_{mn} = \langle \varphi_m, \hat{V}\varphi_n \rangle_{p^2=\mu} = \int_{p^2=\mu}\int_{q^2=\mu} \overline{\varphi_m(\sqrt{\mu}p)}\hat{V}(p-q)\varphi_n(\sqrt{\mu}q)dpdq$, $\varphi_m$ *the* **spherical harmonics** *and*

$$e = \inf \operatorname{spec} M_{mn}.$$

*If* $V$ *commutes with angular momentum, e.g.,* $V = V(|x-y|)$, *then*

$$e = \inf_{\ell \in \mathbb{N}} \frac{1}{2\pi^2} \int_{\mathbb{R}^3} V(x) \left| j_\ell(\sqrt{\mu}|x|) \right|^2 dx$$

$j_\ell$ *are the spherical Bessel Functions.*

- *If* $e < 0$, *then* $T_c(V) > 0$, *i.e.* $\inf \operatorname{spec}(K_T^0 + V) < 0$, *for* $T$ *small enough.*
- *In the weak coupling limit,* $\lambda \to 0$, $T_c(\lambda V) \sim e^{\frac{1}{-\lambda|e|}}$. $e \to a$ *for small* $\mu$ *[HS2]*
- *In 2D the Gap-solution has the symmetry of the linear solution,* $\Delta(p) = e^{i\ell\theta}\Delta_\ell(|p|)$. *[DGHL]*

[FHNS] R.L. Frank, C. Hainzl, S. Naboko, R. Seiringer, J. Geom. Anal. **17**, 559–568 (2007).
[HS1] C. Hainzl, R. Seiringer, Phys. Rev. B **77**, 184517-1–10 (2008).
[HS2] C. Hainzl, R. Seiringer, LMP (2008)
[DGHL] A. Deuchert, A. Geisinger, C. Hainzl, M. Loss, Ann. Henri Poincare 19 (2018), no. 5, 1507–1527

# Non translation invariant case

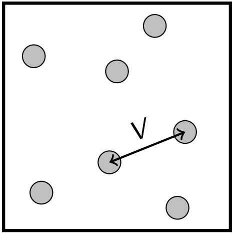



Figure: Add external fields $\mathbf{A}, W$ varying on the size of the box.

The presence of external fields breaks **translation invariance**. In the presence of slowly varying external fields $h\mathbf{A}(hx)$ and $h^2W(hx)$ we proved a famous result of Gorkov [G].

[G] L.P. Gor'kov, Zh. Eksp. Teor. Fiz. **36**, 1918–1923 (1959)

# Non translation invariant case

## Theorem ([FHSS, FHSS2])

*Sei $T = T_c(1 - Dh^2)$. Then in the limit of small $h$ the expectation of Cooper pars in the ground state of the BCS-functional, to leading order, separates into*

$$\boxed{\langle a_y a_x \rangle = \alpha(x,y) = h\psi\left(h\frac{x+y}{2}\right)\alpha_0\,(x-y)}.$$

*where $\psi$ is an (approximate) minimizer of the Ginzburg-Landau-functional and*

$$(K_{T_c}^0 + V)\alpha_0 = 0.$$

The macroscopic ground state $\psi(hx)$ describes the **center-of-mass-motion** of the Cooper-pair-wavefunction $\alpha(x,y)$.


[FHSS] R.L. Frank, C. Hainzl, R. Seiringer, J.P. Solovej, J. Amer. Math. Soc. **25**, 667–713 (2012).
[FHSS2] R.L. Frank, C. Hainzl, R. Seiringer, J.P. Solovej, Oper. Theory Adv. Appl., 227, Birkhäuser/Springer Basel AG, Basel, 2013. 35Q56 (81Q20)

# Ginzburg-Landau

Macroscopic fluctuations of $\alpha(x, y)$ are captured by Ginzburg-Landau.
The influence of external fields $h\mathbf{A}(hx)$ and $h^2 W(hx)$ on the critical temperature is determined by the **linearized GL-operator**:

**Theorem ([FHSS3])**

$$T_c^{\mathrm{BCS}} = T_c(1 - D_c h^2) + o(h^2).$$

$$D_c = \frac{1}{\lambda_2} \inf \mathrm{spec} \left( (-i\nabla + 2\mathbf{A}(x))^2 + \lambda_3 W(x) \right),$$

with the parameters $\lambda_i$ depending on $V, \mu$.

[FHSS3] R.L. Frank, C. Hainzl, R. Seiringer, J.P. Solovej, Commun. Math. Phys. 342 (2016), no. 1, 189–216

Using a linear 2-body operator we also prove a result of Helfand and Werthammer [HW].

## Theorem

*([FHL17]) In the presence of constant magnetic field* $\frac{\mathbf{B}}{2} \wedge x$*, one has*

$$T_c(B) = T_c(1 - \frac{\lambda_0}{\lambda_2} 2B) + o(B),$$

*where*

$$2B = \inf \sigma \left( (-i\nabla + \mathbf{B} \wedge x)^2 \right).$$

With $W(x)$ instead of a magnetic field, we give a similar proof in [FH18].

[HW] E. Helfand, N.R. Werthamer, Phys. Rev. 147, 288 (1966)
[FHL18] R. L. Frank, C. Hainzl, E. Langmann, J. Spectr. Theory
[FH18] R. L. Frank, C. Hainzl, Special Issue in honor of H. Spohn

# Time-dependent BCS-equation

According to the physics literature [R, GE, Cy, S, W] the solution of the time-dependent BCS-equation, with appropriate $F$,

$$ih^2 \dot{\alpha}_t = F(\alpha_t)$$

leads to a diffusive behavior of the center-of-mass part of the Cooper-pair function

$$\psi_t = \frac{1}{h} \langle \alpha_0 | \alpha_t \rangle$$

which supposedly approximately solves the non-linear Ginzburg-Landau-equation

$$\dot{\psi}_t = -(1 + |\psi_t|^2)\psi_t,$$

for $T > T_c$.

[R] Mohit Randeria, Cambridge University Press, July 1996, pp. 355–392. [GE] L. P. Gorkov, G. M. Eliashberg, Sov. Phys.-JETP **27** 328 (1968)
[Cy] Cyrot, 1973 Rep. Prog. Phys. bf 36 103 [S] A. Schmid, Phys. Mat. Cond. **5** 302 (1966)
[W] N. R. Werthamer, Phys. Rev. **132**, 663 (1963)

# Numerics [HSey]

We look at temperatures $T = T_c(1+h^2)$, use as initial state $\alpha|_{t=0}$ the BCS-ground state $\alpha_0$ for $T = T_c(1-h^2)$, and define $\psi_t = \frac{1}{h}\langle\alpha_0|\alpha_t\rangle$.

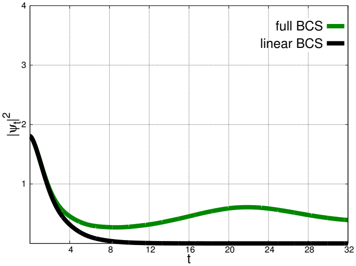



Figure: h=1/4

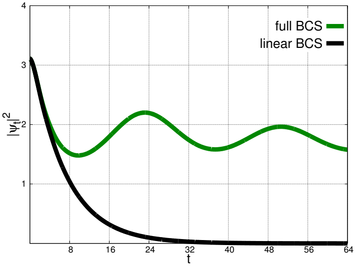



Figure: h=1/8

[HSey] C. Hainzl, J. Seyrich, Eur. Phys. J. B 89 (2016),

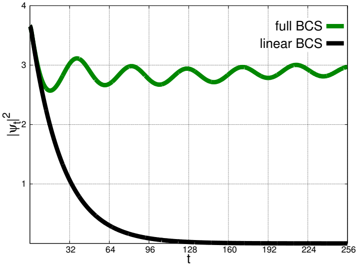



Figure: h=1/16

The linearized BCS-equation leads to a loss of superconductivity due to Fermi's Golden Rule. But the **non-linear equation** does not.

## Theorem ([FHSchS])

*Let* $T = T_c(1 + Dh^2)$*.* $D \in \mathbb{R}$*. Then for all* $t > 0$*,*

$$|\psi_t| = |\psi_0| + O(h^{1/2}).$$

[FHSchS] R.L. Frank, C. Hainzl, B. Schlein, R. Seiringer, Lett. Math. Phys. 106 (2016), no. 7, 913–923

# no symmetry breaking

## Theorem ([DGHL,HS])

- *In 2D there is no breaking of translational symmetry in the neighborhood of $T_c$.*
- *In 3D the same statement holds of the minimizer of the free functional is in an s-state.*

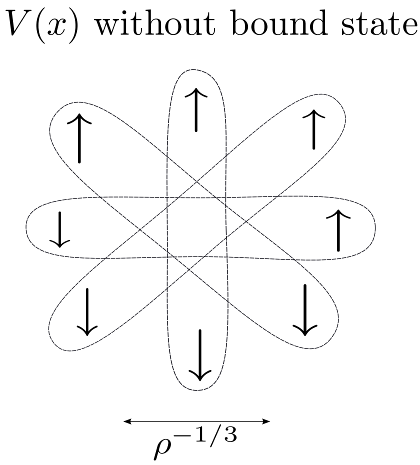
The proof is based on a relative-entropy inequality from [FHSS,HLS].

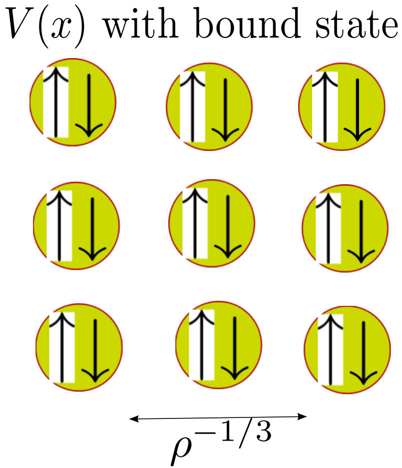
The argument relies on the fact that the $|\cdot|$-value solution of the linear problem is radial. This is true in $2D$ and for the first spherical harmonic in $3D$.

[DGHL] Deuchert, Geisinger, Hainzl, Loss, Ann. Henri Poincare 19 (2018), no. 5, 1507–1527
[HS] Hainzl, Seiringer, PRB (2008)
[HLS] C. Hainzl, M. Lewin, R. Seiringer, RMP (2008)

# BCS-BEC-crossover

In the weak coupling case (or high density case) the “pairing” takes place in momentum space, whereas in the strong coupling and low density case the pairs of Fermions behave as real bosons.



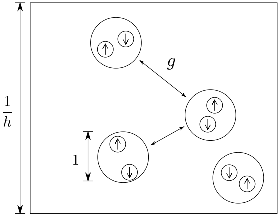
# The strong coupling low density BEC-limit

Let us now take a potential $V$ with a bound state $\alpha_0$ and ground state energy $-E_b$:

$$(-2\Delta + V)\alpha_0 = -E_b\alpha_0.$$

The number of particles is fixed as $1/h$.
Hence the density is

$$\rho = N/|\Omega| = h^2.$$




Energy and evolution in the BCS approach ?

# Condensation of pairs

## Theorem (HS12,BHS14)

*For small h,*

$$\inf_{0\leq\Gamma\leq 1,\,\mathrm{tr}\Gamma=1/h} \mathcal{E}^{\mathrm{BCS}}(\Gamma) = -\frac{E_b}{2h} + h \inf_{\|\psi\|_2=1} \mathcal{E}^{\mathrm{GP}}(\psi) + O(h^{3/2})$$

For an approximate ground state, leading order,

$$\alpha(x,y) = h\psi(\tfrac{h}{2}(x+y))\alpha_0((x-y)),$$

where $\psi(x)$ satisfies the GP-equation with scattering length depending on $\alpha_0$ and $E_b$.

[HS12] C. Hainzl, R. Seiringer, LMP (2012)
[BHS14] G. Bräunlich, C. Hainzl, R. Seiringer, MPAG (2014)

# Time evolution

Time evolution of BCS is governed by the equation

$$ih^2 \partial_t \Gamma_t = [H_{\Gamma_t}, \Gamma_t]$$

for the time-dependent operator $\Gamma_t$. The self-consistent Hamiltonian $H_{\Gamma_t}$ is given here by Let

$$\widetilde{\alpha}_t(X, r) := \alpha_t \left(X + r/2, X - r/2\right),$$

with $X$ the **center-of-mass** coordinate. With B. Schlein [HSch] we show that

$$\psi_t(X) := \frac{e^{itE_b/h^2}}{h} \int dr\, \alpha_0(r/h) \widetilde{\alpha}_t(X, r)$$

satisfies the time-dependent GP-equation to leading order.

C. Hainzl, B. Schlein, J. Funct. Anal. 265 (2013), no. 3, 399–423