Mathematical Aspects of the BCS Theory of Superconductivity

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(4 x 75 min)

1.) Physics background (Superconductivity)

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1. Physics background

(Examples of superfluids: liquid Helium 3 and 4)

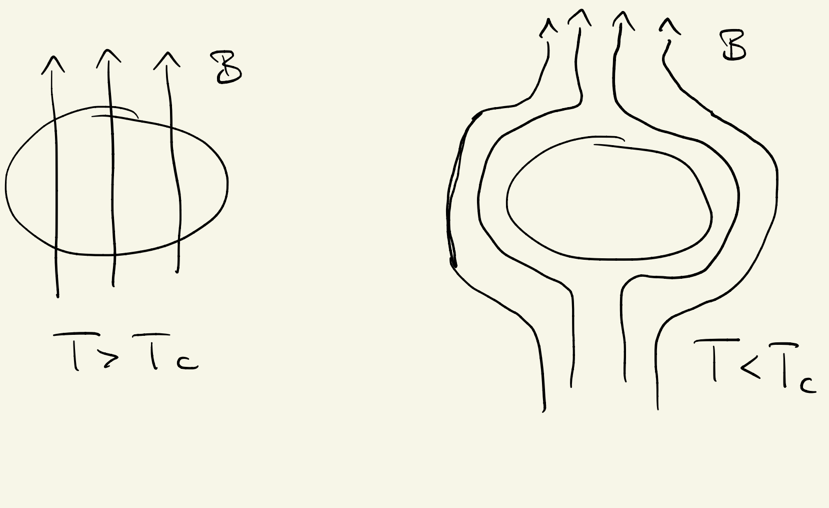
Superfluidity = frictionless flow

Superconductivity = superfluid flow of charged particles

- Superconductivity discovered by Heike Kamerlingh Onnes in 1911. He showed that Mercury is starting to be superconducting at 4.12 Kelvin. (Nobel prize in 1913)

  31 of the known 118 elements are known to be superconducting at low temperature. 18 additional are supercond. at low temp. and high pressure.

- In 1933 W. Meissner and R. Ochsenfeld discovered that samples, in the presence of a magnetic field, expell the magnetic field from their interior after being cooled below their superconducting transition temperature (**Meissner-Ochsenfeld effect**).



type I superconductors: superconducting states breaks down immediately if the external magnetic field reaches a critical value (first order phase transition)

type II superconductors: If one raises the external magnetic field beyond a first critical value one obtains a mixed state, where an increasing amount of localized magnetic flux tubes penetrate the material. However, there remains no resistance to the electric current if it is not too large. Some type II superconductors exhibit a small but finite resistance in the mixed state due to motion of the flux vortices induced by the Lorentz forces from the current. At a second critical field the superconducting states is destroyed.

[·] The **London equations** (F. and H. London, 1935) below have been the first theoretical model that explained the Meissner effect. They read

$\vec{j}_s$ = superconducting current density (vector)

E, B = electric, magnetic field (vectors)

e = electron charge

m = electron mass

n_s = material constant

$$\frac{\partial \vec{j}_s}{\partial t} = \frac{n_s e^2}{m} E, \qquad \mathrm{rot}\, \vec{j}_s = -\frac{n_s e^2}{m} B.$$

- **Isotope effect** (Maxwell, Reynolds 1950-51)

  Critical temperature for superconductivity is, for a given material, approximately inversely proportional to the square root of the mass of the isotope used in the material (Isotopes have the same number of electrons but a different number of neutrons in the nucleus. They therefore have a different mass.).

- **Ginzburg-Landau equations** (Ginzburg, Landau 1950)

  The GL equations have been introduced as a phenomenological theory of superconductivity. The vortex lattice structure that emerges when magnetic vortex tubes penetrate a superconductor can be explained with them (Abrikosov lattice solutions, Nobel prize in 2003). In particular, they describe the superconducting phase transition as a function of the external magnetic field. The GL equations read

magnetic vector potential

$$\left(-i\nabla + A(x)\right)^2 \underbrace{\psi(x)}_{\substack{\text{function from } \mathbb{R}^3 \to \mathbb{C} \\ \text{(order parameter)}}} = \kappa^2 \left(|\psi(x)|^2 - 1 \right) \psi(x)$$

full magnetic field

$$\operatorname{curl}\big[\underbrace{B(x)}_{\operatorname{curl} A(x)} - B_{ext}(x)\big] = \operatorname{Re}\left[\overline{\psi(x)} \left(-i\nabla + A(x)\right) \psi(x) \right].$$

external magnetic field

they carry no charge

In case of a superfluid, the particles cannot create an external magnetic field (the magnetic field in the equation then usually describes a rotation of the system, where the Coriolis force has been compensated by a harmonic potential ωx^2)), and one therefore only considers the first equation (for Ψ) to describe the matter part of the system. This equation successfully predicts that the velocity field $v(x)$ of a superfluid satisfies $\mathrm{rot}\, v(x) = 0$. (irrotational flow)

- **BCS theory of superconductivity** (Bardeen, Cooper, Schrieffer, 1957, Nobel prize 1972). The first microscopic theory of superconductivity. The main ingredients are:

(a) At low temperatures there is an effective attractive interaction between the electrons in a metal or alloy coming from lattice vibrations (**phonons**).

(b) This effective attraction leads to the formation of **Cooper pairs** in the system. These electron pairs are not really bosonic particles because in a typical metal each pair overlaps with order 1000 other pairs. Nevertheless, these pairs do condense as bosons do.

(c) BCS used a clever trial state (we would today call it a quasi-free state) to obtain a model that displays the above phenomenon and can be studied analytically. It describes the superconducting phase transition in many metals and alloys.

- Of the many later developments we only mention the discovery of high-temperature superconductivity by Bednorz and Müller in 1986 at the IBM research lab near Zurich.

  (T_c Mercury 4.2K, highest T_c in 1970s was 20K, Bednorz, Müller: $T_c = 35.1K$, highest T_c as of 2021: 133K (at room pressure))

  To this day there is no satisfactory theoretical explanation for the transition temperatures above. It seems that the superconducting state in these materials is more complicated than the one introduced by BCS.

  In the next section we introduce the class of states of BCS (quasi-free states on the fermionic Fock space) mathematically. Afterward, we give a formal derivation of the BCS functional.

  non-rigorous

2. Fermionic Fock space and quasifree states

Let us consider fermionic particles with spin $1/2$ in the box $\Lambda = [0,L]^3$.

- One particle Hilbert space: $\mathcal{H}_1 = L^2(\Lambda) \otimes \mathbb{C}$.

One element: $\underbrace{\psi(x,\sigma)}_{\text{complex-valued}}$ with $x \in \Lambda$, $\sigma \in \{\uparrow,\downarrow\}$

Inner product: $\langle \varphi, \psi \rangle = \sum_{\sigma \in \{\uparrow,\downarrow\}} \int_\Lambda \overline{\varphi(x,\sigma)} \psi(x,\sigma)\, dx$

- n-particle Hilbert space: $\mathcal{H}_n = \underbrace{\mathcal{H}_1 \wedge \dots \wedge \mathcal{H}_1}_{n\text{-times}}$

One element: $\psi(x_1,\sigma_1, \dots, x_n,\sigma_n)$ with $x_i \in \Lambda$, $\sigma_i \in \{\uparrow,\downarrow\}$ that satisfies

$$\psi(x_1,\sigma_1, \dots, x_i,\sigma_i, \dots, x_j,\sigma_j, \dots, x_n,\sigma_n) \qquad (1)$$

$$= -\psi(x_1,\sigma_1, \dots, x_j,\sigma_j, \dots, x_i,\sigma_i, \dots x_n,\sigma_n)$$

for all $1 \le i < j \le n$.

Fermionic Fock space: $\mathcal{F} = \bigoplus_{n=0}^{\infty} \mathcal{H}_n$ with $\mathcal{H}_0 = \mathbb{C}$.

One element $\Psi = (\Psi_0, \Psi_1, \Psi_2, \dots)$ with $\Psi_n \in \mathcal{H}_n$ and

$$\langle \Psi, \Psi \rangle = \sum_{n=0}^{\infty} \langle \Psi_n, \Psi_n \rangle < +\infty . \qquad (2)$$

The Fock space allows for the description of physical systems with a fluctuating particle number.

Creation and annihilation operators:

For $f \in \mathcal{H}_1$ the creation operator $a^*(f)$ and the annihilation operator $a(f)$ are defined by $(\Psi \in \mathcal{H}_n)$

$$\left(a^*(f)\Psi\right)(x_1, \sigma_1, \dots, x_{n+1}, \sigma_{n+1}) \qquad (3)$$

$$= \frac{1}{\sqrt{n!\,(n+1)!}} \sum_{s \in S_{n+1}} \mathrm{sgn}(s)\, f\left(x_{s(n+1)}, \sigma_{s(n+1)}\right) \Psi\left(x_{s(1)}, \sigma_{s(1)}, \dots, x_{s(n)}, \sigma_{s(n)}\right)$$

and

$$(a(f)\psi)(x_1\sigma_1,\dots,x_{n-1}\sigma_{n-1}) = \sqrt{n}\sum_{\sigma\in\{\uparrow,\downarrow\}}\int_\Lambda \overline{f(x,\sigma)}\,\psi(x,\sigma,x_1,\sigma_1,\dots,x_{n-1}\sigma_{n-1})\,dx,$$

respectively. A short computation shows that $a^*(f)$ is indeed the adjoint of $a(f)$ and that these operators satisfy the **Canonical Anticommutation Relations**

(CAR): $(\{A,B\} = AB+BA;\ f,g\in L^2(\Lambda))$

$$\{a(g),a^*(f)\} = \langle g,f\rangle_{L^2(\Lambda)}\,\mathbb{1}_{\mathcal{F}},$$

$$\{a^*(g),a^*(f)\} = 0 = \{a(g),a(f)\}. \qquad (4)$$

$\boxed{\text{Exercise 1}}$: Please check (4).

- **States**: A bounded operator ρ on $\mathcal{F}$ is called a state if $\rho\geq 0$ and $\operatorname{tr}\rho = 1$. By the spectral theorem it can be written in the form

$$\rho = \sum_{\alpha=1}^{\infty} p_\alpha\,|\psi_\alpha\rangle\langle\psi_\alpha| \qquad (5)$$

with $p_\alpha\geq 0$ for $\alpha\in\mathbb{N}$ and $\sum_{\alpha=1}^{\infty} p_\alpha = 1$. That is, ρ

can be interpreted as a probability distribution over rank one projections. In the following we will use the notation $(A \in \mathcal{B}(\mathcal{F}))$

$$\mathrm{tr}[A\varrho] = \langle A \rangle_\varrho . \qquad (6)$$

Example 1 (Slater determinant): Let $\{\varphi_i\}_{i=1}^N$ be an orthonormal family of vectors in $\mathcal{H}_1$ and define

$$\varrho_\Psi = |\Psi\rangle\langle\Psi| \quad \text{with} \quad \Psi = \varphi_1 \wedge \ldots \wedge \varphi_N . \qquad (7)$$

• **Quasi-free states**: a state ϱ on $\mathcal{F}$ is called quasi-free if the **Wick rule**

$$\langle a_1^\# a_2^\# \ldots a_{2n}^\# \rangle_\varrho = \sum_{p \in S'_{2n}} \mathrm{sgn}(p) \langle a_{p(1)}^\# a_{p(2)}^\# \rangle_\varrho \ldots \langle a_{p(2n-1)}^\# a_{p(2n)}^\# \rangle_\varrho ,$$

$$\langle a_1^\# a_2^\# \ldots a_{2n+1}^\# \rangle_\varrho = 0 \qquad (8)$$

holds. Here $a_j^\#$ stands for either $a^*(f_j)$ or $a(f_j)$ with some $f_j \in \mathcal{H}_1$. S'_{2n} is the subset of the symmetric group S_{2n} containing only permutations which satisfy $p(1) < p(3) < p(5) < \ldots < p(2n-1)$ and $p(2j-1) < p(2j)$ for all $1 \leq j \leq n$.

Example 2 (Wick rule):

$$\langle a^*(f_1)\, a^*(f_2)\, a(f_3)\, a(f_4) \rangle \tag{9}$$

$$= \langle a^*(f_1)\, a^*(f_2) \rangle \langle a(f_3)\, a(f_4) \rangle$$

$$- \langle a^*(f_1)\, a(f_3) \rangle \langle a^*(f_2)\, a(f_4) \rangle$$

$$+ \langle a^*(f_1)\, a(f_4) \rangle \langle a^*(f_2)\, a(f_3) \rangle.$$

Example 3 (Quasi-free state): The Slater determinant introduced in (7) is a quasi-free state.

$\boxed{\textbf{Exercise 2}}$: Please check that ρ_Ψ in (7) is a quasi-free state. Hint: Write the vector Ψ in terms of creation operators as

$$\Psi = \varphi_1 \wedge \ldots \wedge \varphi_N = a^*(\varphi_1) \ldots a^*(\varphi_N)\, \Omega, \tag{10}$$

where $\Omega = (1, 0, 0, \ldots)$ denotes the vacuum vector in $\mathcal{F}$. Then use the CAR.

Let me recall that for $\Psi_1 \in \mathcal{H}_n$ and $\Psi_2 \in \mathcal{H}_m$ we have (for the sake of simplicity I omit spin variables)

$$\Psi_1 \wedge \Psi_2 (x_1, \ldots, x_{n_1+n_2}) = \frac{1}{\sqrt{n_1!\, n_2!\, (n_1+n_2)!}} \times \tag{11}$$

$$\sum_{p \in S_{n_1+n_2}} \mathrm{sgn}(p)\, \Psi_1(x_{p(1)}, \ldots, x_{p(n_1)})\, \Psi_2(x_{p(n_1+1)}, \ldots, x_{p(n_1+n_2)}).$$

Remark 1: A quasi-free state is completely determined if we know $\langle a^*(f) a(g) \rangle_\rho$ and $\langle a(f) a(g) \rangle_\rho$ for all $f, g \in \mathcal{H}_1$. That is, the set of these states has a nice parametrization!

3. Formal derivation of the BCS functional

The **Hamiltonian** of our system of spin ½ fermions in the box $[0,L]^3$ reads (Fourier space, second quantization)

$$H = \underbrace{\sum_{\substack{p \in \frac{2\pi}{L}\mathbb{Z}^3 \\ \sigma \in \{\uparrow,\downarrow\}}} p^2 a^*_{p\sigma} a_{p\sigma}}_{\text{kinetic term}} + \underbrace{\frac{(2\pi)^{3/2}}{2L^3} \sum_{\substack{p,u,v \in \frac{2\pi}{L}\mathbb{Z}^3 \\ \sigma,\tau \in \{\uparrow,\downarrow\}}} \hat{V}(p)\, a^*_{u+p,\sigma} a^*_{v-p,\tau} a_{v,\tau} a_{u,\sigma}}_{\text{interaction potential}} . \qquad (12)$$

(kinetic term: $\sum_{i=1}^{n} -\Delta_i$ in n-particle sector)

(interaction potential: $\sum_{1 \le i < j \le n} V(x_i - x_j)$ in n-particle sector in position space, $\hat{V}(p) = (2\pi)^{-3/2} \int_{[0,L]^3} V(x)\, e^{-ipx}\, dx$)

We are interested in the **grand canonical potential**

$$F = -T \ln\left(\operatorname{tr} \exp\left(-\tfrac{1}{T}(H - \mu N) \right)\right), \qquad (13)$$

T = **temperature**,

μ = **chemical potential**

$$\underbrace{N = \sum_{p,\sigma} a^*_{p\sigma} a_{p\sigma}}_{\text{particle number operator}}$$

which satisfies the Gibbs Variational principle

$$\mathcal{F} = \min \Big\{ \operatorname{tr}[\mathcal{H}\Gamma] - T \underbrace{S(\Gamma)}_{= -\operatorname{tr}\Gamma \ln(\Gamma)} \Big\}, \tag{14}$$

von Neumann entropy

where the minimum is taken over all states on the Fock space. The unique minimizer is the grand canonical Gibbs state

$$G = \frac{\exp\left(-\frac{1}{T}(\mathcal{H} - \mu \mathcal{N})\right)}{\operatorname{tr} \exp\left(-\frac{1}{T}(\mathcal{H} - \mu \mathcal{N})\right)}. \tag{15}$$

The ultimate goal is to show that

$$\lim_{|v| \to \infty} \lim_{L \to \infty} \left\langle a^*(f)\, a^*(g)\, a(\underbrace{T_v g}_{(T_v g)(x) = g(x-v)})\, a(T_v f) \right\rangle_G \neq 0 \tag{16}$$

holds, which would, by physics arguments, imply superconductivity. But this problem is believed to be out of reach of present day mathematics.

The idea of BCS was to restrict attention to quasi-free states in the minimization in (14) to obtain an approximation to the interacting Gibbs state G in (16).

In the following we restrict attention to SU(2) and translation-invariant quasi-free states, which are completely determined by the **one-particle density matrix (1-pdm)**

$$\gamma(p) = \langle a^*_{p,\uparrow} a_{p,\uparrow} \rangle_\rho = \langle a^*_{p,\downarrow} a_{p,\downarrow} \rangle_\rho \qquad (17)$$

and the Fourier transform of the **Cooper pair wave function**

$$\hat{\alpha}(p) = \langle a_{-p,\uparrow} a_{p,\downarrow} \rangle_\rho = -\langle a_{-p,\downarrow} a_{p,\uparrow} \rangle_\rho . \qquad (18)$$

All other expectation values of quadratic expressions are zero under these symmetry assumptions. Using the Cauchy-Schwarz inequality, the CAR, and $\hat{\alpha}(p) = \hat{\alpha}(-p)$ one easily checks that

$$0 \leq \gamma(p) \leq 1 \quad \text{and} \quad |\hat{\alpha}(p)|^2 \leq \gamma(p)\left(1-\gamma(p)\right) \tag{19}$$

holds for al $p \in \frac{2\pi}{L}\mathbb{Z}^3$.

A straight forward computation that uses the Wick theorem shows that the energy of our state reads

$$\begin{aligned}\langle H - \mu N \rangle_\rho = {} & 2 \sum_p (p^2 - \mu)\gamma(p) + \frac{(2\pi)^{3/2}}{2L^3} \sum_{p,k} \hat{v}(k) \overline{\hat{\alpha}(k-p)} \hat{\alpha}(p) \\ & + 2 \frac{(2\pi)^{3/2}}{L^3} \underbrace{\hat{v}(0)}_{\text{direct term}} \left(\sum_p \gamma(p) \right)^2 - \frac{(2\pi)^{3/2}}{L^3} \sum_{p,k} \overbrace{\hat{v}(k)}^{\text{exchange term}} \gamma(p-k) \gamma(p). \end{aligned} \tag{20}$$

It can also be shown (this is more complicated) that the entropy of an SU(2) and translation invariant quasi-free state ρ can be written as

$$S(\rho) = -2 \sum_{p} \mathrm{tr}_{\mathbb{C}^2}\left[\Gamma(p) \ln\left(\Gamma(p)\right)\right], \tag{21}$$

where $\Gamma(p)$ is the 2×2 matrix

$$\Gamma(p) = \begin{pmatrix} \gamma(p) & \hat{\alpha}(p) \\ \overline{\hat{\alpha}(p)} & 1-\gamma(p) \end{pmatrix}, \tag{22}$$

which satisfies the p.w. bound $0 \leq \Gamma(p) \leq 1$.

The next step in the formal derivation of the BCS functional is to discard the two interaction terms that depend on γ (direct and exchange term). When we multiply $\langle H \rangle_\rho - \frac{1}{\beta} S(\rho)$ by $\frac{1}{2}\left(\frac{2\pi}{L}\right)^3$, take the limit $L \to \infty$, and absorb a factor $\frac{1}{2}$ in V, we find the BCS functional

$$\mathcal{F}(\gamma,\alpha) = \int_{\mathbb{R}^3} (p^2-\mu)\,\gamma(p)\,dp + \int_{\mathbb{R}^3} V(x)\,|\alpha(x)|^2\,dx - T\,S(\gamma,\alpha), \tag{23}$$

Sometimes we also write $\mathcal{F}(\Gamma)$ / $S(\Gamma)$

with

here we used the special form of $\Gamma(p)$ to see that if λ is an EV of $\Gamma(p)$ then $1-\lambda$ is one, too.

$$S(\gamma,\alpha) = \frac{1}{2}\int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\Big[\Gamma(p)\ln\Gamma(p) + \big(1-\Gamma(p)\big)\ln\big(1-\Gamma(p)\big)\Big]. \tag{24}$$

In the following we assume $V \in L^{3/2}(\mathbb{R}^3)$. In this case the natural domain of the BCS functional is

$$\mathcal{D} = \Big\{ (\gamma,\alpha) \in L^1\big(\mathbb{R}^3, (1+p^2)dp\big) \times H^1(\mathbb{R}^3, dx) \;\Big|\; \alpha(x) = \alpha(-x),\ 0 \leq \Gamma(p) \leq 1 \Big\}. \tag{25}$$

What is the meaning of superconductivity in the framework of the BCS functional? To answer this question, we replace the interacting Gibbs state G by an $SU(2)$ and translation invariant quasi-free state g in (16). We also replace $a^*(f)$, $a^*(g)$ by $a^*_\uparrow(x)$, $a^*_\downarrow(x)$, where $a^*_\uparrow(x)$ denotes the operator-value distribution

$a^*_\uparrow(x) = \sum_p e^{ipx} a^*_{\uparrow,p}$. A short computation shows

$$\langle a^*_\uparrow(x) a^*_\downarrow(x) a_\downarrow(y) a_\uparrow(y) \rangle = \left[\gamma(x-y)\right]^2 + |\alpha(0)|^2. \tag{26}$$

We have $\int_{\mathbb{R}^3} (1+p^2)\gamma(p)\,dp$, and hence $\lim_{|x|\to\infty} \gamma(x) = 0$

(Riemann-Lebesgue lemma). We conclude that

$$\lim_{|y|\to\infty} \langle a^*_\uparrow(x) a^*_\downarrow(x) a_\downarrow(y) a_\uparrow(y) \rangle \neq 0 \iff \tag{27}$$

$|\alpha(0)|^2 \neq 0$. This motivates the definition that the minimizer of $\mathcal{F}$ is called superconducting iff the minimizer has a non-vanishing Cooper pair wave function (note that this is not exactly the same).

Remark 2: The long range order in (27) can be interpreted as Bose-Einstein condensation of fermion pairs. We recall that BEC can be defined by

$$\lim_{|y|\to\infty} \lim_{L\to\infty} \langle a^*(x) a(y) \rangle_G \neq 0. \tag{28}$$

4. Mathematical analysis of the BCS functional in the translation-invariant case

In this section we study the BCS function $\mathcal{F}(\gamma,\alpha)$ in (23) for $V \in L^{3/2}(\mathbb{R}^3)$ and $(\gamma,\alpha) \in \mathcal{D}$ with $\mathcal{D}$ in (25). As has been shown in

[1] C. Hainzl, E. Hamza, R. Seiringer, J.P. Solovej, The BCS functional for general pair interactions, Commun. Math. Phys. 281, 349–367 (2008)

the BCS functional is bounded from below and attains its infimum in the set $\mathcal{D}$, that is, there exists a pair $(\tilde{\gamma},\tilde{\alpha}) \in \mathcal{D}$ s.t.

$$\inf_{(\gamma,\alpha)\in\mathcal{D}} \mathcal{F}(\gamma,\alpha) = \mathcal{F}(\tilde{\gamma},\tilde{\alpha}). \tag{29}$$

This minimizer need not be unique. The lower bound easily follows from (19) and the inequality $-\Delta + V \geq -C$, which holds in the sense of quadratic forms. The proof of the existence of a minimizer uses the direct method in the calculus of variations and is fairly standard.

If $V \equiv 0$ the BCS functional is minimized by the **normal state**

$$\Gamma_0(p) = \begin{pmatrix} \gamma_0(p) & 0 \\ 0 & 1-\gamma_0(p) \end{pmatrix}, \quad \gamma_0(p) = \frac{1}{e^{\frac{1}{T}(p^2-\mu)}+1}. \tag{30}$$

To prove this statement, we write the BCS functional in the form $(V \equiv 0\,!)$

$$\gamma - \gamma_0$$

$$\mathcal{F}(\Gamma) = \mathcal{F}(\Gamma_0) + \underbrace{\mathcal{F}(\Gamma) - \mathcal{F}(\Gamma_0)}_{}$$

$$\frac{1}{2}\int_{\mathbb{C}^2} \mathrm{tr}_{\mathbb{C}^2}\Big[\underbrace{H_0(p)}_{\begin{pmatrix} p^2-\mu & 0 \\ 0 & -(p^2-\mu) \end{pmatrix}}\big(\Gamma(p) - \Gamma_0(p)\big)\Big]\,dp + \frac{T}{2}\big[S(\Gamma_0) - S(\Gamma)\big]$$

$$= \mathcal{F}_0(\Gamma_0) + \frac{T}{2}\mathcal{H}(\Gamma, \Gamma_0), \quad \text{where} \tag{31}$$

$$\varphi(x) = x\ln(x) + (1-x)\ln(1-x)$$

$$\mathcal{H}(\Gamma,\Gamma_0) = \int_{\mathbb{C}} \mathrm{tr}_{\mathbb{C}^2}\Big[\varphi(\Gamma(p)) - \varphi(\Gamma_0(p)) - \varphi'(\Gamma_0(p))\big(\Gamma(p)-\Gamma_0(p)\big)\Big]\,dp \qquad (32)$$

denotes fermionic relative entropy of Γ w.r.t. Γ_0. We claim that the trace on the r.h.s. is nonnegative and equals zero iff $\Gamma(p) = \Gamma_0(p)$ a.e.. This can be proved with Klein's inequality, whose statement is captured in the following Lemma.

Lemma 1 (Klein's inequality): Let A, B be two self-adjoint operators with spectra $\sigma(A), \sigma(B)$ and let $\{f_k\}, \{g_k\}$ be two families of functions with $f_k : \sigma(A) \to \mathbb{C}$, $g_k : \sigma(B) \to \mathbb{C}$, and assume that

$$\sum_k f_k(a)\, g_k(b) \geq 0 \quad \text{for all } a \in \sigma(A),\ b \in \sigma(B). \qquad (33)$$

Then

$$\mathrm{tr}\Big[\sum_k f_k(A)\, g_k(B)\Big] \geq 0. \qquad (34)$$

Exercise: Prove Klein's inequality in the case of matrices A and B.

The above claims about the relative entropy follow from the strict convexity of the map $x \mapsto \varphi(x)$ and Klein's inequality. This proves that Γ_0 is the unique minimizer of $\mathcal{F}$ if $V \equiv 0$.

The following theorem characterizes phase transitions in the BCS functional and appeared in this form in [1].

Theorem 1: Let $V \in L^{3/2}(\mathbb{R}^3)$, $\mu \in \mathbb{R}$, and $T \in [0,\infty)$.

Then the following statements are equivalent:

(i) The normal state $(\gamma_0, 0)$ is unstable under pair formation, i.e.,

$$\inf_{(\gamma,\alpha)\in \mathcal{D}} \mathcal{F}(\gamma,\alpha) < \mathcal{F}(\gamma_0, 0). \tag{35}$$

(ii) There exists a pair $(\gamma,\alpha) \in \mathcal{D}$, with $\alpha \not\equiv 0$, s.t.

$$\Delta(p) = - \frac{p^2-\mu}{\gamma(p)-\frac{1}{2}} \hat{\alpha}(p) \tag{36}$$

satisfies the BCS gap equation (37)

$$\Delta = -\hat{V} * \left(\frac{\Delta}{E} \tanh\left(\frac{E}{2T} \right) \right) \quad \text{with } E(p) = \sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}.$$

$$f * g(p) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} f(p-q) g(q) \, dq$$

(iii) The linear operator

$$K_{T,\mu} + V \quad , \quad K_{T,\mu} = \frac{p^2-\mu}{\tanh\left(\frac{p^2-\mu}{2T} \right)} , \tag{38}$$

has at least one negative eigenvalue.

Remark 3: The operator in (38) is obtained by taking the second derivative of $\mathcal{F}$ w.r.t. α in the normal state $(\gamma_0, 0)$. Since the normal state is a critical point of $\mathcal{F}$ it is easy to see that (iii) implies (i). The opposite direction says that if $(\gamma_0, 0)$ is not a minimizer then it cannot be locally stable, and it is not immediate.

Let us prove (i) $\Rightarrow$ (iii). To that end, we show that the negation of (iii) implies the negation of (i).

To that end, we need the following lemma, which is a simplified version of Lemma 1 in [FHSS 2012] (see p. 2 in Section on GL theory for the precise reference).

Lemma 2: We have

$$\mathcal{H}(\Gamma,\Gamma_0) \geq \int_{\mathbb{R}^3} \mathrm{tr}_{\mathbb{C}^2}\left[\frac{\frac{1}{T}H_0(p)}{\tanh\left(\frac{H_0(p)}{2T}\right)}\left(\Gamma(p)-\Gamma_0(p)\right)^2\right] dp. \tag{39}$$

The proof of this inequality follows from the bound

$$x\ln\left(\frac{x}{y}\right) + (1-x)\ln\left(\frac{1-x}{1-y}\right) \geq \frac{\ln\left(\frac{1-y}{y}\right)}{1-2y}(x-y)^2 \tag{40}$$

for $0<x,y<1$ and an application of Klein's inequality.

To prove our original claim, we write

$$\mathcal{F}(\Gamma)-\mathcal{F}(\Gamma_0) = \frac{T}{2}\mathcal{H}(\Gamma,\Gamma_0) + \int_{\mathbb{R}^3} V(x)\,|\alpha(x)|^2\,dx$$

$$\underset{\text{Lemma 1}}{\geq} \int_{\mathbb{R}^3} \overbrace{K_{T,\mu}(p)}^{\geq 2T}\left(\gamma(p)-\gamma_0(p)\right)^2 dp + \int_{\mathbb{R}^3} K_{T,\mu}(p)\,|\hat{\alpha}(p)|^2\,dp + \int_{\mathbb{R}^3} V(x)\,|\alpha(x)|^2\,dx$$

$$\geq \langle \alpha, (K_{T,\mu} + V)\alpha \rangle_{L^2(\mathbb{R}^3)} . \qquad (41)$$

If $K_{T,\mu}+V$ has no negative eigenvalues (the essential spectrum of the operator equals $[2T,\infty)$) then the r.h.s. of (41) is nonnegative and we conclude that $\mathcal{F}(\Gamma) - \mathcal{F}(\Gamma_0) \geq 0$. Since this is the negation of (i) the claim is proved.

Remark 4: ⊡ The operator $K_{T,\mu}$ is strictly monotone in T in the sense that

$$\langle \psi, K_{T,\mu} \psi \rangle \leq \langle \psi, K_{T',\mu} \psi \rangle \quad \forall \psi \in H^2(\mathbb{R}^3) \qquad (42)$$

if $T \leq T'$. This allows us to conclude that there exists a unique critical temperature $T_c \geq 0$ s.t. the unique minimizer is the normal state if $T \geq T_c$ and there exists a minimizer Γ with $\alpha \not\equiv 0$ if $T < T_c$.

⊡ The characterization of T_c via the linear operator

$K_{T_{c,\mu}} + V$ is the starting point for several studies of T_c in the weak coupling, the low density, and the high density limit.

• In physics textbook the gap equation in (37) is more prominently featured than the BCS functional. Theorem 1 guarantees that the two approaches are equivalent.

5. The BCS functional in the presence of periodic external fields

In the following we assume that $W : \mathbb{R}^3 \to \mathbb{R}$ is periodic with period a, i.e. $W(x+v) = W(x)$ for all $v \in a\mathbb{Z}^3$, $a > 0$ (lattice constant). To study BCS theory in the presence of W we drop the assumption of translation invariance of the states and rather assume that they are periodic w.r.t. the lattice $a\mathbb{Z}^3$.

In this setting a BCS state is of the form

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \bar{\alpha} & 1-\bar{\gamma} \end{pmatrix} \in \mathcal{B}\left(L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)\right) \tag{43}$$

and satisfies $0 \leq \Gamma \leq 1$. The operator $\bar{\alpha}$ is defined via its integral kernel in position space by $\bar{\alpha}(x,y) = \overline{\alpha(x,y)}$ (the Ops. we will consider have integral kernels).

We highlight that the condition $0 \leq \Gamma \leq 1$ is more complicated here than in the translation invariant case as γ and α are now operators on infinite dimensional Hilbert spaces that need not commute (in the translation invariant case they commute). It implies $\gamma(x,y) = \overline{\gamma(y,x)}$, $\alpha(x,y) = \alpha(y,x)$, and $\alpha\alpha^* \leq \gamma(1-\gamma)$.

We call a BCS state Γ **periodic** (w.r.t. $a\mathbb{Z}^3$) iff

$\left[(T_v f)(x) = f(x+v) \right]$

$$T_v \gamma T_v^* = \gamma \quad \Leftrightarrow \quad \gamma(x+v, y+v) = \gamma(x,y), \tag{44}$$

$$T_v \alpha T_v^* = \alpha \quad \Leftrightarrow \quad \alpha(x+v, y+v) = \alpha(x,y),$$

holds for all $v \in a\mathbb{Z}^3$. A periodic BCS state is called **admissible** if

$$\mathrm{tr}_{Q_a}\left[(-\Delta+1)^{1/2} \gamma (-\Delta+1)^{1/2} \right] < +\infty, \tag{45}$$

that is, if the state has finite trace and finite kinetic energy.

Here tr_{Q_a} denotes the trace per unit volume of a periodic operator A, that is,

$$\mathrm{tr}_{Q_a}[A] = \frac{1}{|Q_a|}\,\mathrm{tr}\left[\chi_{Q_a} A \chi_{Q_a}\right]. \tag{46}$$

Lebesgue measure of Q_a.

multiplication Op. in position space with characteristic function of the set $Q_a = [0,a]^3$.

For an admissible BCS state we define the BCS functional by

$$\mathcal{F}(\Gamma) = \mathrm{tr}_{Q_a}\left[(-\Delta - \mu + W)\gamma\right] - \frac{1}{\beta} S(\Gamma) + \frac{1}{|Q_a|}\int_{\mathbb{R}^3\times Q_a} \alpha(r,X)\, V(r)\, d(r,X). \tag{47}$$

$-\mathrm{tr}_{Q_a}[\Gamma \ln(\Gamma)]$

multiplication operator with $W(x)$

Cooper pair wave function in relative and center of mass coordinates $r = x-y$, $X = \frac{x+y}{2}$.

By a slight abuse of notation we denote it by the same symbol as the original function.

Symmetry

$$\alpha(x,y) = \alpha(y,x)$$

$$\Leftrightarrow \alpha(r,X) = \alpha(-r,X)$$

$$\alpha(x+v, y+v) = \alpha(x,y)$$

$$\Leftrightarrow \alpha(r, X+v) = \alpha(r,X)$$

How do we add an external periodic magnetic field?

We need to replace

leads to constant magnetic field (48)

$\boxdot$ $-\Delta$ by $-\Delta_A = (-i\nabla + A)^2$ with $A(x) = \overbrace{\underbrace{b\begin{pmatrix} -x_2 \\ x_1 \\ 0 \end{pmatrix}}_{A_B(x) \,=\, \underbrace{b e_3}_{B} \wedge x}} + A_{per}(x)$,

wedge or cross product

where $A_{per}(x+v) = A_{per}(x)$ $\forall\, v \in a\mathbb{Z}^d$.

Note that A is <u>not</u> periodic <u>but</u> $B(x) = \operatorname{rot} A(x)$ is.

$\boxdot$ Let us define the magnetic translation

$$T_B(v)\, f(x) = e^{i \frac{B}{2}\cdot(v \wedge x)} f(x+v), \tag{49}$$

which satisfies $T_B^*(v)\left(-i\nabla + A_B(x)\right) T_B(v) = 0$ $\forall\, v \in \mathbb{R}^3$. We need to replace (44) by

$$T_B(v)\,\gamma\, T_B^*(v) = \gamma \iff \gamma(x,y) = e^{i\frac{B}{2}\cdot(v \wedge (x-y))}\,\gamma(x+v, y+v)$$

$$T_B(v)\,\alpha\, \overline{T_B^*}(v) = \alpha \iff \alpha(x,y) = e^{i\frac{B}{2}\cdot(v \wedge (x+y))}\,\alpha(x+v, y+v) \tag{50}$$

$\boxdot$ the BCS functional in (47) by

$$\mathcal{F}(\Gamma) = \operatorname{tr}_{Q_a}\left[\left((-i\nabla + A(x))^2 + W(x) - \mu\right)\gamma\right] - TS(\Gamma)$$
$$+ \int_{\mathbb{R}^3 \times Q_a} V(r)\, |\alpha(r, X)|^2\, d(r, X). \tag{51}$$

Remark 5: The fact that A can be chosen as in (48) and that α can be chosen to be gauge periodic comes from the gauge symmetry of the problem. That is, we choose a certain gauge.

Using this symmetry and Fourier analysis, the following inequality has been proved in [Lemma 3, FHSS 2012]:

$$(*)(0) \geq \text{const.}\ h^2 \int_{\mathbb{R}^3 \times Q_h} |(\nabla_x + \nabla_y)\alpha(x,y)|^2 \, d(x,y). \qquad (104)$$

This would be easy to prove if K_T were replaced by $-\Delta$.

In case of a constant magnetic field we write the Cooper pair wave function as

$$\alpha(r,X) = \alpha_*(r)\cos\left(\tfrac{r}{2}\cdot \Pi_X\right)\Psi(X) + \xi_0(r,X). \qquad (105)$$

Note that the relative- and the center-of-mass wave function are entangled.

$= -i\nabla_X + A_{2B}(X)$

The functions Ψ and ξ_0 are defined via the operator

$$(A\alpha)(X) = \int_{\mathbb{R}^3} \alpha_*(r)\cos\left(\tfrac{r}{2}\cdot \Pi_X\right)\alpha(r,X)\, dr, \qquad (106)$$