STABILITY OF MATTER WITH MAGNETIC SELF-INTERACTIONS

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Many-Body Quantum systems:

N electrons and K nuclei. Hamiltonian:

$$H_{N,K} = H = \sum_{k=1}^{K} T_k + \sum_{i=1}^{N} t_i + V_C.$$

The nuclear kinetic energy operator:

$$T_k = -\frac{1}{2M_k}\Delta_{R_k}, \quad M_k = \text{Nuclear mass}$$

The electron kinetic energy operator:

$$t_i = -\frac{1}{2}\Delta_{x_i}.$$

We shall consider other possible choices for t_i.

The Coulomb potential V_C is the function

$$\begin{aligned} V_C \;=\; & -\sum_{k=1}^{K}\sum_{i=1}^{N} Z_k|x_i - R_k|^{-1} + \sum_{i<j}|x_i - x_j|^{-1} \\ & + \sum_{k<\ell} Z_k Z_\ell |R_k - R_\ell|^{-1} \end{aligned}$$

Units: $m_e = \hbar = e$

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Question: In which Hilbert space $\mathcal{H}$ does $H_{N.K}$ act?

1. case: We could choose $\mathcal{H}$ to be the space of all square integrable functions.

$$\mathcal{H}_{\text{total}} = \bigotimes_{k}^{K} L^2(\mathbb{R}^3_{R_k}) \otimes \bigotimes_{i}^{N} L^2(\mathbb{R}^3_{x_i})$$

(we can always think of $H_{N,K}$ as being defined on the subspace of C_0^∞-functions)

<u>Ground State Energy:</u> The lowest energy of the system is

$$E_{\mathcal{H}}^{N,K} = \inf \{(H\psi, \psi) \ : \ \psi \in \mathcal{H}, \ \|\psi\| = 1, \psi \in C_0^\infty\}$$

<u>Stability of 1st kind:</u> $E_{\mathcal{H}}^{N,K} > -\infty$

<u>Stability of 2nd kind:</u>

$$E_{\mathcal{H}}^{N,K} > C(\max\{Z_k\})(N + K)$$

Explanation: The energy per particle must be bounded.

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Theorem *On the space $\mathcal{H}_{\text{total}}$ of all L^2-functions stability of the first kind holds. Stability of the second kind is false.*

Stability of the first kind, one of the original motivations for quantum mechanics, follows e.g. from the Sobolev inequality. Instability of the 2nd. kind is diffcult, proved by Dyson '67.

<u>The Pauli principle:</u> The missing ingredient to obtain stability of the 2nd kind. The physical Hilbert space is not $\mathcal{H}_{\text{total}}$ but

$$\mathcal{H}_{\text{physical}} = \bigotimes_{k}^{K} L^2(\mathbb{R}^3_{R_k}) \otimes \bigwedge_{i}^{N} L^2(\mathbb{R}^3; \mathbb{C}^2).$$

The electrons are described by *antisymmetric* (the wedge $\bigwedge$) *spinor valued* functions. Spinor valued: here we just mean with values in $\mathbb{C}^2$, but the spinor structure will be important later.

Theorem (Stability of Matter) *If ψ is a normalized C_0^∞ function in the physical Hilbert space $\mathcal{H}_{\text{physical}}$ then*

$$(H\psi, \psi) \geq C(\max\{Z_k\})K$$

Thus on the physical Hilbert space stability of the 2nd kind holds.

Proved originally by Dyson and Lenard '68. Lieb and Thirring gave a simple proof in '75 where the constant is of the correct physical order of magnitude.

<u>Relativistic corrections</u>:

Replace

$$t = -\frac{1}{2}\Delta \;\longrightarrow\; t = \sqrt{-c^2\Delta + c^4} - c^2.$$

Recall $m_e = 1$. In our units the speed of light $c = \alpha^{-1}$, $\alpha =$fine structure constant$\approx 1/137$.

Theorem (Relativistic stability)
(a) $\exists\ \alpha_0 > 0\ :\ \alpha < \alpha_0,\quad \max\{Z_k\}\alpha \le 2/\pi \Rightarrow$ *The relativistic Hamiltonian stable of 2nd kind.*
(b) $\max\{Z_k\}\alpha > 2/\pi$: *unstable of 1st kind.*

First result; Conlon '84. Improved by Fefferman-de la Llave '86. Complete formulation: Lieb-Yau '88

Magnetic self-interactions: Replace

$$t = -\frac{1}{2}\Delta \ \longrightarrow\ \frac{1}{2}\left[(-i\nabla + \mathrm{A})^2 + \sigma\cdot\mathrm{B}\right].$$

Here A is the vector potential for the magnetic field $\mathrm{B} = \nabla\times\mathrm{A}$ generated by the electrons themselves.

$\mathrm{B}\cdot\sigma$ is the interaction of the magnetic field with the spinor components (Clifford multiplication by the vector B).

The Lichnerowiz formula:

$$(-i\nabla + \mathsf{A})^2 + \sigma \cdot \mathsf{B} = [\sigma \cdot (-i\nabla + \mathsf{A})]^2 .$$

$\sigma \cdot (-i\nabla + \mathsf{A})$ is the 3-dimensional Dirac operator.

Magnetic field generated by electrons: Maxwell's equation

$$(8\pi\alpha^2)^{-1}\nabla \times \mathsf{B} = \jmath_\psi$$

$\jmath_\psi$ is the current in the state ψ of the electrons.

Equivalent formulation: The magnetic field minimizes

$$(H\psi, \psi) + (8\pi\alpha^2)^{-1} \int \mathsf{B}^2$$

Recall:

$$H = \frac{1}{2} \sum_{j=1}^{N} \left[\sigma_j \cdot (-i\nabla_j + \mathsf{A}(x_j))\right]^2 + \sum_{k=1}^{K} T_k + V_C$$

Theorem (Magnetic Stability)

(a) $\exists\ \alpha_0, \eta_0 > 0 :\ \alpha < \alpha_0,\ \max\{Z_k\}\alpha^2 \leq \eta_0 \Rightarrow$

$$(H\psi,\psi)+(8\pi\alpha^2)^{-1}\int B^2 \geq C(\max\{Z_k\})(N+K)$$

(b) $\exists\ \eta_1 > 0 :\ \max\{Z_k\}\alpha^2 > \eta_1 \Rightarrow$ *Instability of the 1st kind, i.e.,*

$$\inf_{B,\psi}\left[(H\psi,\psi)+(8\pi\alpha^2)^{-1}\int B^2\right] = -\infty$$

Statement (b) proved by Loss-Yau '86.
Fefferman '95 announced a result similar to (a), ($Z = 1$ and $\alpha_0 \ll (1/137)$.
Lieb-Loss-S.: $\alpha_0 > 1/137$ for $\alpha = 1/137$ stable up to $Z = 1050$.

The instability:

Theorem (Loss-Yau) $\exists\psi$, B: $\int|\psi|^2 < \infty$ *and* $\int B^2 < \infty$ *such that*

$$\sigma \cdot (-i\nabla + A)\psi = 0.$$

The Dirac operator has a non-trivial kernel. Not fromthe index theorem since dimension=3.

The instability follows by scaling. All the non-vanishing terms scale like length^{-1}.

One example of such a B:

The hodge dual $*$B is the two form obtained from stereographic projection of β the two-form on $\mathcal{S}^3$ which is the pull back of the volume form by the Hopf map $\mathcal{S}^3 \to \mathcal{S}^2$.

Sketch of proof of stability:
Two steps:

Step (1) Reducing to a one-body problem:

$$V_C \geq \sum_{j=1}^{N} W(x_j)$$

$$W(x) \approx Z_k |x - R_k|^{-1} \quad \text{for } x \text{ near } R_k.$$

(note not $\sum_k Z_k |x - R_k|^{-1}$. Screening!)

Then

$$(H\psi, \psi) \geq \text{sum of neg. eigenvalues of } \frac{1}{2}[\sigma \cdot (-i\nabla + \mathsf{A})]^2 - W$$

Step(2) Analyzing the one-body-problem:

Theorem (Lieb-Loss-S.)

sum of neg. eigenvalues of $\frac{1}{2}[\sigma\cdot(-i\nabla+A)]^2-W$

$$\geq -C_1\int[W]_+^{5/2} - C_2\int[W]_+^{-4} - C_3\int B^2$$

This is not quite enough to prove stability *but almost*.

Proof:

sum of neg. eigenvalues of $\frac{1}{2}[\sigma\cdot(-i\nabla+\mathsf{A})]^2-W$

$$= -\int_0^\infty \#\text{of neg. ev}[\tfrac{1}{2}(\sigma\cdot(-i\nabla+\mathsf{A}))^2-W+e]de$$

(with $0 \le \mu(e) \le 1/2$)

$$\ge -\int_0^\infty \#\text{of neg. ev}[\mu(e)(\sigma\cdot(-i\nabla+\mathsf{A}))^2-W+e]de$$

(using Lichnerowiz)

$$\begin{aligned} = \; & -\int_0^\infty \#\text{of neg. ev}[\mu(e)((-i\nabla+\mathsf{A}))^2 \\ & +\mu(e)\sigma\cdot\mathsf{B}-W+e]de \end{aligned}$$

(using the Cwikel-Lieb-Rozenblum inequality)

$$\ge -\int\int_0^\infty [-|B|-\mu(e)^{-1}W+\mu(e)^{-1}e]_-^{3/2}dedx.$$

The rest is just a matter of choosing $\mu(e)$. $\mu(e)=1/2$ for small e. $\mu(e)\sim e^{-1}$ for large e.