4 Many-body quantum mechanics and stability of the second kind

- State space of N (spinless) electrons: $L^2(\mathbb{R}^{3N};\mathbb{C})$

namely $L^2(\mathbb{R}^{3N},\mathbb{C}) = \bigotimes_{i=1}^{N} L^2(\mathbb{R}^3)$

Generally: the Hilbert space of the joint system made up of two subsystems with Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$ is

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$$

Universal property: $\mathcal{H}$ is so that for every bilinear map $b: \mathcal{H}_1 \times \mathcal{H}_2 \to K$ there is a unique linear map $\ell: \mathcal{H} \to K$

$$\begin{tikzcd} \mathcal{H}_1 \times \mathcal{H}_2 \arrow[r, "b"] \arrow[d, "\otimes"] & K \\ \mathcal{H}_1 \otimes \mathcal{H}_2 \arrow[ur, "\ell"'] & \end{tikzcd}$$

Note: this determines $\mathcal{H}$ up to isomorphism.

(i)

$$\begin{tikzcd} & \mathcal{H} \arrow[d, dashed, "\ell"] \\ \mathcal{H}_1 \times \mathcal{H}_2 \arrow[ur, "\otimes"] \arrow[r, "\otimes'"'] & \mathcal{H}' \end{tikzcd}$$

use this as b above to get linear $\ell: \mathcal{H} \to \mathcal{H}'$

(ii) invert roles of $\mathcal{H}$ and $\mathcal{H}'$: $\ell': \mathcal{H}' \to \mathcal{H}$

$\Rightarrow$ $\ell' \circ \ell$ is a linear map on $\mathcal{H}$ s.t.

$$(\ell' \circ \ell) \circ \otimes = \ell' \circ \otimes' = \otimes$$

But $\mathrm{id}_{\mathcal{H}}: \mathcal{H} \to \mathcal{H}$ satisfies the same property

by uniqueness
$$\left(\begin{tikzcd} \mathcal{H}_1 \times \mathcal{H}_2 \arrow[r, "\otimes"] \arrow[d, "\otimes"] & \mathcal{H}_1 \otimes \mathcal{H}_2 \\ \mathcal{H}_1 \otimes \mathcal{H}_2 \arrow[ur] & \end{tikzcd}\right)$$

$$\ell' \circ \ell = \mathrm{id}_{\mathcal{H}}$$

so ℓ is an isomorphism

Inner product: $\langle \psi_1 \otimes \psi_2, \varphi_1 \otimes \varphi_2 \rangle := \langle \psi_1, \varphi_1 \rangle \langle \psi_2, \varphi_2 \rangle$

Concretely: for separable Hilbert spaces: if $\{e_i^{(j)}, i \in \mathbb{N}\}$ are a ON basis for $\mathcal{H}^{(j)}$ then so is
$$\{e_i^{(1)} \otimes e_{i'}^{(2)},\ i, i' \in \mathbb{N}\} \quad \text{for} \quad \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$$

- While product vectors $\psi_1 \otimes \psi_2$ form a basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$ not all vectors are of that form $\rightsquigarrow$ "entanglement".
- Back to $L^2(\mathbb{R}^{3N})$: $|\psi(x_1, \dots, x_N)|^2$ is the probability density to find part. "1" at $x_1, \dots,$ part. "N" at x_N.

Marginals:
$$\rho_\psi^{(i)}(x) = \int_{\mathbb{R}^{3(N-1)}} |\psi(x_1, \dots, x_i, \dots, x_N)|^2 dx_1 \dots \widehat{dx_i} \dots dx_N$$
is the proba density to find part "i" at x, and
$$\rho_\psi(x) = \sum_{j=1}^{N} \rho_\psi^{(j)}(x)$$
is the "one-particle density", with $\int \rho_\psi(x)\, dx = N$.

- Kinetic energy: $T(\psi) = \sum_{i=1}^{N} \frac{1}{2} \int |\nabla_{x_i} \psi(x_1, \dots, x_N)|^2 dx$

Potential energy: $V(\psi) = \int V(x_1, \dots, x_N) |\psi(x_1, \dots, x_N)|^2 dx$

- Bosons & fermions

We define an action of S_N on $\mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_N$
$$P_\sigma : \psi_1 \otimes \dots \otimes \psi_N \mapsto \psi_{\sigma^{-1}(1)} \otimes \dots \otimes \psi_{\sigma^{-1}(N)}$$
(and extension to all of $\mathcal{H}$ by linearity)

In fact, unitary representation of S_N on $\mathcal{H}$, with
$$P_{id} = \mathbb{1}, \quad P_\sigma P_\tau = P_{\sigma\tau}, \quad (P_\sigma)^* = P_{\sigma^{-1}}$$

Identical particles are indistinguishable: there is no observable that distinguishes $P_\sigma \psi$ from ψ

$\to$ Postulate: Physical states are those that
$$P_\sigma \psi = \chi(\sigma) \psi$$

with $|\chi(\sigma)| = 1$

It follows that $\chi(\sigma)\chi(\tau) = \chi(\sigma\tau)$

namely $\chi : S_N \to U(1)$ is a one-dimensional representation of the permutation group.

Lemma: There are only two such repr:

$$\chi(\sigma) = 1 \quad \text{or} \quad \chi(\sigma) = \mathrm{sgn}(\sigma)$$

Proof (quick)
+ $\chi(\sigma)\chi(id) = \chi(\sigma)$ implies $\chi(id) = 1$
+ For a transposition (ij): $(ij)^2 = id$ implies

$$\chi((ij)) = \pm 1$$

+ For any $\sigma \in S_N$: $\sigma \circ (ij) = (\sigma(i)\sigma(j)) \circ \sigma$ implies that the alternative ± 1 is global for all transpositions.
+ Conclude: every σ is the product of transpositions and $\mathrm{sgn}(\sigma)$ is the number of transpositions $\square$

This yields two possible types of particles:

(i) Bosons with Hilbert space:

$$\mathcal{H}_s^N = \{\Psi \in \mathcal{H}^N : P_\sigma \Psi = \Psi \quad \forall \sigma \in S_N\}$$

(ii) Fermions

$$\mathcal{H}_a^N = \{\Psi \in \mathcal{H}^N : P_\sigma \Psi = \mathrm{sgn}(\sigma)\Psi \quad \forall \sigma \in S_N\}$$

In the case of $\mathcal{H} = L^2(\mathbb{R}^3)$:
+ Bosonic wavefunctions

$$\Psi(x_1, .., x_N) = \Psi(x_{\sigma(1)}, ..., x_{\sigma(N)})$$

+ Fermionic wavefunctions

$$\Psi(x_1, .., x_N) = \mathrm{sgn}(\sigma)\Psi(x_{\sigma(1)}, ..., x_{\sigma(N)}).$$

$\hookrightarrow$ Pauli Principle: $|\Psi(x_1, \underset{i}{x}, \underset{j}{x}, x_N)|^2 = 0$

Proba density to find two fermions at the same location vanishes: "exclusion principle".

Note: electrons, protons, neutrons are all fermions

We now consider

$$H_N = \frac{1}{2}\sum_{i=1}^{N}(-\Delta_i) + \alpha V(x, R) \qquad (\mathrm{Ham\,N})$$

where

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$$V(x,R) = \sum_{1\le i<j\le N} \frac{1}{|x_i-x_j|} - \sum_{i=1}^{N}\sum_{j=1}^{M} \frac{Z_j}{|x_i-R_j|} + \sum_{1\le k<l\le M} \frac{Z_k Z_l}{|R_k-R_l|}$$

repulsive (positive) electron-electron interaction; attractive electron-nuclei interaction; positive constant

acts on $\Lambda^N L^2(\mathbb{R}^3)$

Stability of matter of the second kind holds if $\exists\, C$ independent of N, M such that

$$\langle \Psi, H_N \Psi\rangle \geq -C\,(N+M) \qquad \forall \Psi \in \Lambda^N L^2(\mathbb{R}^3),\ \|\Psi\|$$

in particular: the ground state energy per particle

$$\frac{1}{N} \inf_{\|\Psi\|=1} \langle \Psi, H_N \Psi\rangle$$

is bounded in N.

Key ingredients:

(i) Uncertainty Principle. Potential energy bounded by kinetic energy $\rightsquigarrow$ Stability of first kind

(ii) Electrostatic screening $\rightsquigarrow$ effective cancelations of negative and positive charges in the potential "at infinity"
"Baxter's inequality"

(iii) Pauli Principle $\rightsquigarrow$ "Lieb-Thirring inequality"

We start with some heuristics:

* N particles on a single nucleus: $\sum_i -\frac{1}{2}\Delta_i - \frac{Z}{|x_i|}$
Ground state for one electron

$$\Psi_0(x) \propto \exp(-Z|x|/2) \quad \text{because of kinetic energy}$$

has energy $E(\Psi_0) = -Z^2/4$

Without interactions and on all of $L^2(\mathbb{R}^{3N})$
The ground state is $\Psi_0(x_1,\dots,x_N) = \Psi_0(x_1)\cdots\Psi_0(x_N)$
namely symmetric and

$$E_0^N = -\frac{Z^2}{4}\cdot N$$

* Neglecting the nucleus-nucleus repulsion, but having M nuclei on top of each other and non-interact

electrons $E_0^N = -\frac{1}{4}(Z_1 + \dots Z_M)^2 N$
$$\geq -\frac{1}{4} Z^2 M^2 N$$
where $Z = \max\{Z_i\}$

By the arithmetic-geometric mean inequality
$$\sqrt[3]{M \cdot M\, N} \leq \frac{1}{3}(M+M+N)$$
$$\Rightarrow M^2 N \leq \frac{1}{27}(2M+N)^3 \leq \frac{8}{27}(M+N)^3$$
$$E_0^N \geq -C(M+N) \; (3) \; \triangle!$$

* Taking electrostatics into account (repulsive energy): $-C(M+N)^{5/3}$

so a $\frac{4}{3}$ gain

* Pauli Principle: The Hamiltonian $-\Delta + \frac{Z}{|x|}$ has eigenvalues
$$\varepsilon_j = -\frac{C}{j^2}$$
with degeneracies j^2 $(l = 1, \dots j^2)$

On the full Hilbert space $L^2(\mathbb{R}^{3N})$, $H^N = \Sigma(\dots)$ has eigenvectors
$$\Psi_{j_1, \dots j_\ell} = \Psi^{(1)}_{j_1} \otimes \dots \otimes \Psi^{(r_1)}_{j_1} \otimes \dots \otimes \Psi^{(1)}_{j_\ell} \otimes \dots \otimes \Psi^{(r_\ell)}_{j_\ell}$$
with $\sum_{i=1}^{\ell} r_i = N$ and $\left(-\Delta + \frac{Z}{|x|}\right)\Psi^{(r_i)}_{j_i} = \varepsilon_{j_i}$

and

eigenvalues $\sum_{i=1}^{\ell} r_i \, \varepsilon_{j_i}$ "orbitals"

Such a vector can be antisymmetrized iff $\Psi^{(r_k)}_{j_i} \neq \Psi^{(r_\ell)}_{j_m}$ (all "orbitals" different) so that the ground state energy is obtained by filling the lowest N "orbitals"

For fixed N the largest 1-particle energy obtained in this way is the Fermi energy E_F

It is given by
$$N = \sum_{j=1}^{j_0} j^2 \qquad E_F = E_{j_0}$$

Specifically: $N = \sum^{j_0} j^2 = \frac{1}{6} j_0(j_0+1)(2j_0+1) \sim j_0^3$

Ground state energy

$$\sum_{j=1}^{j_0} \underbrace{j^2}_{\text{degeneracy}} \underbrace{\frac{C}{j^2}}_{\text{eigenvalue}} \sim j_0 \sim N^{1/3}$$

If we again stack all nuclei on top of each other

$$E_0^N \geq -CZ^2 M^2 N^{1/3} \geq -CZ^2 (6M^{1/3} + N^{1/3})^7$$
$$\geq -CZ^2 (M+N)^{7/3}$$

$\to$ The Pauli principle yields a $\frac{2}{3}$ gain

$\rightsquigarrow$ Electrostatics + Pauli give a $\frac{4}{3} + \frac{2}{3}$ gain, namely $3 - 6/3 = 1 \rightsquigarrow$ stability ♡

We shall now do this in details, and from scratch.

Lemma Let $\psi \in H^1(\mathbb{R}^3) = \{\psi \in L^2(\mathbb{R}^3) : \nabla\psi \in L^2(\mathbb{R}^3)\}$.
Then $\int \frac{|\psi(x)|^2}{|x|} dx \leq \|\nabla\psi\|_2 \|\psi\|_2$

The proof relies on the formal identity

$$\frac{2}{|x|} = \sum_{j=1}^3 [\partial_j, \frac{x_j}{|x|}]$$

Proof: We note

$$\langle\psi, \frac{1}{|x|}\psi\rangle = \left(\int_{B_\varepsilon(0)} + \int_{B_\varepsilon(0)^c}\right)\left(\frac{|\psi(x)|^2}{|x|}\right) dx$$

Let $\psi \in C_c^\infty(\mathbb{R}^3)$

• Since ψ is bounded: $\int_{B_\varepsilon(0)} (\cdot) \leq 4\pi \|\psi\|_\infty^2 \int_0^\varepsilon r\,dr \xrightarrow{\varepsilon \to 0} 0$

• $2\int_{B_\varepsilon(0)^c} (\cdot) = \int_{B_\varepsilon(0)^c} \bar\psi(x)\left(\partial_j \frac{x_j}{|x|}\psi(x) - \frac{x_j}{|x|}\partial_j \psi(x)\right) dx$

$$\left(\text{Since } \sum_j \partial_j \frac{x_j}{|x|} = \frac{3}{|x|} - \sum_j \frac{x_j^2}{|x|^3} = \frac{3}{|x|} - \frac{1}{|x|}\right)$$

$$= \int_{B_\varepsilon(0)^c} \left(\operatorname{div}\left(\frac{x}{|x|}|\psi(x)|^2\right) - \frac{x}{|x|} \cdot 2\operatorname{Re}(\nabla\psi(x))\bar\psi(x)\right) dx$$

The divergence term is bounded by

$$\int_{\partial B_\varepsilon(0)} |\psi(x)|^2 d\sigma \le 4\pi\varepsilon^2 \|\psi\|_\infty^2 \xrightarrow{\varepsilon\to 0} 0$$

For the other one: $2\mathrm{Re}(\ldots) \le 2|\ldots|$ and

then $\sum_{j=1}^{3} |\langle \partial_j \psi, \frac{x_j}{|x|}\psi\rangle|$

$$\le \sum_{j=1}^{3} \|\partial_j \psi\|_2 \left\| \frac{x_j}{|x|}\psi \right\|_2 \quad (\text{C-S in } L^2)$$

$$\le \|\nabla\psi\|_2 \|\psi\|_2 \quad (\text{C-S in } \mathbb{C}^3)$$

The bound extends to H^1 by density of $C_c^\infty(\mathbb{R}^3)$ $\boxtimes$

Prop Let $Z > 0$ and

$$E_0 = \inf\left\{ \int |\nabla\psi|^2 - \frac{Z}{|x|}|\psi|^2 : \psi \in H^1, \|\psi\|_2 = 1 \right\}$$

Then E_0 is finite and in fact $E_0 = -\frac{Z^2}{4}$.

Moreover:

$E_0 = E(\psi_0)$ where $\psi_0 = \frac{Z^{3/2}}{\sqrt{8\pi}} e^{-Z\frac{|x|}{2}}$

Proof $E(\psi) \ge \|\nabla\psi\|_2^2 - Z\|\nabla\psi\|_2$ (by lemma)

$= (\|\nabla\psi\|_2 - \frac{Z}{2})^2 - \frac{Z^2}{4}$ (complete square)

$\ge Z^2/4$ indeed

A calculation yields that the first inequality is an equality if $\psi = C\exp(-c|x|)$ and the second if $\|\nabla\psi\|_2 = \frac{Z}{2}$. This and $\|\psi\|_2 = 1$ yield the constants. $\boxtimes$

Theorem [Stability of the first kind for atoms & molecule]

Let $Z_1, \ldots, Z_M > 0$ and

$E(\psi) = \langle \psi, H_N \psi \rangle$ with H_N from (Ham N)

for $\psi \in H^1(\mathbb{R}^{3N})$

Let $E_0(R) = \inf\{ E(\psi) : \psi \in H^1(\mathbb{R}^{3N}), \|\psi\|_2 = 1 \}$

Then $E_0(R) > -\infty$ for any $R \in \mathbb{R}^{3M}$ and

$$E_0 = \inf\{ E_0(R) : R \in \mathbb{R}^{3M} \} > -\infty.$$

Note: Nuclei are static. Adding their kinetic energy would only increase the G.S.E.

Proof. Neglecting the positive terms of $V(x,R)$, we consider
$$\sum_{j=1}^{N}\int|\nabla_j\Psi(x)|^2dx-\sum_{i=1}^{M}\sum_{j=1}^{N}\int\frac{z_i|\Psi(x)|^2}{|x_j-R_i|}dx. \quad (*)$$

and let $Z=\max z_i$ and pick j. Then $(*)$ can be lower bounded by $\sum_j\int dx_1\ldots\cancel{dx_j}\ldots dx_N\,\mathcal{E}_j(x_1,\ldots\cancel{x_j},\ldots x_N)$ where
$$\mathcal{E}_j=\underbrace{\int dx_j\left(|\nabla_j\Psi(x)|^2-\frac{MZ}{|x_j-R_0|}|\Psi(x)|^2\right)}$$

see Ψ as a function
$g_j: x_j\mapsto\Psi(x_1,\ldots x_j,\ldots x_N)$
with parameters $x_1,\ldots\cancel{x_j},\ldots x_N$.

$$\mathcal{E}_j=\int dx\left(|\nabla g_j(x)|^2-\frac{MZ}{|x-R_0|}|g_j(x)|^2\right)$$

By previous proposition: $\mathcal{E}_j\geq\frac{(MZ)^2}{4}\|g_j\|_2^2$ uniformly in R_0

Since
$$\int\|g_j\|_2^2\,dx_1\ldots\cancel{dx_j}\,dx_N=\int|\Psi(x_1\ldots x_N)|^2dx=1,$$
we conclude that
$$(*)\geq-\frac{1}{4}NM^2Z^2\quad\text{uniformly in }R_1,\ldots,R_M.$$

Notes: * We recover the cubic dependence on $(M+N)$ obtained by approximation before.
* It can be shown that the minimizer belongs to the unphysical symmetric subspace.

• We now turn to the stability of the second kind.

Theorem [Lieb-Thirring inequalities]. Let $\gamma\geq0$ and $V=V_+-V_-$ with $V_\pm(x)\geq0$ $\forall x$. Assume that $V_-\in L^{\gamma+\frac{d}{2}}(\mathbb{R}^d)$. Let $E_0\leq E_1\leq\ldots$ be the negative eigenvalues of $-\Delta+V$ in $L^2(\mathbb{R}^d)$.
Then $\exists\, L_{\gamma,d}>0$ s.t.

$$\sum_j |E_j|^\gamma \leq L_{\gamma,d} \int_{\mathbb{R}^d} V_-(x)^{\gamma+\frac{d}{2}}\,dx$$

with conditions: * $\gamma \geq \frac{1}{2}$ if $d=1$
* $\gamma > 0$ if $d=2$
* $\gamma \geq 0$ if $d \geq 3$

- Remarks: * "One-body" estimate
  * Explicit upper bounds for $L_{\gamma,d}$ are known, but not all sharp values.
  * The case $\gamma=0$ is special: "CLR bound"
  * A scaling argument shows that $\gamma+\frac{d}{2}$ is the only possible exponent. Let ψ be s.t. $(-\Delta-V_-)\psi = E\psi$, and let $\psi_\lambda(x) = \psi(\lambda x)$. Then $(-\Delta-V_\lambda)\psi_\lambda = E_\lambda\psi_\lambda$ for $V_\lambda(x) = \lambda^2 V(\lambda x)$
  $E_\lambda = \lambda^2 E$

  So if an LT bound holds, then for all $\lambda > 0$:

$$\lambda^{2\gamma}\sum_j |E_j|^\gamma = \sum_j |E_{\lambda,j}|^\gamma \leq L \int V_\lambda(x)^\alpha\,dx$$
$$= L \cdot \lambda^{2\alpha}\lambda^{-d}\int V_-(x)\,dx$$

  This is only possible if $2\alpha-d-2\gamma = 0$, namely $\alpha = \gamma+\frac{d}{2}$.

- We now rephrase the eigenvalue problem in terms of the so-called Birman-Schwinger operator, here for $d=3$.

  Let $-e$, $e>0$ be a negative eigenvalue of $-\Delta-V_-$. Then

$$(-\Delta+e)\psi = V_-\psi$$

  which we understand in a weak sense for $\psi \in H^1$, $\|\psi\|_2 = 1$: $(-\Delta+e)\psi$ might not be in L^2, but it is in H^{-1}, the set of bounded linear functionals on H^1: Indeed, $(-\Delta+e)\psi$ acts on H^1 by $\xi \mapsto \int(\overline{\nabla\psi}\nabla\xi + e\bar{\psi}\xi)$

Let $\varphi(x) = \sqrt{-V(x)}\,\psi(x)$.

<u>Claim 1</u> $\varphi \in L^2(\mathbb{R}^3)$ if $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$

Indeed if $\psi \in H^1$, then $\int |\sqrt{V_-}\,\psi|^2 = \int V_-(x)|\psi(x)|^2\,dx$

$$\Rightarrow \|\sqrt{V_-}\,\psi\|_2^2 \leq \|V_1\|_{3/2} \underbrace{\||\psi|^2\|_3}_{=\|\psi\|_6^2 \,\leq\, C\|\nabla\psi\|_2^2 \text{ by Sobolev.}} + \|V_2\|_\infty \|\psi\|_2^2$$

Hence $\psi \in H^1 \Rightarrow \varphi \in L^2$ indeed $\square$

Since $-\Delta \geq 0$ and $-e < 0$, we have that $-e \in \rho(-\Delta)$ and so $(-\Delta + e)^{-1}$ is bounded, from L^2 to H^2. Since L^2 is a dense subspace of H^{-1}, $(-\Delta+e)^{-1}$ extends to a bounded operator on H^{-1}, with range H^1 indeed. If $\xi \in H^{-1}$, then $\psi = (-\Delta+e)^{-1}\xi \iff \xi = (-\Delta+e)\psi$.

Finally $\varphi \in L^2 \Rightarrow \sqrt{V_-}\,\varphi \in H^{-1}$ (since $\xi \in H^1 \Rightarrow \sqrt{V_-}\,\xi \in L^2$) and we conclude from

$$(-\Delta+e)\psi = \sqrt{V_-}\,\varphi \qquad \text{(as eq. in } H^{-1})$$

that

$$\psi = (-\Delta+e)^{-1}\sqrt{V_-}\,\varphi \qquad \text{(as eq. in } H^1)$$

and hence

$$\varphi = \underbrace{\sqrt{V_-}\,(-\Delta+e)^{-1}\sqrt{V_-}}_{=K_e \text{ the Birman-Schwinger operator}}\,\varphi \qquad \text{(as eq. in } L^2).$$

<u>Claim 2</u> K_e is compact if $V_- \in L^2(\mathbb{R}^3)$

Indeed: K_e is given by a square-integrable kernel. The kernel of $(-\Delta+e)^{-1}$ is $\frac{1}{4\pi}\frac{1}{|x-y|}\exp(-\sqrt{e}\,|x-y|)$ and so the kernel of K_e^2 is given by

$$\frac{1}{16\pi^2}\sqrt{V_-(x)}\int_{\mathbb{R}^3}\frac{1}{|x-y|}e^{-\sqrt{e}|x-y|}\,V_-(y)\,e^{-\sqrt{e}|y-t|}\frac{1}{|y-t|}\,dy\,\sqrt{V_-(t)}$$

and

$$\mathrm{Tr}(K_e^2) = \|K_e\|_2^2 = \int_{\mathbb{R}^6} G_e(|x-y|)^2\, V_-(x) V_-(y)\, dx\, dy$$

where $G_e(t) = \frac{1}{4\pi}\frac{1}{|t|} e^{-\sqrt{e}|t|}$

By Cauchy-Schwarz (in $\mathbb{R}^6$): $\|K_e\|_2^2 \leq \left(\int V_-(x)^2 G_e(|x-y|)^2 dx\,dy\right)^{1/2} \cdot (x \leftrightarrow y)$

and since $\int V_-(x)^2 G_e(|x-y|)^2 dx\,dy = \int V_-(x)^2 dx \int G_e(|t|)^2 dt$

we conclude that, if $V_- \in L^2(\mathbb{R}^3)$, then

(i) K_e is compact

(ii) $\mathrm{Tr}(K_e^2) \leq \|V_-\|_2^2 \cdot \frac{C}{\sqrt{e}}$ by explicit integration of G_e^2. ☒

We have now seen: if $\psi \in H^1$ is s.t. $(-\Delta + e)\psi = V_-\psi$, then $\varphi \in L^2$ is s.t. $\varphi = K_e\varphi$.

Reciprocally: Let φ be as ↗. Then $\psi := (-\Delta+e)^{-1}\sqrt{V_-}\varphi \in H^1$

and $(-\Delta+e)\psi = \sqrt{V_-}\varphi = \sqrt{V_-}K_e\varphi$

$= V_-(-\Delta+e)^{-1}\sqrt{V_-}\varphi = V_-\psi$.

⇒ There is a one-to-one correspondence between $\{\psi \in H^1 \text{ s.t. } (-\Delta+e)\psi = V_-\psi\}$ and $\{\varphi \in L^2 \text{ s.t. } \varphi = K_e\varphi\}$.

In fact, let N_e = # eigenvalues of $-\Delta - V_-$ that are $\leq -e$

B_e = — " — K_e — " — ≥ 1

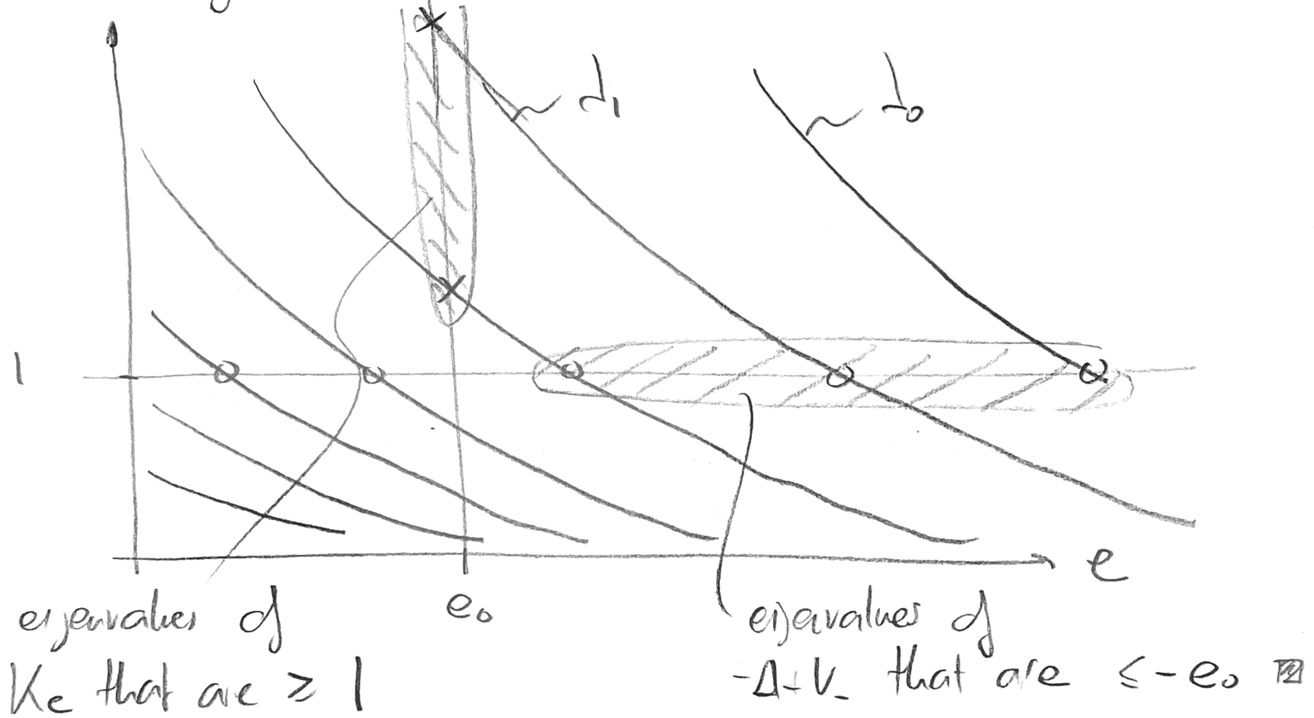
<u>Claim 3</u>: [Birman-Schwinger Principle]: $B_e = N_e$

<u>Indeed</u>. The identity $(-\Delta+e')^{-1} - (-\Delta+e)^{-1} = (e-e')(-\Delta+e')^{-1}(-\Delta+e)^{-1}$ and the positivity of $-\Delta+e$, $-\Delta+e'$, imply that $e \mapsto (-\Delta+e)^{-1}$ is decreasing and therefore so is $e \mapsto K_e$. It follows that the eigenvalues $\lambda_j(e)$

of K_e are also decreasing, with $\lim_{e \to \infty} \lambda_j(e) = 0$.

⌈Note: K_e compact $\Rightarrow$ the eigenvalues can be enumerated:
$\lambda_0(e) \geq \lambda_1(e) \geq \dots \lambda_n(e) \geq \dots \geq 0$ and they may only accumulate at 0 ⌋

Hence:



We are now equipped to prove the LT-inequality for the case $d = 3$, $\gamma > 0$ and $V_- \in L^{3/2} + L^\infty$.

By arguments in part I, $-\Delta - V_-$ is bounded below. Hence $N_e = 0$ for e large enough. Moreover, it is a piecewise constant function and so

$$\int_0^\infty e^{\gamma - 1} N_e \, de = \sum_j \frac{1}{\gamma} j \left(|E_{j-1}|^\gamma - |E_j|^\gamma \right) = \frac{1}{\gamma} \sum_j |E_j|^\gamma$$

(in the case of degenerate eigenvalues j must be replaced by the degeneracy of the j^{th} eigenvalue)

With the Birman-Schwinger Principle:

$$\sum_j |E_j|^\gamma = \gamma \int_0^\infty e^{\gamma - 1} B_e \, de$$

By definition of B_e:

$$B_e \le \sum_{j:\lambda_j(e)\ge 1} \lambda_j(e)^2 \le \mathrm{Tr}(K_e^2)$$

add all eigenvalues in $[0,1)$.

Now instead of considering V_-, we use

$$W_e(x) = \left(V(x)+\frac{e}{2}\right)_- = \max\left\{0, -V(x)-\frac{e}{2}\right\}$$

which is so that: (i) $W_e(x) \ge 0 \quad \forall x$

(ii) $W_e(x) \ge V_-(x) - \frac{e}{2}$

and "=" holds whenever $V(x) \le -\frac{e}{2}$

Hence: $N_e(-V_-) = N_{\frac{e}{2}}\left(-V_- + \frac{e}{2}\right) \le N_{e/2}(-W_e)$

(indeed: if $A \le B$, then # of e.v. of $A \le \mu$ is greater than # e.v. of $B \le \mu$.)

and we can apply the B.-S. Principle:

$$\sum_j |E_j|^\gamma = \gamma \int_0^\infty e^{\gamma-1} N_e \, de \le \gamma \int_0^\infty e^{\gamma-1} N_{e/2}(-W_e)\, de$$

$$\le C \int_0^\infty e^{\gamma-1-\frac{1}{2}} \int_{\mathbb{R}^3} W_e(x)^2 \, dx$$

Since $W_e(x) = 0$ for all (e,x) s.t. $e > -2V(x)$

$$\sum_j |E_j|^\gamma \le C \int_{\mathbb{R}^3} dx \int_0^{-2V(x)} \underbrace{W_e(x)^2}_{\text{in this domain: } = V_-(x) - \frac{e}{2}} e^{\gamma-\frac{3}{2}} \, de$$

changing variables: $e = -2V(x)u = 2V_-(x)u$ in domain:

$$\int_0^{-2V(x)} \cdots de = C \int_0^1 V_-(x)^{\gamma-\frac{3}{2}+2+1} u^{\gamma-\frac{3}{2}+1}(1-u)^2 \, du$$

since $V_- - \frac{e}{2} = V_-(1-u)$.

Hence:

$$\sum_j |E_j|^\gamma \leq C \int_{\mathbb{R}^3} V_-(x)^{\gamma+\frac{3}{2}} dx$$

since $\int_0^1 u^{\gamma-\frac{1}{2}}(1-u)^2 du$ is convergent for all $\gamma > 0$ $\blacksquare$

- With L-T, we have an lower bound on the eigenvalues of a one-body Hamiltonian. The following inequality gives a lower bound on the full many-body Hamiltonian by an effective one-body operator.

Theorem [Baxter] Let $V(x,R)$ be as in (Ham N) with $Z_j = Z$ $\forall 1 \leq j \leq M$. Then

$$V(x,R) \geq -(2Z+1)\sum_{i=1}^{N} \frac{1}{D(x_i)} + \frac{Z^2}{8}\sum_{j=1}^{M} \frac{1}{D_j}$$

where: & $D(x) = \min\{|x-R_j| : 1 \leq j \leq M\}$
(distance from x to closest nucleus)
& $D_j = \frac{1}{2}\min\{|R_i - R_j| : 1 \leq i \leq M\}$
(half-distance to nearest neighbour)

Remark For a lower bound, the electrostatic interactions effectively cancel out leaving only the interactions to the nearest nucleus.

- Proof of stability of matter:

By Baxter

$$H_N \geq \sum_{j=1}^{N}\left(-\frac{1}{2}\Delta_j - (2Z+1)\frac{\alpha}{D(x_j)}\right) = \sum_{j=1}^{N} h_j$$

where we dropped the non-negative term of the potential

Now $\mathcal{D}(x)^{-1}$ is not in $L^{5/2}$ (at infinity) so as before

$$-\mathcal{D}(x)^{-1} = -\left(\mathcal{D}(x)^{-1} - b\right) - b \qquad (b > 0)$$

and $\left(\mathcal{D}(x)^{-1} - b\right)_+ \in L^{5/2}$ (because the local singularity is integrable in $d=3$)

So now

$$H_N \geq \sum_{j=1}^{N} \left(-\tfrac{1}{2}\Delta_j - (2Z+1)\frac{\alpha}{\mathcal{D}(x_j) - b} \right) - bN\alpha(2Z+1)$$

We are looking for an estimate on $\langle \psi, H_N \psi \rangle$ over all antisymmetric wave functions: in fact

$$\inf_{\psi \in L^2_a(\mathbb{R}^{3N})} \langle \psi, H_N \psi \rangle \geq \sum_{j=1}^{N} E_j \geq \sum_{j=1} E_j$$

which can be bounded by LT inequalities

$$\inf_{\psi} \langle \psi, \textstyle\sum(\ldots)\psi_N \rangle \geq C\left(\alpha(2Z+1)\right)^{5/2} \int \left(\frac{1}{\mathcal{D}(x)} - b\right)_+^{5/2} dx$$

Now: crude bound

$$\left(\mathcal{D}(x)^{-1} - b\right)_+^{5/2} = \max_j \left(|x - R_j|^{-1} - b\right)_+^{5/2} \leq \sum_j \left(|x - R_j|^{-1} - b\right)_+^{5/2}$$

yields

$$\int_{\mathbb{R}^3} \left(\mathcal{D}(x)^{-1} - b\right)_+^{5/2} dx \leq M \int \left(|x|^{-1} - b\right)_+^{5/2} dx$$

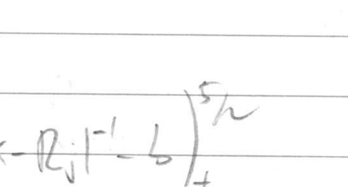
$$= M \int_{|x| \leq 1/b} \left(|x|^{-1} - b\right)^{5/2} dx = CM \int_0^{1/b} \left(\frac{1}{r} - b\right)^{5/2} r^2 \, dr$$

$$= CM \int_0^{\infty} \frac{u^{5/2}}{(u+b)^4} du = C \frac{5\pi}{16\sqrt{b}} \cdot M$$

Hence

$$\langle \psi, H_N \psi \rangle \geq -\left(C_1 \alpha^{5/2} (2Z+1)^{5/2} \frac{M}{\sqrt{b}} + \alpha(2Z+1)Nb \right)$$

as a function of b:



Critical point at $b_0 = C\left(\frac{M}{N}\right)^{2/3} \alpha(2Z+1)$
for an extremal value

$$C\beta^2 M^{2/3} N^{1/3}$$

- Comments on stability

(i) Bosons are not stable. In fact: for any $R_1, \dots R_M$, there is $\Psi \in \mathcal{H}_s^{(N)}$ s.t.

$$E(\Psi) \leq -C\alpha^2 Z^{4/3} \min\{N, ZM\}^{5/3}$$

The upper bound is explicit, using a product wave function.

(ii) Magnetic fields. Introduced by replacing

$$-i\nabla \rightsquigarrow (-i\nabla + A(x))$$

magnetic potential

where $(\mathrm{curl}\, A)(x) = B(x)$ magnetic field

We have the diamagnetic inequality

$$|((-i\nabla + A)\Psi)(x)| \geq |\nabla|\Psi|(x)|$$

pointwise almost everywhere. Hence A can only improve stability.

Somewhat informally: if $\Psi(x) \neq 0$:

$$\partial_j |\Psi(x)|^2 = (\partial_j \bar{\Psi}(x))\Psi(x) + \bar{\Psi}(x)\partial_j\Psi(x) = 2|\Psi(x)|\partial_j|\Psi(x)|$$

so that $\nabla|\Psi(x)| = \mathrm{Re}\left(\frac{\bar{\Psi}(x)}{|\Psi(x)|}\nabla\Psi(x)\right)$

Hence $|\nabla|\Psi|| = \left|\mathrm{Re}\left(\frac{\bar{\Psi}}{|\Psi|}(\nabla + iA)\Psi\right)\right|$

$$\leq \left|\frac{\bar{\Psi}}{|\Psi|}(\nabla + iA)\Psi\right| = |(\nabla + iA)\Psi|.$$

(all rigorous with $A \in L^2_{loc}$)

(iii) When electrons have 'spin' (see next chapter) things get complicated and stability does not hold for very heavy atoms.
(But then the internal structure of the nuclei should be taken into account)

(iv) The electromagnetic field can also be treated as an independent quantum mechanical object and stability holds for not too heavy atoms.