The energy of Charged Matter

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Charged matter in Quantum Mechanics

The **Hamiltonian** for charged matter in quantum mechanics:

$$H_N = \sum_{i=1}^{N} T_i + \sum_{1\le i<j\le N} \frac{e_i e_j}{|x_i - x_j|} + \mathcal{U}$$

T_i = **Kinetic energy** operator for particle i.

$x_i \in \mathbb{R}^3$ = **Position** of particle i.

e_i = **Charge** of particle i=± 1 (for simplicity). *Considered as variable.*

Different kinetic energies (all masses$= 1$ (unusual setup), $\hbar = 1$):

$$\begin{aligned} T_i &= -\tfrac{1}{2}\Delta_i & \qquad T_i^{\mathrm{Mag}} &= \tfrac{1}{2}(-i\nabla_i + \tfrac{e_i}{c}\mathbf{A}(x_i))^2 \\ T_i^{\mathrm{Rel}} &= \sqrt{-c^2\Delta_i + c^4} & \qquad T_i^{\mathrm{Pauli}} &= \tfrac{1}{2}\left((-i\nabla_i + \tfrac{e_i}{c}\mathbf{A}(x_i))\cdot\sigma_i\right)^2 \end{aligned}$$

$$\mathcal{U} = \frac{1}{8\pi}\int |\nabla \times \mathbf{A}|^2 = \text{ Field Energy}$$

The Hilbert space and the energy

H_N acts in the **Hilbert Spaces**

$$\mathcal{H}_N^{(0)} = \bigotimes^N \mathcal{H}_1, \qquad \mathcal{H}_N^{\mathrm{Bose}} = \bigotimes^N_{\mathrm{sym}} \mathcal{H}_1, \qquad \mathcal{H}_N^{\mathrm{Fermi}} = \bigwedge^N \mathcal{H}_1$$

$$\mathcal{H}_1 = L^2(\mathbb{R}^3 \times \underbrace{\{-1,1\}}_{\text{charge}}), \qquad \mathcal{H}_1^{\mathrm{Spin}} = L^2(\mathbb{R}^3 \times \underbrace{\{-1,1\}}_{\text{charge}}; \mathbb{C}^2)$$

In general one may have mixtures of Fermions and Bosons (usual setup).

The **ground state energy**

$$E(N) := \inf_{\mathbf{A}} \inf \operatorname{spec}_{\mathcal{H}_N} H_N$$

Remark: For $T = -\frac{1}{2}\Delta$ or T^{Rel} we have

$$E^{(0)}(N) = E^{\mathrm{Bose}}(N)$$

Stability of Matter for Fermions

THEOREM 1 (Stability of Matter). *On the Fermionic space* $\mathcal{H}_N^{\text{Fermi}}$ *we have the estimate*

$$E^{\text{Fermi}}(N) \geq -CN.$$

If

1. $T = -\frac{1}{2}\Delta$ *with* $\mathcal{H}_1$ *or* $\mathcal{H}_1^{\text{Spin}}$
   Dyson-Lenard '66-67, Lieb-Thirring '75, Federbush '75)
2. T^{Mag} *with* $\mathcal{H}_1$ *or* $\mathcal{H}_1^{\text{Spin}}$ (Avron-Herbst-Simon '81 ?)
3. T^{Rel} *with* $\mathcal{H}_1$ *or* $\mathcal{H}_1^{\text{Spin}}$ *and c large enough.*
   (Conlon '84, Fefferman-de la Llave '86, Lieb-Yau '88)
4. T^{Pauli} *with* $\mathcal{H}_1^{\text{Spin}}$ *and c large enough.*
   (Fefferman (unpublished), Lieb-Loss-Sol. '95)

Remark on the proof: Uses one-body techniques, i.e., compares with an effective (mean field) non-interacting system.

Energy estimates for Bosons

THEOREM 2 (*Dyson-Lenard '66***).** *With* $T = -\frac{1}{2}\Delta$

$$E^{\mathrm{Bose}}(N) \geq -CN^{5/3}.$$

Remark on the proof: Again uses one-body techniques.

THEOREM 3 (*Lieb '79***).** *The exponent* $5/3$ *is sharp if we ignore the kinetic energy of (say) the positively charged particles.*

BUT:

THEOREM 4 ($N^{7/5}$**-instability of charged Bose gas,** *Dyson '67***).**

$$E^{\mathrm{Bose}}(N) \leq -CN^{7/5}. \qquad \textit{NOTE: } 7/5 < 5/3$$

Remark on the proof: Dyson uses a complicated **BCS** type trial wave function. A **simple product wave function** (accurat for non-interacting systems) only gives $\leq -CN$ (**no instability**).

The sharp $N^{7/5}$-law

THEOREM 5 (Dyson's sharp $N^{7/5}$-conjecture *(Lieb-Sol. in prep.)***).** *If* $T = -\frac{1}{2}\Delta$

$$E^{\mathrm{Bose}}(N) \geq -AN^{7/5} + o(N^{7/5}).$$

$$A = -\inf\left\{ \tfrac{1}{2}\int |\nabla\phi|^2 - J\int \phi^{5/2} \;\middle|\; \phi \geq 0,\ \int \phi^2 = 1 \right\}$$

$$J = \left(\frac{2}{\pi}\right)^{3/4} \int_0^\infty 1 + x^4 - x^2\left(x^4+2\right)^{1/2} dx = \left(\frac{4}{\pi}\right)^{3/4} \frac{\Gamma(\frac{1}{2})\Gamma(\frac{3}{4})}{5\Gamma(\frac{5}{4})}.$$

Remark: Conlon-Lieb-Yau '88 proved $E^{\mathrm{Bose}}(N) \geq -CN^{7/5}$, but $C > A$.

Remark: Dyson also conjectured a similar upper bound.

Heuristics behind the $N^{7/5}$-law

(1) **Condensation**: Almost all particles are in the same one particle state $\widetilde{\phi} \in L^2(\mathbb{R}^3)$ with kinetic energy $N \int |\nabla \widetilde{\phi}|^2$.

(2) There are few particles excited into **Cooper pairs** correlating on a scale ℓ_0 on which $\widetilde{\phi}$ is essentially constant. This correlation gives rise to the attractive energy. The electrostatic interaction may be ignored on scales larger than ℓ_0.

(3) To calculate the **correlation energy** we consider a box of some size $\ell \gg \ell_0$ on which $\widetilde{\phi}$ is still nearly constant. In this box we can write the Hamiltonian in **second quantized form** (expanding in plane waves)

$$\sum_p \tfrac{1}{2} p^2 (a_{p+}^* a_{p+} + a_{p-}^* a_{p-})$$

$$+\tfrac{1}{2} \sum_{pq,\mu\nu} \widehat{w}_{pq,\mu\nu} \left(a_{p+}^* a_{q+}^* a_{\nu+} a_{\mu+} + a_{p-}^* a_{q-}^* a_{\nu-} a_{\mu-} - 2 a_{p+}^* a_{q-}^* a_{\nu-} a_{\mu+} \right)$$

The Bogolubov approximation (Foldy's method)

(4) Ignore all quartic terms with only 0 or 1 of the operators $a_{0\pm}$, $a^*_{0\pm}$ (represents the creation or annihilation of the state $\widetilde{\phi}$). Replace $a_{0\pm}$ and $a^*_{0\pm}$ by the c-number $(N\widetilde{\phi}^2\ell^3)^{1/2}$. Using explicitly the Coulomb potential we arrive at the **effective Bogolubov Hamiltonian**:

$$
\begin{aligned}
&\ell^3(2\pi)^{-3}\int \tfrac{1}{4}k^2\left(a^*_{k+}a_{k+} + a^*_{-k+}a_{-k+} + a^*_{k-}a_{k-} + a^*_{-k-}a_{-k-}\right)\\
&+\tfrac{1}{2}(2\pi)N\widetilde{\phi}^2|k|^{-2}\Big[(a^*_{k+}a_{k+} + a^*_{-k+}a_{-k+} + a^*_{k+}a^*_{-k+} + a_{k+}a_{-k+})\\
&\qquad + (a^*_{k-}a_{k-} + a^*_{-k-}a_{-k-} + a^*_{k-}a^*_{-k-} + a_{k-}a_{-k-})\\
&\qquad - (a^*_{k+}a_{k-} + a^*_{-k+}a_{-k-} + a^*_{k-}a_{k+} + a^*_{-k-}a_{-k+})\\
&\qquad - (a^*_{k+}a^*_{-k-} + a^*_{-k+}a^*_{k-} + a_{k+}a_{-k-} + a_{-k+}a_{k-})\Big]dk
\end{aligned}
$$

Completing squares and **CCR** give lower bound: $-JN^{5/4}\widetilde{\phi}^{5/2}\ell^3$

The $N^{7/5}$ scaling

Summing over different boxes gives energy $-JN^{5/4}\int \widetilde{\phi}^{5/2}$. The total energy is thus

$$N\int |\nabla\widetilde{\phi}|^2 - JN^{5/4}\int \widetilde{\phi}^{5/2} = N^{7/5}\left(\int |\nabla\phi|^2 - J\int \phi^{5/2}\right)$$

where

$$\phi(x) = N^{-3/10}\widetilde{\phi}(xN^{-1/5}).$$

Remark: **The length scale** of the charged Bose cloud is $N^{-1/5}$.

Remark: **The correlation length scale** of the Cooper pairs is $\ell_0 \sim N^{-2/5}$.

Rigorizing the argument: On the next slides we discuss techniques to reduce to the Bogolubov Hamiltonian in cubes. The replacement of a_0, a_0^* by c-numbers is easily achieved by rewriting in terms of the operator $b_p = \nu^{-1/2}a_p a_0^*$ (ν = number of particles in cube).

One-body techniques: The kinetic energy

Sobolev Inequality:

$$\int |\nabla\psi|^2 \geq C\left(\int |\psi|^6\right)^{1/3}, \; \psi \in C_0(\mathbb{R}^3)$$

Implies

$$-\Delta - V \geq -C_{\mathrm{S}}\int V(x)^{5/2}dx, \; V \leq 0$$

Stability of matter require taking into account the Pauli exclusion principle.

Lieb-Thirring ('76) inequality:

$$\underbrace{\mathrm{Tr}(-\Delta - V)_-}_{\text{Sum of negative eigenvalues}} \qquad \geq -C_{\mathrm{LT}}\int V(x)^{5/2}dx$$

Remarks: Holds also for $-\Delta \to T^{\mathrm{Mag}}$. Similar results for T^{Rel} (Daubechies '83). There are several versions for the Pauli operator.

One-body techniques: Controlling electrostatics

Using harmonicity and postive type of Coulomb potential give

$$\sum_{1\leq i<j\leq N} \frac{e_i e_j}{|x_i - x_j|} \geq -\sum_{i=1}^{N} W_i,$$

$$W_i \text{``}=\text{''} C \max\{|x_i - x_j|^{-1} \mid e_i e_j = -1\}$$

I.e., W_i is *essentially* the attraction of the i-th particle to the nearest particle of the opposite charge.

THEOREM 6 (*Lieb-Yau '88, Baxter '80***).** *The above inequality holds also if we sum only over negatively (positively) charged particles on the right.*

This theorem and the Lieb-Thirring inequality prove stability of matter even if we ignore the kinetic energy of the positive particles.

The Sobolev inequality and the electrostatic estimate can control the irrelevant terms in the Bose case, after reducing to a box.

The sliding electrostatic estimate

In order to ignore the interaction between boxes of size ℓ one may use the following estimate of Conlon-Lieb-Yau '88.

THEOREM 7 (The sliding method). *Let X_z be the characteristic funtion of a cube with side ℓ centered at $z \in \mathbb{R}^3$. Then*

$$\sum_{1\leq i<j\leq N} \frac{e_i e_j}{|x_i - x_j|} \text{``}\geq\text{''} \int \sum_{1\leq i<j\leq N} X_z(x_i) \frac{e_i e_j}{|x_i - x_j|} X_z(x_j) dz - C\frac{N}{\ell}$$

Note: $N/\ell \ll N^{7/5}$ if $\ell \gg \ell_0 \sim N^{-2/5}$.

Remarks:

Conlon-Lieb-Yau '88: Proved for Coulomb $\rightarrow$ Yukawa and smoothed characteristic funtion.

Graf-Schenker '95: Proved for cubes $\rightarrow$ simplices and integrating also over rotations.

A many-body kinetic energy localization

One may restrict the kinetic energy to boxes by introducing **Neumann boundary conditions**. But this is **too crude**: It will ignore the term $\int |\nabla\widetilde{\phi}|^2$. Better estimate:

THEOREM 8 (A many body kinetic energy bound).
$\chi_z =$ *"smooth characteristic" function of unit cube centered at* $z \in \mathbb{R}^3$. $a^*(z)$ *creation operator of constant in cube.* $\mathcal{P}_z$ =*projection orthogonal to constants in cube.* $\Omega \subset \mathbb{R}^3$. e_1, e_2, e_3 *standard basis.*
For all $0 < s < 1$

$$(1+\varepsilon(\chi,s))\sum_{i=1}^N -\Delta_i \geq \int_\Omega \Big[\sum_{i=1}^N \mathcal{P}_z^{(i)}\chi_z^{(i)}\frac{(-\Delta_i)^2}{-\Delta_i+s^{-2}}\chi_z^{(i)}\mathcal{P}_z^{(i)}$$

$$+\sum_{j=1}^3\left(\sqrt{a_0^*(z+e_j)a_0(z+e_j)+1/2}-\sqrt{a_0^*(z)a_0(z)+1/2}\right)^2\Big]dz$$

$$-3vol(\Omega), \qquad \varepsilon(\chi,s)\to 0 \text{ as } s\to 0.$$