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Stability of Matter Through an Electrostatic Inequality

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Abstract Stability of matter is proved using an electrostatic inequality which is a manifestation of screening.

Dedicated to Klaus Hepp and Walter Hunziker

1. Introduction

Nonrelativistic matter is described by the Hamiltonian

$$H = -\sum_{i=1}^{N} \Delta^{(i)} + \sum_{\substack{i,j=1 \\ i<j}}^{N+M} \frac{e_i e_j}{|x_i - x_j|} ,$$

accounting for N fermionic electrons $i = 1, \dots , N$ and M nuclei $i = N+1, \dots N+M$ with positions $x_i \in \mathbb{R}^3$ and charges $e_i = -1$, resp. $1 \le e_i \le$ const. Stability of matter is the statement:

Theorem 1. *There is a constant* C *such that*

$$H \ge -C(N+M) . \tag{1}$$

This result has first been proved by Dyson and Lenard [3] and subsequently by Lenard [10], Federbush [5], Eckmann [4], Lieb and Thirring [14] and Fefferman [6]. We refer to [11] for the implications of this result. More recently, stability of matter in magnetic field has been proved [7] (but see [13] for another proof), thereby extending previous results [8, 12]. Here we propose a fairly direct proof of (1) based on an electrostatic inequality: Essentially, Coulomb energies are lowered as $\mathbb{R}^3$ is decomposed into simplices and the interaction is restricted to pairs belonging to the same simplex. This procedure is then repeated until only a few nuclei are left in each simplex.

2. Inequalities

Let $\mathcal{L}$ be a lattice in $\mathbb{R}^3$ with unit cell of unit volume: $|\mathbb{R}^3/\mathcal{L}| = 1$. An open simplex, i.e., a tetrahedron, is a bounded set

$$\Delta = \{x \in \mathbb{R}^3 \mid a_i x < c_i,\ i = 1, \dots, 4\} \tag{2}$$

with $a_i \in \mathbb{R}^3$, $c_i \in \mathbb{R}$. A periodic tiling of $\mathbb{R}^3$ is a collection $T_0 = \{\Delta_\alpha\}$ of disjoint simplices, finitely many up to congruences, such that

$$\bigcup_{\alpha \in T_0} \overline{\Delta}_\alpha = \mathbb{R}^3$$

$$T_0 + u := \{\Delta_\alpha + u\} = T_0 \qquad (u \in \mathcal{L})\ .$$

An example is the tiling given by the $\mathbb{Z}^3$-translations of the simplices obtained by cutting the unit cube $W = [0,1]^3$ with all planes passing through the centre and an edge or a face diagonal of W. This tiling contains just one simplex up to congruences.

We now regard $\mathcal{L}$, T_0 as fixed and define a tiling T of scale $l > 0$ to be one congruent to lT_0. Its simplices are also said to be of scale l. Given a tiling T (of any scale) let

$$\delta_T(x_1, x_2) = \begin{cases} 1 & \text{if } x_1, x_2 \text{ belong to the same simplex of } T\ , \\ 0 & \text{otherwise}\ . \end{cases}$$

The average of a function $f(T)$ of the tilings T of scale l is defined as

$$\langle f \rangle = \int_{\mathrm{SO}(3) \times \mathbb{R}^3/\mathcal{L}} d\mu(R) dy\, f(lR(T_0 + y))\ ,$$

where $d\mu(R)$ is the Haar measure on $R \in \mathrm{SO}(3)$. This definition is Euclidean invariant in the sense that it is not affected if $\mathcal{L}$, T_0 are replaced by $R\mathcal{L}$, $R(T_0 + y)$ for some $R \in \mathrm{SO}(3)$, $y \in \mathbb{R}^3$.

Theorem 2. *There is $C > 0$ such that for any $N \in \mathbb{N}$, any $x_i \in \mathbb{R}^3$, $e_i \in \mathbb{R}$, $(i = 1, \dots, N)$ and any $l > 0$*

$$\sum_{\substack{i,j=1 \\ i<j}}^{N} \frac{e_i e_j}{|x_i - x_j|} \geq \Big\langle \sum_{\substack{i,j=1 \\ i<j}}^{N} \frac{e_i e_j}{|x_i - x_j|} \delta_T(x_i, x_j) \Big\rangle - \frac{C}{l} \sum_{i=1}^{N} e_i^2\ , \tag{3}$$

where the average is over tilings T of scale l.

This result, although not explicitely stated, is contained in [9]. Previously, similar inequalities were derived in [1] and in [2]: There the tiling is made of cubes, the average is over translations and the interaction on the r.h.s. is of Yukawa type but, as here, the two sides of the inequality differ by an interaction of positive type.

The proof of (3) is based on the following two lemmas, whose proof is given in the Appendix. The spherical average of a function $f : \mathbb{R}^3 \to \mathbb{R}$ is the function $\bar{f} : [0, +\infty) \to \mathbb{R}$ given by

$$\bar{f}(|x|) = \int_{\mathrm{SO}(3)} d\mu(R) f(R^{-1}x) \, . \tag{4}$$

Lemma 3. *Let Δ be a simplex with characteristic function χ. Set $\chi_-(x) = \chi(-x)$ and let $h(r)$ be the spherical average of $\chi * \chi_-$. Then $h \in \mathrm{C}_0^2[0, +\infty)$, $h(0) = |\Delta|$ and $h''(r)$ is non-increasing in r.*

Lemma 4. *Let $h \in \mathrm{C}^2[0, +\infty)$ with $\lim_{r\to+\infty} h(r) = 0$ and let $h''(r)$ be non-increasing. Then*

$$w(x) = \frac{h(0) - h(|x|)}{|x|} \, , \qquad (x \in \mathbb{R}^3)$$

has positive Fourier transform: $\widehat{w}(p) \geq 0$.

Proof of Theorem 2. By scaling it suffices to prove (3) for $l = 1$. In this case it follows from the fact that the function $w(x)$ given by

$$w(x_1 - x_2) = \frac{1}{|x_1 - x_2|}(1 - \langle \delta_T(x_1, x_2)\rangle)$$

is of positive type, and that $C = w(0)/2 < +\infty$. The proof of these properties is as follows: T_0 consists of finitely many simplices $\Delta^{(i)}$, $(i = 1, \ldots, n)$ up to $\mathcal{L}$-translations. Let $\chi^{(i)}$ (resp. χ_α) be the characteristic function of $\Delta^{(i)}$, (resp. Δ_α). Using $\delta_{T_0}(x_1, x_2) = \sum_{\alpha\in T_0} \chi_\alpha(x_1)\chi_\alpha(x_2)$ and $\delta_{R(T_0+y)}(x_1, x_2) = \delta_{T_0}(R^{-1}x_1 - y, R^{-1}x_2 - y)$ we get

$$\begin{aligned}
\langle \delta_T(x_1, x_2)\rangle &= \int_{\mathrm{SO}(3)\times\mathbb{R}^3/\mathcal{L}} d\mu(R)dy \sum_{\alpha\in T_0} \chi_\alpha(R^{-1}x_1 - y)\chi_\alpha(R^{-1}x_2 - y) \\
&= \sum_{i=1}^{n} \int_{\mathrm{SO}(3)\times\mathbb{R}^3} d\mu(R)dy\, \chi^{(i)}(R^{-1}x_1 - y)\chi^{(i)}(R^{-1}x_2 - y) \\
&= \sum_{i=1}^{n} \int_{\mathrm{SO}(3)} d\mu(R)\, \chi^{(i)} * \chi_-^{(i)}(R^{-1}(x_1 - x_2)) \, .
\end{aligned}$$

The claim now follows from the above lemmas, together with $\langle \delta_T(x, x)\rangle = 1$. ∎

For the sake of simplicity we shall from now on assume that all Δ_α, $\alpha \in T$ are congruent to a single one $\Delta = l\Delta_0$, as in the example previously mentioned. We fix an open cube $Q_0 \supset \overline{\Delta}_0$ and let Q (resp. Q_α) be a cube in a fixed relative position to Δ (resp. Δ_α), i.e., if $\Delta_\alpha = lR(\Delta_0 + y)$ then $Q_\alpha = lR(Q_0 + y)$.

Lemma 5. *Let Δ_B be the Neumann-Laplacian for an open set $B \subset \mathbb{R}^3$. Then*

$$-\Delta_B \geq \left\langle \frac{|\Delta_0|}{|Q_0|} \sum_{\alpha \in T} (-\Delta_{Q_\alpha \cap B}) \right\rangle , \tag{5}$$

where the average is over tilings T of scale l.

Proof. This follows from integrating $|\nabla\psi|^2$ against

$$\left\langle \sum_{\alpha \in T} \chi_{Q_\alpha \cap B}(x) \right\rangle = \left\langle \sum_{\alpha \in T} \chi_{Q_\alpha}(x) \right\rangle \chi_B(x) = \frac{|Q_0|}{|\Delta_0|} \chi_B(x) .$$ ■

Let Δ be the simplex of scale l. We shall consider Hamiltonians of the form

$$H_{\Delta,S} = \kappa l^2 K_Q + l V_S ,$$

where $\kappa > 0$ will be fixed later, $S \subset \Delta$ and

$$K_Q = \sum_i{}^{*} (-\Delta_Q^{(i)}) , \qquad V_S = \sum_{i<j} \frac{e_i e_j}{|x_i - x_j|} \chi_S(x_i) \chi_S(x_j) ,$$

with the $*$ indicating that the sum is over electrons only. Scaling yields the unitary equivalence $H_{l\Delta_0,lS} \cong H_{\Delta_0,S}$. We also set $H_\Delta = H_{\Delta,\Delta}$. Moreover, let M_B, resp. N_B be the number of nuclei, resp. electrons in $B \subset \mathbb{R}^3$.

From (3, 5) we obtain a decoupling inequality for tilings T of scale l,

$$H \geq l^{-1} \left(\left\langle \sum_{\alpha \in T} H_{\Delta_\alpha} \right\rangle - C(N + M) \right) , \tag{6}$$

provided $\kappa l \leq |\Delta_0| / |Q_0|$.

3. Stability of Matter

We shall prove that the 'energy in finite volume' is bounded below:

Proposition 6. *There are κ, $C > 0$ such that*

$$H_{\Delta_0} \geq -C . \tag{7}$$

Proof of Theorem 1. By scaling, the bound (7) holds for Δ of any scale and can be replaced by $H_\Delta \geq -CM_\Delta$, since $H_\Delta \geq 0$ if $M_\Delta = 0$. Together with (6) this proves stability of matter (1). ■

i) One electron, one nucleus: The uncertainty principle. For the simplex Δ_0 we have

$$-\Delta_{Q_0} - \frac{e}{|x-y|}\chi_S(x) \geq -C \tag{8}$$

for some $C > 0$, uniformly in $y \in \mathbb{R}^3$, $e \leq$ const and $S \subset \Delta_0$. To show this [6], let $V(x) = |x-y|^{-1}\chi_S(x)$ and ψ, $\nabla\psi \in \mathrm{L}^2(Q_0)$. Set $\bar{\psi} = |Q_0|^{-1}\int_{Q_0}\psi$. Then, for any $\varepsilon > 0$,

$$\begin{aligned}(V\psi,\psi) &\leq 2\varepsilon^{-1}(V\bar{\psi},\bar{\psi}) + 2\varepsilon(V(\psi-\bar{\psi}),\psi-\bar{\psi}) \leq 2\varepsilon^{-1}\|V\|_1|\bar{\psi}|^2 + 2\varepsilon\|V\|_{3/2}\|\psi-\bar{\psi}\|_6^2 \\ &\leq 2\varepsilon^{-1}|Q_0|^{-1}\|V\|_1\|\psi\|_2^2 + 2C'\varepsilon\|V\|_{3/2}\|\nabla\psi\|_2^2\end{aligned}$$

by Hölder and Sobolev inequalites, where the p-norms are those of $\mathrm{L}^p(Q_0)$. This proves (8).

ii) Many electrons, no nuclei: The Pauli principle. For the cube Q_0 we have

$$K_{Q_0} \geq c(N_{Q_0} - 1)_+^{5/3} \tag{9}$$

for some $c > 0$. This follows from the Pauli principle by filling one-particle levels.

iii) Many electrons, many nuclei: Screening.

Lemma 7. *Given $C_0, K > 0$ there are $C_1, \kappa > 0$ depending respectively on C_0 and K only, such that*

$$H_{\Delta_0,S} \geq C_0(N_S + M_S) - C_1 \tag{10}$$

for any $S \subset \Delta_0$, provided

$$M_S \leq K\ . \tag{11}$$

Proof. Let y_j, $j = 1,\dots, M_S$ be the positions of the nuclei in S. By dropping the repulsion between electrons we have for $\kappa \geq 2K$

$$\begin{aligned}H_{\Delta_0,S} &\geq \frac{\kappa}{2}K_{Q_0} + \sum_{j=1}^{M_S}\sum_i{}^{\bullet}\Big(-\frac{\kappa}{2M_S}\Delta_{Q_0}^{(i)} - \frac{e_j}{|x_i - y_j|}\chi_S(x_i)\Big) + \sum_{j<k}\frac{e_j e_k}{|y_j - y_k|} \\ &\geq \frac{c\kappa}{2}(N_{Q_0} - 1)_+^{5/3} - CM_S N_{Q_0} + \mathrm{const}\, M_S(M_S - 1)\ ,\end{aligned}$$

by using (8, 9) and $\mathrm{diam}(\Delta_0) < +\infty$. Due to $M_S N_{Q_0} \leq M_S + K(N_{Q_0} - 1)_+^{5/3}$ we see that if $c\kappa/2 \geq CK + 1$ in addition then

$$H_{\Delta,S} - C_0(N_{Q_0} + M_S) \geq (N_{Q_0} - 1)_+^{5/3} - C_0 N_{Q_0} + \mathrm{const}\, M_S(M_S - 1) - (C + C_0)M_S\ .$$

The r.h.s. has a lower bound $-C_1$ depending on C_0 only. Clearly, $N_S \leq N_{Q_0}$. ∎

Lemma 8. *There is $\kappa > 0$ such that (10) holds for some C_0, $C_1 > 0$ without the restriction (11).*

Remark. This implies Proposition 6.

Proof. We choose $0 < l < \min(|\Delta_0|/|Q_0|, 1/2)$ such that if Δ is any simplex of scale l intersecting Δ_0 then $Q \subset Q_0$. Let ω be the maximal number of such Δ's occurring in any tiling of scale l. Using (3, 5) once more we have

$$H_{\Delta_0,S} \geq l^{-1}\Big(\Big\langle \sum_{\substack{\alpha\in T \\ Q_\alpha\subset Q_0}} H_{\Delta_\alpha,S_\alpha}\Big\rangle - C(N_S + M_S)\Big) , \tag{12}$$

where $S_\alpha = S \cap \Delta_\alpha$ and the average is over tilings $T = \{\Delta_\alpha\}$ of scale l. Here we dropped any $\alpha \in T$ with $Q_\alpha \not\subset Q_0$ since their contribution is purely kinetic.

We shall prove prove the lemma by induction in $n = 0, 1, \dots$, the induction assumption being: (10) holds provided $M_{S\cap\Delta^{(n)}} \leq K$ for any simplex $\Delta^{(n)}$ of scale l^n, where K will be fixed below. Clearly any given configuration of non-coinciding nuclei satisfies this condition for some $n \in \mathbb{N}$. The case $n = 0$ corresponds to Lemma 7. We may thus assume $M_S > K$. If $n \geq 1$ the induction assumption applies to the simplices $\Delta_\alpha \supset S_\alpha$ of scale l, after scaling them to scale 1. The r.h.s. of (12) is thus the average of

$$l^{-1} \sum_{\substack{\alpha\in T \\ Q_\alpha\subset Q_0}} \Big(H_{\Delta_\alpha,S_\alpha} - C(N_{S_\alpha} + M_{S_\alpha})\Big) \geq l^{-1}\Big((C_0 - C)(N_S + M_S) - C_1\omega\Big)$$

$$= 2C_0(N_S + M_S) - \frac{C_1\omega}{l} ,$$

where we set $C_0 = C(1 - 2l)^{-1}$. Now C_1 is fixed by the previous lemma, but not K. By taking it large enough (independent of n) we have

$$\frac{C_1\omega}{lM_S} \leq \frac{C_1\omega}{lK} \leq C_0$$

and hence $H_{\Delta_0,S} \geq C_0(N_S + M_S)$. ∎

Appendix

For the convenience of the reader we include the proofs [9] of Lemma 3 and 4. We remark that $a_i \in \mathbb{R}^3$, $c_i \in \mathbb{R}$ in (2) can be normalized as

$$\sum_{i=1}^{4} a_i = 0 , \tag{13}$$

$$|\det(a_i, a_j, a_k)| = \frac{1}{6} . \tag{14}$$

Here i, j, k is some (and, by (13), any) triple of distinct integers in $\{1, \dots, 4\}$. Elementary considerations show that the volume of Δ is

$$|\Delta| = \Big(\sum_{i=1}^{4} c_i\Big)_+^3 , \tag{15}$$

where $x_+ = \max(x, 0)$. The spherical average (4) of a function $f : \mathbb{R}^3 \to \mathbb{R}$ is also given by $\bar{f}(r) = \int_{S^2} d\omega f(r\omega)$, where $d\omega$ is the normalized surface measure on the unit sphere $S^2 = \{\omega \in \mathbb{R}^3 \mid |\omega| = 1\}$.

Proof of Lemma 3. We begin with

$$\chi * \chi_-(x) = \int dy \chi(x-y)\chi(-y) = \int dy \chi(y)\chi(y+x) = |\Delta \cap (\Delta - x)| .$$

Note that $y \in \Delta \cap (\Delta - x)$ iff $a_i y < c_i$ and $a_i y < c_i - a_i x$ for $i = 1, \dots, 4$, i.e., iff

$$a_i y < \min(c_i, c_i - a_i x) = c_i - (a_i x)_+ \qquad (i = 1, \dots, 4) .$$

Hence $\Delta \cap (\Delta - x)$ is again a simplex. According to (15) its volume is

$$|\Delta \cap (\Delta - x)| = \Big(\sum_{i=1}^{4} c_i - (a_i x)_+\Big)_+^3 = |\Delta|(1 - k(\omega)r)_+^3 ,$$

where we set $x = r\omega$ ($r \geq 0$, $\omega \in S^2$) and $k(\omega) = |\Delta|^{-1/3}\sum_{i=1}^{4}(a_i\omega)_+$. This last function is continuous on S^2 and has a positive minimum there. Indeed, if $k(\omega) = 0$ for some $\omega \in S^2$ then $a_i\omega = 0$ for $i = 1, \dots, 4$ because of (13). Together with (14), this would imply that the four vectors a_1, a_2, a_3, $\omega \in \mathbb{R}^3$ are linearly independent, which is impossible. As a result,

$$h(r) = |\Delta| \int_{S^2} d\omega (1 - k(\omega)r)_+^3$$

has compact support. Its second derivative $h''(r) = 6|\Delta| \int_{S^2} d\omega k(\omega)^2 (1 - k(\omega)r)_+$ is continuous and non-increasing in r. ∎

Proof of Lemma 4. We note that $h, -h', h'' \geq 0$. Passing to spherical coordinates we find for $p \neq 0$

$$\begin{aligned}
\widehat{w}(p) &= \lim_{\varepsilon \downarrow 0} \int dx e^{-ipx} e^{-\varepsilon|x|} w(x) = \frac{4\pi}{|p|} \lim_{\varepsilon \downarrow 0} \int_0^\infty dr \sin(|p|r) e^{-\varepsilon r}(h(0) - h(r)) \\
&= -\lim_{\varepsilon \downarrow 0} \frac{4\pi}{\varepsilon^2 + |p|^2} \int_0^\infty dr (\cos(|p|r) + \frac{\varepsilon}{|p|}\sin(|p|r)) e^{-\varepsilon r} h'(r) = -\frac{4\pi}{|p|^2} \int_0^\infty dr \cos(|p|r) h'(r) \\
&= \frac{4\pi}{|p|^3} \int_0^\infty dr \sin(|p|r) h''(r) = \frac{4\pi}{|p|^4} \sum_{k=0}^{\infty} (-1)^k \int_0^\pi dt \sin t \, h''\Big(\frac{k\pi + t}{|p|}\Big) \geq 0 .
\end{aligned}$$

The third and fifth equalities are obtained by partial integration. The series above is alternating because $h'' \geq 0$ is non-increasing. Hence the final inequality. ∎

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References

[1] J.G. Conlon, E.H. Lieb, H.T. Yau, The $N^{7/5}$ law for charged bosons, Commun. Math. Phys. **116**, 417-448 (1988).

[2] J.G. Conlon, E.H. Lieb, H.T. Yau, The Coulomb gas at low temperature and low density, Commun. Math. Phys. **125**, 153-180 (1989).

[3] F.J. Dyson, A. Lenard, Stability of matter, I, J. Math. Phys. **8**, 423-434 (1967).

[4] J.P. Eckmann, Sur la stabilité de la matière, Lecture notes (unpublished).

[5] P. Federbush, A new approach to the stability of matter problem, J. Math. Phys. **16**, 347-351, 706-709 (1975).

[6] C.L. Fefferman, The uncertainty principle, Bull. A.M.S. **9**, 129-206 (1983).

[7] C.L. Fefferman, unpublished.

[8] J. Fröhlich, E.H. Lieb, M. Loss, Stability of Coulomb systems with magnetic fields I. The one-electron atom, Commun. Math. Phys. **104**, 251-270 (1986).

[9] G.M. Graf, D. Schenker, On the molecular limit of Coulomb gases, Commun. Math. Phys., to appear.

[10] A. Lenard, in *Statistical Mechanics and Mathematical Problems*, A. Lenard ed., Springer (1973).

[11] E.H. Lieb, The stability of matter, Rev. Mod. Phys. **48**, 553-569 (1976).

[12] E.H. Lieb, M. Loss, Stability of Coulomb systems with magnetic fields II. The many-electron atom and the one-electron molecule, Commun. Math. Phys. **104**, 271-282 (1986).

[13] E.H. Lieb, M. Loss, J.P. Solovej, Stability of matter in magnetic fields, Phys Rev. Lett. **75**, 985-989 (1995).

[14] E.H. Lieb, W. Thirring, Bound for the kinetic energy of fermions which proves the stability of matter, Phys. Rev. Lett. **35**, 687-689 (1975). Errata **35**, 1116 (1975).