

Magnetic Schrödinger operators and magnetic density functional theory

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Non-magnetic Hamiltonian for N -electrons:

$$H(v) = \underbrace{\sum_{i=1}^N -\frac{1}{2}\Delta_i}_{\text{kinetic energy}} + \underbrace{\sum_{1 \leq i < j \leq N} |\mathbf{r}_i - \mathbf{r}_j|^{-1}}_{\text{interaction energy}} + \underbrace{\sum_{i=1}^N v(\mathbf{r}_i)}_{\text{external potential}} .$$

Example: For Helium placed at the origin,

$$H = \underbrace{-\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2}_{\text{kinetic energy}} + \underbrace{-\frac{2}{|\mathbf{r}_1|} - \frac{2}{|\mathbf{r}_2|}}_{\text{attraction with He}} + \underbrace{\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}}_{\text{electronic interaction}}$$

$H(v)$ is linear and acts on the fermionic space $\bigwedge_{i=1}^N L^2(\mathbb{R}^3)$. Its domain is $\bigwedge_{i=1}^N H^1(\mathbb{R}^3)$:

$$\Psi \in \bigwedge_{i=1}^N H^1(\mathbb{R}^3) \implies \Psi(\mathbf{r}_{p(1)}, \mathbf{r}_{p(2)}, \dots, \mathbf{r}_{p(N)}) = \varepsilon(p)\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N).$$

Problem: Ψ lives in \mathbb{R}^{3N} !

Example: 10 DOFs/direction, Uranium ($N = 92$): $10^{3 \times 92}$ DOFs

Impossible for a computer

- 1 Introduction of the Density Functional Theory
- 2 The question of representability
- 3 Pure states and Mixed states
- 4 The magnetic case

Usually, one main object of interest is the **ground state energy**,

$$E(v) = \min_{\Psi \in \Lambda, H^1, \|\Psi\|_{L^2}=1} \langle \Psi | H(v) | \Psi \rangle.$$

We have

$$\langle \Psi | H(v) | \Psi \rangle = \langle \Psi | T + W | \Psi \rangle + \int_{\mathbb{R}^3} v(\mathbf{r}) \rho(\mathbf{r}) \, d^3\mathbf{r}$$

with the **electronic density**

$$\rho_{\Psi}(\mathbf{r}) := N \int_{\mathbb{R}^{3(N-1)}} |\Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N)|^2 \, d^3\mathbf{r}_2 \dots d^3\mathbf{r}_N$$

so that

$$E(v) = \inf_{\rho \in \mathcal{I}_N} \left\{ \int v\rho + \underbrace{\inf_{\Psi \in \Lambda, H^1(\mathbb{R}^3), \rho_{\Psi}=\rho} \{ \langle \Psi | T + W | \Psi \rangle \}}_{F(\rho)} \right\}$$

Question: What is the set \mathcal{I}_N ?

(question of **representability**)

Theorem (Hohenberg-Kohn 65)

If Ψ_1 (resp. Ψ_2) is a ground state for $H(v_1)$ (resp. $H(v_2)$), with $v_1 \neq v_2$, then $\rho_1 \neq \rho_2$.

Corollary : There exists a map $\rho \rightarrow v \rightarrow \Psi$.

Proof (very easy)

Recall that

$$\langle \Psi | H(v) | \Psi \rangle = \langle \Psi | T + W | \Psi \rangle + \int_{\mathbb{R}^3} v(\mathbf{r}) \rho(\mathbf{r}) d^3\mathbf{r}$$

Assume the **non degeneracy** of the ground state, and suppose that $\rho_1 = \rho_2 := \rho$, so that

$$\langle \Psi_1 | H(v_1) | \Psi_1 \rangle < \langle \Psi_2 | H(v_1) | \Psi_2 \rangle = \langle \Psi_2 | H(v_2) | \Psi_2 \rangle + \langle \Psi_2 | H(v_1) - H(v_2) | \Psi_2 \rangle$$

or

$$E(v_1) < E(v_2) + \int (v_1(\mathbf{r}) - v_2(\mathbf{r})) \rho(\mathbf{r}) d^3\mathbf{r}.$$

In a similar way, we get

$$E(v_2) < E(v_1) + \int (v_2(\mathbf{r}) - v_1(\mathbf{r})) \rho(\mathbf{r}) d^3\mathbf{r}$$

which is a contradiction!

According to the Hohenberg-Kohn theorem, there is a map $\rho \rightarrow \Psi$, so that we can work with the variable $\rho \in L^1(\mathbb{R}^3)$ instead of $\Psi \in \bigwedge_{i=1}^N H^1(\mathbb{R}^3)$:

We have transform the linear problem on a high dimensional space:

$$\inf_{\Psi \in \bigwedge_{i=1}^N H^1(\mathbb{R}^3), \|\Psi\|_{L^2}=1} \{ \langle \Psi | T + W + V | \Psi \rangle \}$$

into the non linear one on a three dimensional space:

$$\inf_{\rho \in \mathcal{I}_N} \left\{ \int v\rho + F(\rho) \right\} \quad \text{with} \quad F(\rho) = \inf_{\Psi \in \bigwedge_{i=1}^N H^1(\mathbb{R}^3), \|\Psi\|_{L^2}=1} \{ \langle \Psi | T + W | \Psi \rangle \}$$

and both problems are equivalent.

Problems:

- We do not know an explicit form for $F(\rho)$
But we know some very accurate approximations of F (large literature).
- We do not know an explicit form for \mathcal{I}_N (question of representability).

What is the space \mathcal{I}_N ?

According to the Hohenberg-Kohn theorem, we should introduce

$$\mathcal{V}_N = \{v \text{ measurable, } H(v) \text{ has a unique ground state}\}$$

and

$$\mathcal{A}_N = \left\{ \Psi \in \bigwedge_{i=1}^N H^1(\mathbb{R}^3), \quad \|\Psi\|_{L^2} = 1, \quad \exists v \in \mathcal{V}_N, \quad \psi \text{ is the ground state of } H(v) \right\}$$

to finally take

$$\mathcal{I}_N^v = \{ \rho \in L^1(\mathbb{R}^3), \quad \exists \Psi \in \mathcal{A}_N, \quad \rho = \rho_\Psi \}.$$

This problem is called the **v-representability**, and is very difficult. We prefer to take the **N-representability**:

$$\mathcal{I}_N = \left\{ \rho \in L^1(\mathbb{R}^3), \quad \exists \Psi \in \bigwedge_{i=1}^N H^1(\mathbb{R}^3), \quad \|\Psi\|_{L^2} = 1, \quad \rho = \rho_\Psi \right\}$$

Remark : Of course, $\mathcal{I}_N^v \subsetneq \mathcal{I}_N$, so that

$$\inf_{\rho \in \mathcal{I}_n} F(\rho) \leq \inf_{\rho \in \mathcal{I}_n^v} F(\rho)$$

Theorem (Gilbert '75, Lieb '81)

$$\mathcal{I}_N = \left\{ \rho \in L^1(\mathbb{R}^3) \cap L^3(\mathbb{R}^3), \quad \rho \geq 0, \quad \int \rho = N, \quad \sqrt{\rho} \in H^1(\mathbb{R}^3) \right\}.$$

Remarks:

- \mathcal{I}_N is a convex set (while \mathcal{I}_N^v is not).
- $F(\rho)$ is well-defined on \mathcal{I}_n :

$$F(\rho) = \inf_{\Psi, \Psi \rightarrow \rho} \langle \Psi | T + W | \Psi \rangle$$

Theorem (Gilbert '75, Lieb '81)

$$\mathcal{I}_N = \left\{ \rho \in L^1(\mathbb{R}^3) \cap L^3(\mathbb{R}^3), \quad \rho \geq 0, \quad \int \rho = N, \quad \sqrt{\rho} \in H^1(\mathbb{R}^3) \right\}.$$

Idea of the proof (Harriman).

If $\{\Phi_1, \dots, \Phi_N\}$ is in H^1 and is a L^2 -orthonormal, then

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \det(\Phi_i(\mathbf{r}_j))_{1 \leq i, j \leq N} \quad \text{satisfies} \quad \Psi \in \bigwedge_{i=1}^N H^1(\mathbb{R}^3) \quad \text{and} \quad \|\Psi\|_{L^2} = 1.$$

For this Ψ , we can calculate

$$\rho_\Psi(\mathbf{r}) = \sum_{i=1}^N |\Phi_i(\mathbf{r})|^2$$

We choose

$$\Phi_k(\mathbf{r}) = \sqrt{\frac{\rho(\mathbf{r})}{N}} \cdot \exp(2\pi i k f(\mathbf{r}))$$

where f is carefully chosen to ensure orthogonality.

We want to do the same work for the magnetic case

We want to do the same work for the magnetic case
Before that, let us introduce some new mathematical objects

For $\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \in \bigwedge_{i=1}^N H^1(\mathbb{R}^3)$ such that $\|\Psi\|_{L^2} = 1$, we introduce the **one body density matrix**

$$\gamma_{\Psi}(x, y) = N \int_{\mathbb{R}^{3(N-2)}} \Psi(x, x_2, \dots, x_N) \overline{\Psi(y, x_2, \dots, x_N)} dx_2 \dots dx_N$$

Remarks:

- We have $\rho_{\Psi}(x) = \gamma_{\Psi}(x, x)$
- $\gamma(y, x) = \overline{\gamma(x, y)}$
- $\int \gamma(x, x) = N$

Now, we think of γ as an operator acting on $L^2(\mathbb{R}^3)$ via

$$(\gamma f)(x) = \int_{\mathbb{R}^3} \gamma(x, y) f(y) dy.$$

Example: If $\Psi(x_1, \dots, x_N) = \frac{1}{\sqrt{N}} \det(\Phi_i(x_j))$, then

$$\gamma(x, y) = \sum_{i=1}^N \Phi_i(x) \overline{\Phi_i(y)}$$

and, as an operator, γ is the projector on the space spanned by $\{\Phi_1, \dots, \Phi_n\}$.

The set of γ we can obtain with this method is the set of projectors on N -dimensional subspace of $H^1(\mathbb{R}^3)$:

$$\gamma \in \mathcal{P}_N := \{\gamma \in \mathcal{S}(L^2(\mathbb{R}^3)), \quad \gamma \text{ is a projector,} \quad \text{Tr}(\gamma) = N, \quad \text{Tr}(-\Delta\gamma) < \infty\}$$

where

$$\text{Tr}(\gamma) = \int_{\mathbb{R}^3} \gamma(x, x) dx \quad \text{and} \quad \text{Tr}(-\Delta\gamma) = \sum_{i=1}^N \|\nabla\Phi_i\|_{L^2}^2.$$

Now, note that the map $\gamma \rightarrow \rho$ is linear ($\rho(x) = \gamma(x, x)$), and that, according to **N -representability**, the image of \mathcal{P}_N is exactly \mathcal{I}_N . Because \mathcal{I}_N is a convex set, the image of the convex hull of \mathcal{P}_N is also \mathcal{I}_N .

We define the **set of mixed states** as the convex hull of \mathcal{P}_N :

$$\mathcal{D}_N := \{\gamma \in \mathcal{S}(L^2(\mathbb{R}^3)), \quad 0 \leq \gamma \leq 1, \quad \text{Tr}(\gamma) = N, \quad \text{Tr}(-\Delta\gamma) < \infty\}$$

This space is very useful for **finite temperature systems**: it allows Boltzmann statistic superposition of states (different from quantum superposition).

Set of **mixed states**:

$$\mathcal{D}_N := \{\gamma \in \mathcal{S}(L^2(\mathbb{R}^3)), \quad 0 \leq \gamma \leq 1, \quad \text{Tr}(\gamma) = N, \quad \text{Tr}(-\Delta\gamma) < \infty\}$$

According to the spectral theorem, we can write, for $\gamma \in \mathcal{D}_N$,

$$\gamma(x, y) = \sum_{i=1}^{\infty} n_i \Phi_i(x) \overline{\Phi_i(y)}, \quad 0 \leq n_i \leq 1, \quad \sum_{i=1}^{\infty} n_i = N$$

where Φ_i is a base of $H^1(\mathbb{R}^3)$ (for the L^2 scalar product).

With this notation,

$$\rho(x) = \sum_{i=1}^{\infty} n_i |\phi(x)|^2 \quad \text{and} \quad \text{Tr}(-\Delta\gamma) = \sum_{i=1}^{\infty} n_i \|\nabla\Phi_i\|_{L^2}^2$$

Remark: The condition $0 \leq n_i \leq 1$ may be interpreted as the **Pauli principle**, stating that maximum one fermion can be at a given state.

It is useful to work with mixed states, and \mathcal{D}_N is convex while \mathcal{P}_N is not

Finally, we can see how to translate the DFT arguments into Hamiltonian with a magnetic field

According to the **Dirac equation**, the Hamiltonian for N -electrons is

$$H(v, \mathbf{A}) = \underbrace{\sum_{i=1}^N \frac{1}{2} \left(\sigma_i \cdot \left(-i\nabla_i + \frac{1}{c} \mathbf{A}(\mathbf{r}_i) \right) \right)^2}_{\text{kinetic energy}} + \underbrace{\sum_{1 \leq i < j \leq N} |\mathbf{r}_i - \mathbf{r}_j|^{-1}}_{\text{interaction energy}} + \underbrace{\sum_{i=1}^N v(\mathbf{r}_i)}_{\text{external potential}}$$

It is linear, and acts on the fermionic space $\bigwedge_{i=1}^N H^1(\mathbb{R}^3, \mathbb{C}^2)$:

$$\Psi \in \bigwedge_{i=1}^N H^1(\mathbb{R}^3, \mathbb{C}^2) \text{ has } 2^N \text{ components: } \begin{pmatrix} \Psi(\mathbf{r}_1, \uparrow, \mathbf{r}_2, \uparrow, \dots, \mathbf{r}^N, \uparrow) \\ \Psi(\mathbf{r}_1, \uparrow, \mathbf{r}_2, \uparrow, \dots, \mathbf{r}^N, \downarrow) \\ \vdots \\ \Psi(\mathbf{r}_1, \downarrow, \mathbf{r}_2, \downarrow, \dots, \mathbf{r}^N, \downarrow) \end{pmatrix}$$

and still satisfies

$$\Psi(\mathbf{r}_{p(1)}, \alpha_{p(1)}, \mathbf{r}_{p(2)}, \alpha_{p(2)}, \dots, \mathbf{r}_{p(N)}, \alpha_{p(N)}) = \varepsilon(p) \Psi(\mathbf{r}_1, \alpha_1, \mathbf{r}_2, \alpha_2, \dots, \mathbf{r}_N, \alpha_N).$$

\mathbf{A} is the magnetic **potential vector** (recall that $\text{rot}(\mathbf{A}) = \mathbf{B}$ is the magnetic field), and σ_i contains the **Pauli-matrices** acting on the i -th spin.

We changed the **Hilbert space**, it is now

$$\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^2) := \{\Phi = (\phi^\uparrow, \phi^\downarrow) \in L^2(\mathbb{R}^3), \quad \|\Phi\|_{\mathcal{H}} < \infty\}$$

with

$$\langle \Phi | \Psi \rangle = \int_{\mathbb{R}^3} \left(\overline{\phi^\uparrow}(x) \psi^\uparrow(x) + \overline{\phi^\downarrow}(x) \psi^\downarrow(x) \right) dx.$$

For instance, for one-body density matrices are acting on this Hilbert space. We write

$$\gamma(x, y) = \begin{pmatrix} \gamma^{\uparrow\uparrow} & \gamma^{\uparrow\downarrow} \\ \gamma^{\downarrow\uparrow} & \gamma^{\downarrow\downarrow} \end{pmatrix} (x, y) \quad \text{with} \quad \gamma^{\alpha\beta}(x, y) = \gamma(x\alpha, y\beta) = \sum_{i=1}^{\infty} n_i \phi_i^\alpha(x) \overline{\phi_i^\beta(y)}$$

and the set of mixed states is

$$\tilde{\mathcal{D}}_N := \{\gamma \in \mathcal{S}(L^2(\mathbb{R}^3, \mathbb{C}^2)), \quad 0 \leq \gamma \leq 1, \quad \text{Tr}(\gamma) = N, \quad \text{Tr}(-\Delta\gamma) < \infty\}.$$

The **Pauli matrices** are also acting on this Hilbert space. We have

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

This time, we write :

$$\langle \Psi | H(v, \mathbf{A}) | \Psi \rangle = \langle \Psi | T + W | \Psi \rangle + \int \left(v(\mathbf{r}) + \frac{1}{2} \frac{|\mathbf{A}(\mathbf{r})|^2}{c^2} \right) \rho(\mathbf{r}) d^3 \mathbf{r} + \int_{\mathbb{R}^3} \mathbf{A}(\mathbf{r}) \cdot \mathbf{j}_p(\mathbf{r}) d^3 \mathbf{r} + \mu_B \int_{\mathbb{R}^3} \mathbf{B}(\mathbf{r}) \cdot \mathbf{m}(\mathbf{r}) d^3 \mathbf{r}$$

where new objects have appeared:

- ρ is still the **electronic density**
- \mathbf{j}_p is the **paramagnetic current**
- \mathbf{m} is the **spin density**

$$\left\{ \begin{array}{l} \rho(x) = \gamma^{\uparrow\uparrow}(x, x) + \gamma^{\downarrow\downarrow}(x, x) = \sum n_i \left(|\phi_k^{\uparrow}(x)|^2 + |\phi_k^{\downarrow}(x)|^2 \right) \\ \mathbf{j}_p(x) = \text{Im} \left(\nabla_2 \gamma^{\uparrow\uparrow}(x, x) + \nabla_2 \gamma^{\downarrow\downarrow}(x, x) \right) = \sum n_i \text{Im} \left(\phi^{\uparrow}(x) \nabla \overline{\phi_i^{\uparrow}(x)} + \dots \right) \\ \mathbf{m}_z = \gamma^{\uparrow\uparrow}(x, x) - \gamma^{\downarrow\downarrow}(x, x) = \sum n_i \left(|\phi_k^{\uparrow}(x)|^2 - |\phi_k^{\downarrow}(x)|^2 \right) \\ \mathbf{m}_x = \gamma^{\uparrow\downarrow}(x, x) + \gamma^{\downarrow\uparrow}(x, x) = 2 \sum n_i \text{Re} \left(\phi_i^{\uparrow}(x) \overline{\phi_i^{\downarrow}(x)} \right) \\ \mathbf{m}_y = -i \left(\gamma^{\uparrow\downarrow}(x, x) - \gamma^{\downarrow\uparrow}(x, x) \right) = -2 \sum n_i \text{Im} \left(\phi_i^{\uparrow}(x) \overline{\phi_i^{\downarrow}(x)} \right) \end{array} \right.$$

Recall that \mathbf{A} and \mathbf{B} satisfy $\mathbf{B} = \text{rot } \mathbf{A}$. However, as \mathbf{A} acts on the orbitals, whereas \mathbf{B} acts on the spin, we usually study the two effects separately and choose:

- $\mathbf{A} = \mathbf{0}$ and $\mathbf{B} \neq \mathbf{0}$ for spin effects. **Spin Density Functional Theory** (SDFT).
- $\mathbf{B} = \mathbf{0}$ and $\mathbf{A} \neq \mathbf{0}$ for orbital effects. **Current Density Functional Theory** (CDFT).

In this presentation, I will present SDFT:

$$\langle \Psi | H(v, \mathbf{B}) | \Psi \rangle = \langle \Psi | T + W | \Psi \rangle + \int_{\mathbb{R}^3} v(\mathbf{r}) \rho(\mathbf{r}) d^3 \mathbf{r} + \mu_B \int_{\mathbb{R}^3} \mathbf{B}(\mathbf{r}) \cdot \mathbf{m}(\mathbf{r}) d^3 \mathbf{r}$$

For $\Psi \in \bigwedge_{i=1}^N H^1(\mathbb{R}^3)$, we introduce

$$R_\Psi(\mathbf{r}) = \begin{pmatrix} \rho^{\uparrow\uparrow}(\mathbf{r}) & \rho^{\uparrow\downarrow}(\mathbf{r}) \\ \rho^{\downarrow\uparrow}(\mathbf{r}) & \rho^{\downarrow\downarrow}(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} \gamma^{\uparrow\uparrow}(\mathbf{r}, \mathbf{r}) & \gamma^{\uparrow\downarrow}(\mathbf{r}, \mathbf{r}) \\ \gamma^{\downarrow\uparrow}(\mathbf{r}, \mathbf{r}) & \gamma^{\downarrow\downarrow}(\mathbf{r}, \mathbf{r}) \end{pmatrix}.$$

Then, R_Ψ is hermitian, positive, satisfies $\int \text{Tr}(R_\Psi) = N$, and we have

$$\langle \Psi | H(v, \mathbf{B}) | \Psi \rangle = \langle \Psi | T + W | \Psi \rangle + \int_{\mathbb{R}^3} \text{Tr} \left(\underbrace{\begin{pmatrix} v + \mu_B \mathbf{B}_z & \mu_B \mathbf{B}_x + i\mu_B \mathbf{B}_y \\ \mu_B \mathbf{B}_x - i\mu_B \mathbf{B}_y & v - \mu_B \mathbf{B}_z \end{pmatrix}}_{\mathcal{V}(v, \mathbf{B})}(\mathbf{r}) R_\Psi(\mathbf{r}) \right)$$

Similarly to standard DFT, we write:

$$E(v, \mathbf{B}) := \inf_{\Psi \in \wedge^N H^1(\mathbb{R}^3, \mathbb{C}^2), \|\Psi\|=1} \langle \Psi | H(v, \mathbf{B}) | \Psi \rangle = \inf_{R \in \mathcal{J}_N} \{F(R) + (\mathcal{V}(v, \mathbf{B}) | R)\}$$

with

$$F(R) := \inf_{\Psi \in \wedge^N H^1(\mathbb{R}^3, \mathbb{C}^2), \|\Psi\|=1, R_\Psi=R} \langle \Psi | T + W | \Psi \rangle$$

Problems

- We still do not know the functional F .
- What is the set \mathcal{J}_N ?

We are looking for N -representability, i.e.

$$\mathcal{J}_N^p := \left\{ R \in \mathcal{M}_{2 \times 2}(L^1(\mathbb{R}^3)), \quad \exists \Psi \in \bigwedge^N H^1(\mathbb{R}^3, \mathbb{C}^2), \quad \|\Psi\| = 1, \quad R = R_\Psi \right\} \text{ (pure states)}$$

or

$$\mathcal{J}_N^m := \left\{ R \in \mathcal{M}_{2 \times 2}(L^1(\mathbb{R}^3)), \quad \exists \gamma \in \tilde{\mathcal{D}}_N, \quad R = R_\gamma \right\} \text{ (mixed states)}$$

We recall that, by definition, \mathcal{J}_N^m is the convex hull of \mathcal{J}_N^p .

Remark:

- For $N = 1$, \mathcal{J}_1^p only contains rank-1 matrices, while \mathcal{J}_1^m contains more matrices.

We chose to work with mixed states only (and the proof is easier, due to convexity)

Theorem

$$\mathcal{J}_N^m = \left\{ R \in \mathcal{M}_{2 \times 2}(L^1(\mathbb{R}^3)), R \text{ is hermitian positive, } \int \text{Tr}(R) = N, \sqrt{R} \in \mathcal{M}_{2 \times 2}(H^1(\mathbb{R}^3)) \right\}$$

- The $\sqrt{}$ is in the hermitian matrices sense
- Very beautiful analog of the previous DFT ($\{\rho, \dots, \sqrt{\rho} \in H^1(\mathbb{R}^3)\}$).

Idea of the proof

- Construct representability for rank-1 matrices using the previous construction.
- Show that all $R \in \mathcal{J}_N^m$ is the convex combination of two matrices of rank-one.
- Use convexity to conclude.

Remark

The fact that this \mathcal{J}_N^m is a convex set is not obvious. Actually, I cannot prove it!

Future work

- Do the proof for CDFT: N -representability for (ρ, \mathbf{j}_ρ) .
- Study the model with some used approximations of $F(R)$

For this point, the problem is not convex. For instance, for the free spinless electron gas, we have the translational invariant problem:

$$\mathcal{E}(\gamma) = \frac{1}{2} \text{Tr}(-\Delta\gamma) + \int \int \frac{\rho(x)\rho(y)}{|x-y|} dx dy - c_x \int \rho^{4/3} + \underbrace{\int V_0 \rho}_{=cst}$$

and we can prove the following two facts:

- If V_0 is large enough, then the gas is the only minimizer
- If V_0 is small enough, then the gas is not the minimizer (Wigner crystals)

THANK YOU FOR YOUR ATTENTION