What is Superconductivity?

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PLAN of the LECTURE

- Physics background & phenomenological models
- Mathematical set-up: Fermionic Fock space
- The BCS functional
- State of the art
- The translation invariant case
- Open problems

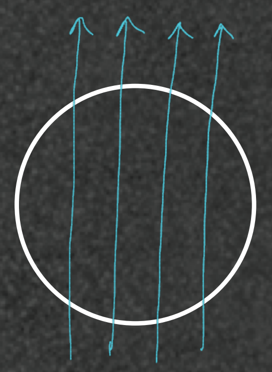
1. Physics background & pheonomenological models

Frictionless flows of charged particles $\rightarrow$ superconductors

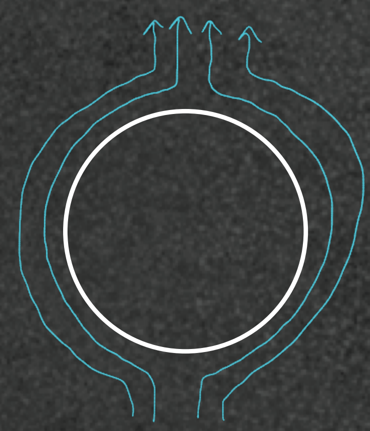
History:

- 1911 K. Onnes
  compute resistence of mercury at $\approx 4\,K$
  no resistence $\rightarrow$ "superconducting state"
  } Nobel Prize 1913

- 1933 Meissner & Ochsenfeld



$T > T_c$



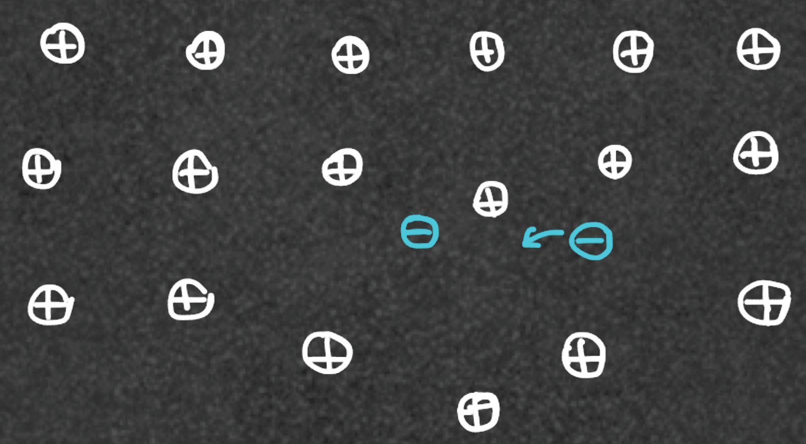
$T < T_c$

Two characteristics of superconductivity

- resistence approaching zero below a certain temperature;
- magnetic flow pushed out from the interior of a sample below a certain temperature.

- 1935 London : penetration length of the magnetic field

- 1950s Fröhlich : superconductivity comes from ion vibration (phonons)



- 1950 Ginzburg & Landau : phenomenological theory

- 1957 Bardeen, Cooper, Schreiffer
  microscopic theory of superconductivity } Nobel Prize 1972

BCS Theory of Superconductivity

Observations

(1) $T < T_c$: effective attractive interaction between electrons

(2) effective attractive interaction $\Rightarrow$ formation of Cooper pairs

(3) BCS used a trial state to obtain a model with (1) & (2)

(quasi-free state)

2. Mathematical set-up

Fermions with spin 1/2 in the box $\Lambda = [0,L]^3$.

- one-particle Hilbert space

$$\mathcal{H} := L^2(\Lambda) \otimes \mathbb{C}$$

$\psi \in \mathcal{H}$, $\psi = \psi(x,\sigma)$, $x \in \Lambda$, $\sigma \in \{\uparrow, \downarrow\}$

inner product : $\forall \varphi, \psi \in \mathcal{H}$

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

- N-particle Hilbert space

$$\mathcal{H}_N := \underbrace{\mathcal{H} \wedge \ldots \wedge \mathcal{H}}_{N \text{ times}}$$

$\psi \in \mathcal{H}_N$, $\psi = \psi(x_1, \sigma_1, \ldots, x_N, \sigma_N)$ $\quad x_i \in \Lambda$, $\sigma_i \in \{\uparrow, \downarrow\}$

antisymmetric: $\forall \quad i,j = 1 \ldots N$

$$\psi(x_1, \sigma_1, \ldots, x_j, \sigma_j, \ldots, x_i, \sigma_i, \ldots, x_N, \sigma_N)$$

$$= (-1)\, \psi(x_1, \sigma_1, \ldots, x_i, \sigma_i, \ldots, x_j, \sigma_j, \ldots, x_N, \sigma_N)$$

- Fermionic Fock Space

$$\mathcal{F} := \bigoplus_{n \geq 0} \mathcal{H}_n \qquad \text{with} \quad \mathcal{H}_0 \in \mathbb{C}$$

$$\mathcal{F} \ni \Psi = (\Psi_0, \Psi_1, \Psi_2, \dots), \quad \Psi_n \in \mathcal{H}_n \quad (n\text{-sector of } \mathcal{F})$$

inner product : $\Psi, \varphi \in \mathcal{F}$

$$\langle \Psi, \varphi \rangle_{\mathcal{F}} := \sum_{n \geq 0} \langle \Psi_n, \varphi_n \rangle < +\infty$$

- Remark: # of particles not fixed

  good set up to study fluctuations

- Creation and annihilation operators

Let $\psi \in \mathcal{H}_m$ and $f \in \mathcal{H}$.

$$(a^*(f)\psi)(x_1,\sigma_1,\dots,x_{n+1},\sigma_{n+1})$$

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

$$(a(f)\psi)(x_1,\sigma_1,\dots,x_{n-1},\sigma_{n-1})$$

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

EXERCISE 1

(i) $a^*(f)$ is the adjoint of $a(f)$

(ii) a^* and a satisfy the canonical anticommutation relation (C.A.R.), i.e. $\forall f, g \in L^2(\Lambda)$

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

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

where

$$\{A, B\} = AB + BA$$

- ## Quasi-free States

STATE $:=$ ρ bounded operator on $\mathcal{F}$

$\rho \geqslant 0$ and $\operatorname{tr} \rho = 1$

Spectral theorem $\Rightarrow$ $\rho = \sum_{j=1}^{\infty} \lambda_j \, |\psi_j\rangle\langle\psi_j|$

$\lambda_j \geqslant 0$ for $j \in \mathbb{N}$, $\sum_{j\geqslant 1} \lambda_j = 1$

Probability distribution over rank one projections.

Remark. $(|\psi\rangle\langle\varphi|)(f) = \langle\varphi|f\rangle|\psi\rangle$

- Slater Determinant:

let $\{\varphi_j\}_{j=1,\dots N}$ be an orthonormal family of functions in $\mathcal{H}_1$. let $\Psi = \varphi_1 \wedge \dots \wedge \varphi_N$ and

$$\rho_\Psi := |\Psi\rangle\langle\Psi|$$

- Quasi-free States:

a state ρ on $\mathcal{F}$ is quasi-free if the Wick rule holds $^{\circledast}$.

⊛ Wick's rule:

$$\mathrm{tr}\left(a_1^\# a_2^\# \dots a_{2n}^\# \rho\right)$$

$$= \sum_{\pi \in S'_{2n}} \mathrm{sgn}(\pi) \langle a^\#_{\pi(1)} a^\#_{\pi(2)} \rangle_\rho \dots \langle a^\#_{\pi(2n-1)} a^\#_{\pi(2n)} \rangle_\rho$$

$$\mathrm{tr}\left(a_1^\# a_2^\# \dots a_{2n+1}^\# \rho\right) = 0$$

where

- $a^\#_j$ either $a^*(f_j)$ or $a(f_j)$, $f_j \in \mathcal{H}$
- $S'_{2n} \subset S_{2n}$ permutations s.t.

$$\pi(1) < \pi(3) < \pi(5) < \dots < \pi(2n+1)$$

and $\pi(2j-1) < \pi(2j)$ $\forall\, j = 1, \dots, n$.

EXERCISE 2.

Check that ρ_ψ (Slater determinant) is a quasi-free state.

Hint: write $\psi = a^*(\varphi_1)\dots a^*(\varphi_n)\Omega$, where $\Omega = (1,0,0\dots) \in \mathcal{F}$

and use the C.A.R.

Remark.

From Wick's rule we deduce that quasi-free states can be parametrized in terms of

$$\underbrace{\mathrm{tr}\,(a^*(f)\,a(g)\,\rho)}_{\text{one-particle operator}} \quad \text{and} \quad \underbrace{\mathrm{tr}\,(a(f)\,a(g)\,\rho)}_{\text{expectation value of pairs of particles}}$$

3. The BCS energy functional

Trial states (BCS states)

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \bar{\alpha} & 1-\bar{\gamma} \end{pmatrix} \qquad 0 \leq \Gamma \leq 1$$

γ one-particle density matrix of the system, operator on $L^2(\Lambda) \otimes \mathbb{C}^2$

α bounded operator on $L^2(\Lambda) \otimes \mathbb{C}^2$

↳ describes the expectation values of pairs

(Cooper pair wave function)

SU(2)-invariant states

let $S \in SU(2)$ rotation in spin-space. Then Γ is SU(2) invariant if

$$\mathcal{S}^* \Gamma \mathcal{S} = \Gamma \quad , \quad \text{where } \mathcal{S} = \begin{pmatrix} S & 0 \\ 0 & \bar{S} \end{pmatrix}$$

For γ and α:

$$S^* \gamma S = \gamma \qquad \text{and} \qquad S^* \alpha \bar{S} = \alpha$$

EXERCISE 3

(i) If $M \in \mathbb{C}^{2\times 2}$ is s.t. $S^* M S = M \quad \forall S \in SU(2)$, then $M = \lambda \mathbb{1}$.

(ii) If $M \in \mathbb{C}^{2\times 2}$ is s.t. $S^* M \bar{S} = M \quad \forall S \in SU(2)$, then $M = \lambda \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

In terms of γ and α $\Rightarrow$ spins factor out

Under the SU(2)-invariance assumption, we can express the energy functional in terms of spin-independent quantities

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

where now γ, α are operators on $L^2(\Lambda)$ and not on $L^2(\Lambda) \otimes \mathbb{C}^2$.

The BCS Functional

$$\mathcal{F}(\Gamma) = \mathrm{tr}\left[(-\Delta-\mu)\gamma\right] - \frac{2}{\beta} S(\Gamma) + \boxed{2\iint_{\Lambda\times\Lambda} \gamma(x,x)\,\gamma(y,y)\,V(x-y)\,dx\,dy}$$

$$- \boxed{\iint_{\Lambda\times\Lambda} |\gamma(x,y)|^2\, V(x-y)\,dx\,dy}$$

$$+ \iint_{\Lambda\times\Lambda} |\alpha(x,y)|^2\, V(x-y)\,dx\,dy$$

Goal: minimize $\mathcal{F}(\Gamma)$ on the set of Γ translation invariant and $SU(2)$ invariant. Under which assumptions on V, β and Γ is $\alpha \neq 0$? Difficult!

Remark.

$\alpha \neq 0 \;\leftrightarrow\;$ correlation of pairs over macroscopic distances (Long Range Order) responsible for the vanishing resistance in a metal

Definition.

We say that the system is in a superconducting phase if the minimizer has a NON-ZERO PAIR WAVE FUNCTION α.

Simplified BCS energy functional

$$\mathcal{F}(\Gamma) = \operatorname{tr}\left[(-\Delta - \mu)\gamma\right] - \frac{2}{\beta} S[\Gamma]$$

$$+ \iint_{\Lambda \times \Lambda} V(x-y)\, |\alpha(x,y)|^2 \, dx\, dy$$

where

$$S(\Gamma) = - \operatorname{tr}\left[\Gamma \ln \Gamma\right]$$

Goal:

$$\min_{\Gamma : 0 \leq \Gamma \leq 1} \mathcal{F}(\Gamma) = F(\beta, \mu) \qquad \text{with } \alpha \neq 0$$

4. State of the art (see also Hainzl, Seiringer 2015)

- translation invariant case

$$\gamma(x,y) = \gamma(x-y) \quad \text{and} \quad \alpha(x,y) = \alpha(x-y)$$

→ Hainzl, Hamza, Seiringer, Solovej 2008

($\exists\, T_c$ s.t. $\alpha \neq 0$ for $T < T_c$)

- weak and slow varying fields

→ Frank, Hainzl, Seiringer, Solovej 2012

BCS minimizer ⟷ Ginzburg-Landau minimizer

- translation invariant + magnetic field/periodic ext. fields/...
- high temperature (cfr. recent experiments in the IBM lab in Zurich)

5. BCS Functional for translation-invariant states

- one-particle density matrix $\quad \gamma(x-y)$
- Cooper pair wave function $\quad \alpha(x-y)$

$\Rightarrow$ Fourier transform:

$$\left.\begin{aligned}
\gamma(x-y) &= (2\pi)^{-3} \int_{\mathbb{R}^3} \hat{\gamma}(p)\, e^{ip\cdot(x-y)}\, dp \\
\alpha(x-y) &= (2\pi)^{-3} \int_{\mathbb{R}^3} \hat{\alpha}(p)\, e^{ip\cdot(x-y)}\, dp
\end{aligned}\right\} \quad \Gamma(p) = \begin{pmatrix} \hat{\gamma}(p) & \hat{\alpha}(p) \\ \overline{\hat{\alpha}(p)} & 1-\hat{\gamma}(-p) \end{pmatrix}$$

Recall the BCS functional:

$$\mathcal{F}(\Gamma) = \operatorname{tr}_{L^2(\Lambda)}\left[(-\Delta - \mu)\gamma\right] - \frac{1}{\beta} S[\Gamma]$$

$$+ \iint_{\Lambda \times \Lambda} V(x-y)\, |\alpha(x,y)|^2 \, dx\, dy$$

and plug $\Gamma(p)$ into it (EXERCISE 4)

$$\int_{\mathbb{R}^3} (p^2 - \mu)\, \hat{\gamma}(p) \frac{dp}{(2\pi)^3} + \int_{\mathbb{R}^3} |\alpha(x)|^2 V(x)\, dx + \frac{1}{\beta} \int_{\mathbb{R}^3} \operatorname{Tr}_{\mathbb{C}^2}\left[\Gamma(p) \ln \Gamma(p)\right] \frac{dp}{(2\pi)^3}$$

$\Rightarrow$ TRANSLATION INVARIANT BCS FUNCTIONAL

$$\boxed{\mathcal{F}(\Gamma) = \int (p^2 - \mu)\, \hat{\gamma}(p)\, dp + \int |\alpha(x)|^2 V(x)\, dx - \frac{1}{\beta} S(\Gamma)}$$

EXISTENCE of MINIMIZERS

<u>Theorem</u> (Hainzl, Hamza, Seiringer, Solovej 2008)

For $V \in L^{3/2}(\mathbb{R}^3)$, the BCS functional is bounded from below and attains its infimum $(\tilde{\gamma}, \tilde{\alpha})$ on

$$\mathcal{D} = \left\{ \Gamma \;\middle|\; \hat{\gamma} \in L^1(\mathbb{R}^3, (1+p^2)\,dp),\ \alpha \in H^1(\mathbb{R}^3, dx),\ 0 \le \Gamma \le 1 \right\}$$

i.e.

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

Sketch of the proof.

- $\mathcal{F}$ bounded from below

$$\mathcal{F}(\Gamma) \geq C_1 + \frac{3}{4} \int (p^2 - \mu)\, \hat{\gamma}(p)\, dp + \int |\alpha(x)|^2\, V(x)\, dx$$

$$C_1 := \inf_{(\gamma,\alpha) \in \mathcal{D}} \left(\frac{1}{4} \int (p^2 - \mu)\, \hat{\gamma}(p)\, dp - \frac{1}{\beta} S(\Gamma) \right)$$

$$= -\frac{1}{\beta} \int \ln \left(1 + e^{-\frac{\beta}{4}(p^2 - \mu)} \right) dp$$

Since $V \in L^{3/2}$, we have

$$0 \geq \underbrace{\inf \operatorname{spec} \left(\frac{p^2}{4} + V \right)}_{=: C_2} > -\infty \qquad \text{(EXERCISE 5)}$$

Use that $\hat{\gamma}(p) \geq |\hat{\alpha}(p)|^2$

$$\frac{1}{4}\int p^2 \hat{\gamma}(p)\,dp + \int V(x)\,|\alpha(x)|^2\,dx \geq C_2 \int |\hat{\alpha}(p)|^2\,dp \geq C_2 \int \hat{\gamma}(p)\,dp$$

Use that $\hat{\gamma}(p) \leq 1$:

$$\mathcal{F}(\Gamma) \geq -A + \frac{1}{8}\|\alpha\|^2_{H^1(\mathbb{R}^3, dx)} + \frac{1}{8}\|\gamma\|_{L^1(\mathbb{R}^3, (1+p^2)dp)}$$

with $A = -C_1 - \int [p^2/4 - 3\mu/4 - 1/4 + C_2]_-\,dp$

Then $\mathcal{F}(\Gamma)$ is bounded from below.

EXERCISE 6. Show that $\exists$ a minimizer of $\mathcal{F}(\Gamma)$

(Hint: lower semicontinuity of $\mathcal{F}$)

The non-interacting case

If $V=0$, the minimizer of the BCS functional is given by the Fermi-Dirac distribution, i.e.

$$\Gamma = \begin{pmatrix} \gamma_0 & 0 \\ 0 & 1-\gamma_0 \end{pmatrix} \qquad \gamma_0(p) = \frac{1}{1+e^{\beta(p^2-\mu)}}$$

Notice that $\alpha = 0$.

Proof.

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

$$\mathcal{F}(\Gamma) - \mathcal{F}(\Gamma_0) = \frac{1}{2}\int \operatorname{tr}_{\mathbb{C}^2}\left[H_0(p)\left(\Gamma(p) - \Gamma_0(p)\right)\right]dp + \frac{1}{2\beta}\left[S(\Gamma_0) - S(\Gamma)\right]$$

where

$$H_0(p) = \begin{pmatrix} p^2-\mu & 0 \\ 0 & -(p^2-\mu) \end{pmatrix}$$

Then

$$\mathcal{F}(\Gamma) = \mathcal{F}(\Gamma_0) + \frac{1}{2\beta}\mathcal{H}(\Gamma, \Gamma_0)$$

with

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

RELATIVE ENTROPY of Γ w.r.t. Γ_0

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

(EXERCISE 7)

Claim:

$$\Gamma(p) = \Gamma_0(p) \text{ a.e.} \Leftrightarrow \mathcal{H}(\Gamma, \Gamma_0) = 0$$

Lemma 1 (Klein's inequality)

Let A, B self-adjoint operators with spectra $\sigma(A)$, $\sigma(B)$.

Let $\{f_r\}$ and $\{g_r\}$ two families of functions s.t.

$$f_k : \sigma(A) \to \mathbb{C} \qquad g_k : \sigma(B) \to \mathbb{C}$$

and assume

$$\sum_k f_k(a)\, g_k(b) \geq 0 \qquad \forall\, a \in \sigma(A),\ b \in \sigma(B).$$

Then

$$\operatorname{tr}\left[\sum_k f_k(a)\, g_k(b)\right] \geq 0$$

EXERCISE 8

prove the lemma for A, B matrices.

Back to the claim

$$\text{"} \Gamma(p) = \Gamma_0(p) \text{ a.e.} \Leftrightarrow \mathcal{H}(\Gamma, \Gamma_0) = 0 \text{"}$$

we use that

- $x \mapsto \varphi(x)$ is strictly convex
- Klein's inequality

$\Rightarrow$ Γ_0 is the unique minimizer of $\mathcal{F}$ if $V = 0$.

Theorem (Hainzl, Hamza, Seiringer, Solovej 2008)

The following statements are equivalent:

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

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

non vanishing α

(ii) The linear operator

$$K_{\beta,\mu} + V \quad \text{with} \quad K_{\beta,\mu} := \frac{p^2-\mu}{\tanh\left(\frac{p^2-\mu}{2}\beta\right)}$$

effective attractive interaction

has at least one negative eigenvalue.

EXERCISE 9

Compute the second derivative of $\mathcal{F}$ with respect to α in the state $(\gamma_0, 0)$ to obtain $K_{\beta,\mu} + V$.

proof of the Theorem.

$(ii) \Rightarrow (i)$ Exercise 7, together with the observation that $(\gamma_0, 0)$ is a critical point of $\mathcal{F}$, shows that (ii) implies

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

$(i) \Rightarrow (ii)$ we will prove that negative (ii) implies negative (i).

Lemma 2 (Frank, Hainzl, Seiringer, Solovej 2012)

$$\mathcal{H}(\Gamma, \Gamma_0) \geq \int \mathrm{tr}_{\mathbb{C}^2} \left[\frac{\beta H_0(p)}{\tanh(H_0(p)\beta/2)} (\Gamma(p) - \Gamma_0(p))^2 \right] dp$$

(see slide 28 for $\mathcal{H}(\Gamma, \Gamma_0)$)

proof.

Notice that

$$x \ln \frac{x}{y} + (1-x) \ln \frac{(1-x)}{(1-y)} \geq \frac{\ln\left(\frac{1-y}{y}\right)}{1-2y} (x-y)^2 \quad \text{for } 0 < x, y < 1$$

Then, by Klein's inequality, the statement follows.

EXERCISE 10

Rule out the details of the proof of the above lemma.

We are left with the proof of (ii) $\Rightarrow$ (i), equivalently

if $T_{\beta,\mu} + V$ has no negative eigenvalues, than $\mathcal{F}(\gamma, \alpha) \geq \mathcal{F}(\gamma_0, 0)$.

Look at

$$\mathcal{F}(\Gamma) - \mathcal{F}(\Gamma_0) = \frac{1}{2\beta} \mathcal{H}(\Gamma, \Gamma_0) + \int_{\mathbb{R}^3} V(x) |\alpha(x)|^2 dx$$

Lemma 2

$$\geq \int K_{\beta,\mu}(p) \left(\gamma(p) - \gamma_0(p)\right)^2 dp$$

(*) essspec $(K_{\beta,\mu})$ $= [2/\beta, +\infty)$

$$+ \int K_{\beta,\mu}(p) |\hat{\alpha}(p)|^2 dp$$

$$+ \int V(x) |\alpha(x)|^2 dx$$

(*) $K_{\beta,\mu} \geq 2/\beta$

$$\geq \langle \alpha, (K_{\beta,\mu} + V) \alpha \rangle \overset{\text{by assumption}}{\geq} 0$$

Then

$$\mathcal{F}(\Gamma) - \mathcal{F}(\Gamma_0) \geq 0$$

and (i) follows. ■

Remark.

$K_{\beta,\mu}$ is strictly monotone in β, i.e. $\forall \psi \in H^2(\mathbb{R}^3)$

$$\langle \psi, K_{\beta,\mu} \psi \rangle \leq \langle \psi, K_{\beta',\mu} \psi \rangle \quad \text{if } \beta \geq \beta'$$

$\Rightarrow \exists\, \beta_c \geq 0$ s.t. the unique minimizer is $(\gamma_0, 0)$ if $\beta < \beta_c$

and $\exists$ minimizers Γ with $\alpha \neq 0$ if $\beta > \beta_c$.

6. Open Problems

* General setting for $\alpha \neq 0$?

* Dynamics ?

  → Hainzl, Schlein '13

  → Marcantoni, Porta, Sabin '24

  → Chong, Laflèche, C.S. '24

Non-vanishing α : Bogoliubov de Gennes equation