Stability of matter p. 8

12. Pauli's principle
13. Ideal Fermi gas
14. Kinetic LT for anti-symmetric fcts.

12. Pauli's exclusion principle

The Pauli exclusion principle states that "two quantum particles cannot occupy the same quantum state"

In a traditional QM course this is said to be a consequence of the anti-symmetry of the wave function, that is if $x_i = x_j$, $i \neq j$ then

$$\Psi_N(x_1, \dots, x_i, \dots, x_j, \dots, x_N) = -\Psi_N(x_1, \dots, x_j, \dots, x_i, \dots, x_N) = 0$$

However, there is more that follows from anti-symmetry of the wave function than the vanishing on the diagonal set.

Thm (Pauli's exclusion principle)

For any normalized wave function $\Psi_N \in L^2_a(\mathbb{R}^{dN})$, we have

$$\boxed{0 \leq \gamma^{(1)}_{\Psi_N} \leq 1 \quad \text{on } L^2(\mathbb{R}^d)}$$

Remarks

- without the anti-symmetry assumption, $\gamma^{(1)}_{\Psi_N}$ may have an eigenvalue as large as N. In fact if $\Psi_N(x_1, \dots, x_N) = u(x_1) \dots u(x_N)$, $\|u\|_2 = 1$,

then
$$\gamma^{(1)}_{\Psi_N} = N|u\rangle\langle u| \quad (\rightsquigarrow \text{Bose-Einstein Condensation})$$

•) Recall that if $\{u_i\}_{i=1}^N$ - ON and $\Psi_N = u_1 \wedge \dots \wedge u_N$,
then
$$\gamma^{(1)}_{\Psi_N} = \sum_{i=1}^N |u_i\rangle\langle u_i|$$

Thus, $f \in L^2(\mathbb{R}^d)$, $f = \sum_i a_i u_i$, $\sum |a_i|^2 = 1$

$$\Rightarrow \quad \langle f, \gamma^{(1)}_{\Psi_N} f\rangle = \sum_{i=1}^N |a_i|^2 \leq 1.$$

Proof of theorem

Note that
$$\langle u, \gamma^{(1)}_{\Psi_N} u\rangle = \langle \Psi_N, \sum_{j=1}^N (P_u)_{x_j} \Psi_N\rangle, \quad P_u = |u\rangle\langle u|$$

Indeed
$$LHS = \iint \bar{u}(x)\, \gamma(x,y)\, u(y)\, dy\, dx =$$
$$= N \int\int \bar{u}(x) u(y)\, \Psi(x, x_2, \dots, x_N) \overline{\Psi(y, x_2, \dots, x_N)}\, dx_2 \dots dx_N$$

RHS =
$$\int \cdots \int \overline{\Psi(x_1, \dots, x_N)} \sum_j u(x_j) \bar{u}(y) \Psi(x_1, \dots, \overset{j}{\downarrow}{y}, \dots, x_N)$$
$$= \int \cdots \int \bar{\Psi}(x_1, \dots, x_N)\, u(x_1)\, \bar{u}(y)\, \Psi(y, x_2, \dots, x_N)$$
$$+ \int \cdots \int \bar{\Psi}(x_1, \dots, x_N)\, u(x_2)\, \bar{u}(y)\, \Psi(x_1, y, x_3, \dots, x_N)$$
$$+ \cdots + \int \cdots \int \bar{\Psi}(x_1, \dots, x_N)\, u(x_N)\, \bar{u}(y)\, \Psi(x_1, \dots, x_{N-1}, y)$$
$$= N \int \cdots \int \bar{\Psi}(y, x_2, \dots, x_N)\, \Psi(x_1, x_2, \dots, x_N)\, \bar{u}(x)\, u(y) = LHS$$

Thus we need to prove that

$$A = \sum_{j=1}^{N} (P_u)_{x_j} \leq 1 \quad \text{on} \quad L^2_a(\mathbb{R}^{dN})$$

Take an ONB $\{u_i\}_{i=1}^{\infty}$ for $L^2(\mathbb{R}^d)$ such that $u_1 = u$.
We claim that

$$A = \sum_{1 = i_1 < i_2 < \dots < i_N} |u_{i_1} \wedge \dots \wedge u_{i_N} \rangle \langle u_{i_1} \wedge \dots \wedge u_{i_N}|$$

and the result then follows from the fact that Slater determinants form an ONB for $L^2_a(\mathbb{R}^{dN})$. Indeed, for every $1 \leq i_1 < i_2 < \dots < i_N$ we have

$$A\, u_{i_1} \wedge \dots \wedge u_{i_N} = \sum_{j=1}^{N} (P_u)_{x_j} \sum_{\sigma \in S_N} \frac{1}{\sqrt{N!}} \operatorname{sign}(\sigma) u_{i_{\sigma(1)}}(x_1) \dots u_{i_{\sigma(N)}}(x_N)$$

$$= \sum_{j=1}^{N} \sum_{\sigma \in S_N} \frac{\operatorname{sign}(\sigma)}{\sqrt{N!}} u_{i_{\sigma(1)}}(x_1) \dots \left(P_u u_{i_{\sigma(j)}}(x_j) \right) \dots u_{i_{\sigma(N)}}(x_N)$$

$$= \sum_{j=1}^{N} \sum_{\sigma \in S_N} \frac{1}{\sqrt{N!}} \operatorname{sign}(\sigma) u_{i_{\sigma(1)}}(x_1) \dots \left(\delta_{1, i_{\sigma(j)}} u_{i_{\sigma(j)}}(x_j) \right) \dots u_{i_{\sigma(N)}}(x_N)$$

$$= \mathbb{1}(1 \in \{i_1, \dots, i_N\}) \sum_{\sigma \in S_N} \frac{1}{\sqrt{N!}} \operatorname{sign}(\sigma) u_{i_{\sigma(1)}}(x_1) \dots u_{i_{\sigma(N)}}(x_N)$$

$$= \begin{cases} u_{i_1} \wedge \dots \wedge u_{i_N} & 1 = i_1 \\ 0 & \text{otherwise} \end{cases}$$

$\blacksquare$

The following result tells that the condition $0 \leq \gamma \leq 1$ in Pauli's exclusion principle is optimal.

Thm (Coleman 1963)

Let γ be a trace class operator on $L^2(\mathbb{R}^d)$ such that $0 \leq \gamma \leq 1$ on $L^2(\mathbb{R}^d)$, $\mathrm{Tr}\,\gamma = N \in \mathbb{N}$. Then there exists a mixed state Γ_N on $L^2_a(\mathbb{R}^{dN})$, namely a non-negative operator on $L^2_a(\mathbb{R}^{dN})$ with $\mathrm{Tr}\,\Gamma_N = 1$, such that its one-body density matrix $\Gamma_N^{(1)} = \gamma$.

(here $\Gamma_N^{(1)} = N \mathrm{Tr}_{2 \to N} \Gamma_N$)

$\boxtimes$

Remarks

- If γ is a projection, namely $\gamma = \gamma^2$, then Γ_N can be chosen to be a pure state $\Gamma_N = |\varphi_N\rangle\langle\varphi_N|$ and φ_N is a Slater determinant.

- In general, it might not be possible to choose Γ_N to be a pure state.

$\boxtimes$

In general, one can also define higher order reduced density matrices. For example, if φ_N is a normalized wave function in $L^2_a(\mathbb{R}^{dN})$, then the two-body reduced density matrix $\gamma^{(2)}_{\varphi_N}$ is a trace class operator on $L^2_a(\mathbb{R}^{2d})$ with kernel

$$\gamma^{(2)}_{\psi_N}(x_1, x_2; y_1, y_2) = \frac{N(N-1)}{2} \int_{\mathbb{R}^{d(N-2)}} \psi_N(x_1, x_2, x_3, \dots, x_N) \overline{\psi_N(y_1, y_2, x_3, \dots, x_N)} \, dx_3 \dots dx_N$$

then for every two-body operator W on $L^2_a(\mathbb{R}^{2d})$ we can write

$$\langle \psi_N, \sum_{1 \le i < j \le N} w_{ij} \psi_N \rangle = \mathrm{Tr}\,(W \gamma^{(2)}_{\psi_N}).$$

For general mixed states

$$\gamma^{(2)}_{\Gamma_N} = \frac{N!}{(N-2)!} \mathrm{Tr}^{(N-2)} \Gamma_N$$

k-th reduced density matrix:

$$\gamma^{(k)}_{\Gamma_N} = \frac{N!}{(N-k)!} \mathrm{Tr}^{(N-k)} \Gamma_N$$

In practice, these are much harder to use because there is no complete characterization for $p > 1$ reduced density matrices.

This is the so-called N-representability problem: how to recognize whether a given pth-order reduced density matrix is derivable from an anti-symmetric N-particle wave function / N-body state.

13. Ideal Fermi gas

The Hamiltonian of a non-interacting Fermi gas is of the form

$$H_N = \sum_{i=1}^{N} h_i \quad \text{on} \quad L^2(\mathbb{R}^{dN}).$$

Thm Assume the one-body Hamiltonian h has at least N negative eigenvalues $e_0 \leq \dots \leq e_{N-1}$. Then the ground state energy of H_N is

$$E_N = \sum_{j=0}^{N-1} e_j.$$

Proof

Recall that

$$\langle \psi_N, \sum_{i=1}^{N} h_i \psi_N \rangle = \mathrm{Tr}\left(h \gamma_{\psi_N}^{(1)} \right)$$

Since $\gamma_{\psi_N}^{(1)}$ is positive and trace class, there exist ONB $\{u_i\}$ such that

$$\gamma_{\psi_N}^{(1)} = \sum \lambda_i |u_i\rangle\langle u_i|, \quad \sum \lambda_i = N, \ \lambda_i \geq 0.$$

We obtain

$$\mathrm{Tr}\left(h \gamma_{\psi_N}^{(1)} \right) \geq \inf \left\{ \sum_{i=1}^{\infty} \lambda_i \langle u_i, h u_i \rangle \right\} =$$

$$= \inf \left\{ \sum_{i=1}^{N} \langle u_i, h u_i \rangle \right\} = e_0 + \dots + e_{N-1}.$$

For an upper bound we consider the Slater determinant

$$\varphi_N = u_1 \wedge \dots \wedge u_N \,,$$ where u_i's are

eigenfunctions corresponding to the energies $e_0, \dots, e_{N-1}$.

We have

$$E_N \leq \langle u_1 \wedge \dots \wedge u_N, H_N\, u_1 \wedge \dots \wedge u_N \rangle = \mathrm{Tr}\left(h\, \gamma^{(1)}_{u_1 \wedge \dots \wedge u_N}\right) =$$

$$= \mathrm{Tr}\left(h \sum_{i=1}^{N} |u_i\rangle\langle u_i|\right) = \sum_{i=1}^{N} \langle u_i, h u_i \rangle = \sum_{j=0}^{N-1} e_j .$$

∎

Exemple

$$H_N = \sum_{i=1}^{N} \left(-\Delta_{x_i} + \frac{N}{|x_i|}\right) \quad \text{on} \quad L^2_a(\mathbb{R}^{3N}).$$

Then

$$E_N = -N^{7/3}\left(\frac{\sqrt[3]{3}}{4} + o(1)_N\right) \quad \text{as } N \to \infty$$

Indeed, we know that the spectrum of $-\Delta + \frac{N}{|x|}$ is of the form $-\frac{N^2}{4k^2}$ with multiplicity k^2, $k = 1, 2, \dots$

Because of degeneracy!

$$N = 1 + 2^2 + \dots + M^2 + M' \,, \quad 0 \leq M' < (M+1)^2$$

Then

$$E_N = \sum_{k=1}^{M} -\frac{N^2}{4k^2}\cdot k^2 - \frac{M' N^2}{4(M+1)^2} = -\frac{MN^2}{4} - \frac{M' N^2}{4(M+1)^2}$$

Using:

$$1^2 + 2^2 + \dots + M^2 = \frac{M(M+1)(2M+1)}{6} \implies M = (3N)^{1/3} + o(N)$$

$$\implies E_N = -N^{7/3}\left(\frac{3^{1/3}}{4} + o(1)\right)_{N \to \infty}$$

14. Kinetic LT inequality for antisymmetric fcts

Recall the kinetic LT inequality:

$$\sum_{n=1}^{N} \int_{\mathbb{R}^d} |\nabla u_n|^2 \, dx \geq K \int_{\mathbb{R}^d} \Big(\sum_{n=1}^{N} |u_n(x)|^2 \Big)^{1+\frac{2}{d}} dx.$$

Proposition

One has

$$\sum_{n=1} \nu_n \int_{\mathbb{R}^d} |\nabla u_n|^2 \, dx \; \|\nu\|_\infty^{2/d} \geq K \int_{\mathbb{R}^d} \Big(\sum_n \nu_n |u_n|^2 \Big)^{1+\frac{2}{d}} dx$$

$\forall \; 0 \leq \nu \in \ell^1(\mathbb{N})$ and $L^2(\mathbb{R}^d)$-ON u_n's.

Proof: Write $M := \|\nu\|_\infty$ and observe that

$$\sum_n \nu_n \|\nabla u_n\|^2 = \int_0^M \sum_{\nu_n > \tau} \|\nabla u_n\|^2 \, d\tau$$

(layer cake with discrete measure). For each fixed $\tau > 0$ we have

$$\sum_{\nu_n > \tau} \|\nabla u_n\|^2 \geq K \int_{\mathbb{R}^d} \Big(\sum_{\nu_n > \tau} |u_n|^2 \Big)^{1+\frac{2}{d}} dx$$

and consequently

$$\sum_n \nu_n \|\nabla u_n\|^2 \geq K \int_{\mathbb{R}^d} \int_0^M \Big(\sum_{\nu_n > \tau} |u_n|^2 \Big)^{1+\frac{2}{d}} d\tau \, dx$$

We now have by Hölder's inequality

$$M^{-\frac{2}{d}} \left(\sum_n \nu_n |u_n|^2 \right)^{1+\frac{2}{d}} = M^{-\frac{2}{d}} \left(\int_0^M \sum_{\nu_n > \tau} |u_n|^2 \, d\tau \right)^{1+\frac{2}{d}}$$

$$\leq M^{-\frac{2}{d}} M^{\frac{1}{\alpha}(1+\frac{2}{d})} \int_0^M \left(\sum_{\nu_n > \tau} |u_n|^2 \right)^{1+\frac{2}{d}}$$

where $\frac{1}{\alpha} + \frac{1}{1+\frac{2}{d}} = 1 \Rightarrow \frac{1}{\alpha} = 1 - \frac{d}{d+2} = \frac{2}{d+2}$

$$\Rightarrow \frac{1}{\alpha}\left(1+\frac{2}{d}\right) = \frac{2}{d+2} \frac{d+2}{d} = \frac{2}{d} \Rightarrow M^{-\frac{2}{d}} M^{\frac{1}{\alpha}(1+\frac{2}{d})} = 1$$

$$\Rightarrow \int_0^M \left(\sum_{\nu_n > \tau} |u_n|^2 \right)^{1+\frac{2}{d}} \geq M^{-2/d} \left(\sum_\nu \nu_n |u_n|^2 \right)^{1+\frac{2}{d}}$$

$\square$

Corollary

Let $\gamma \geq 0$ be a trace class operator on $L^2(\mathbb{R}^d)$ then one has

$$(\mathrm{Tr}\,(-\Delta)\gamma)\, \|\gamma\|_1^{2/d} \geq K_d \int_{\mathbb{R}^d} \rho_\gamma(x)^{1+2/d}\, dx$$

Here we use the definition $\mathrm{Tr}\,(-\Delta)\gamma = \sum_j \nu_j \|\nabla \varphi_j\|^2$ and $\rho_\gamma = \sum_j \nu_j |\varphi_j|^2$ for $\gamma = \sum_j \nu_j |\varphi_j\rangle\langle\varphi_j|$

$\square$

We immediately recognize the crucial role of the antisymmetry of ψ_N or rather the bound

$$\|\gamma\|_1 \le 1 .$$

Indeed, recall the (bosonic) Hartree state

$$\psi_N(x_1, \dots, x_N) = u(x_1) \cdots u(x_N)$$

then $\gamma_{\psi_N} = N |u\rangle\langle u|$ and $\|\gamma_{\psi_N}\|_1 = N$

$$\Rightarrow \left(\mathrm{Tr}(-\Delta)\gamma\right) \ge N^{-2/d} K_d \int \rho_\gamma(x)^{1+2/d} \, dx .$$

which becomes obvious for $N \to \infty$.