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An electrostatic inequality with applications to the constitution of matter

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Abstract. We discuss an electrostatic inequality, based on tetrahedra, which is a manifestation of the screening property of the Coulomb interaction. Several known features of the constitution of matter can be understood as an application of this inequality.

The inequality

The statement which is at the center of this contribution is essentially as follows: Let a periodic tiling of $\mathbb{R}^3$ into simplices, i.e., tetrahedra, be given. Then the electrostatic energy of an arbitrary number of charged particles becomes smaller if the interaction is restricted to particles belonging to the same simplex in the tiling. At least, this is (almost) true on average w.r.t. translations and rotations of the tiling. We should now present the precise statement:

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 is a bounded set

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

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

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

where $d\mu(R)$ is the Haar measure on $R \in SO(3)$. 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 $R \in SO(3)$, $y \in \mathbb{R}^3$.

Theorem 1. [8, 9] *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 $l > 0$*

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

where the average is over tilings T of scale l.

Related inequalities were derived in [1] and in [2]: There the tiling is made of (smeared out) cubes, the average is over translations and the interaction on the r.h.s. is of Yukawa type.

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

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

has positive Fourier transform $\hat{w}(p) \geq 0$, and that $C = w(0)/2 < +\infty$. The proof of these properties is as follows: T_0 consists of finitely many simplices $\Delta^{(i)}$, $(i = 1, \dots, n)$ up to $\mathcal{L}$-translations. Let $[0, +\infty) \ni r \mapsto h_\Delta(r)$ be the spherical average of the function $\mathbb{R}^3 \ni x \mapsto |\Delta \cap (\Delta - x)|$. It is a matter of computation to verify that

$$w(x) = \sum_{i=1}^{n} \frac{h_{\Delta^{(i)}}(0) - h_{\Delta^{(i)}}(|x|)}{|x|} \,.$$

The next two observations are crucial:

i) Let Δ be a simplex. Then $h''_\Delta(r)$ is non-increasing in r.

ii) Let $h \in C^2[0, +\infty)$ with $\lim_{r \to +\infty} h(r) = 0$ and let $h''(r)$ be non-increasing. Then $v(x) = |x|^{-1}(h(0) - h(|x|))$ has positive Fourier transform.

The first claim depends on the fact that $\Delta \cap (\Delta - x)$ is geometrically similar to Δ, a property which characterizes simplices. The second one follows by an integration by parts:

$$\widehat{v}(p) = \frac{4\pi}{|p|^3} \int_0^\infty dr \sin(|p| r) h''(r) = \frac{4\pi}{|p|^4} \sum_{k=0}^{\infty} (-1)^k \int_0^\pi dt \sin t \, h''\Big(\frac{k\pi + t}{|p|}\Big) \geq 0 \,. \qquad \blacksquare$$

Applications

The applications we present are concerned with Hamiltonians of Coulomb systems. The above inequality allows to obtain lower bounds for those Hamiltonians in terms of finite volume Hamiltonians.

1. Stability of matter. Non-relativistic 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. $1 \le e_i \le \text{const}$. Stability of matter is the statement:

Theorem 2. *There is a constant C such that*

$$H \ge -C(N+M) . \tag{2}$$

This result has first been proved by Dyson and Lenard [3] and subsequently by Lenard [11], Federbush [5], Eckmann [4], Lieb and Thirring [14] and Fefferman [6]. We refer to [12] for the implications of this result. A proof [8] of (2) can be obtained by applying the above inequality repeatedly — at ever smaller scales — until only a few nuclei are left in each simplex. At this point the uncertainty principle and the Pauli principle guarantee stability.

2. The molecular limit of Coulomb gases. A mixture of electrons and various kinds of nuclei consists of individual atoms and molecules, provided the temperature and the density are sufficiently low. Put differently, a gas of elementary particles is effectively described in this thermodynamic regime in terms of an ideal gas of composite particles. Different mathematical formulations and verifications of this fact have been given by Fefferman [7], by Conlon, Lieb and Yau [2], and by Macris and Martin [15]. See also [16, 17] for a discussion of the issues involved.

The mixture shall consist of S species of spinless particles with masses $\mathbf{M} = (M_1, \dots , M_S)$ and charges $\mathbf{Q} = (Q_1, \dots , Q_S) \in \mathbb{Z}^S$. We assume that all negatively charged particles are fermions, whereas the statistics of the other particles is irrelevant. Let $N_k \in \mathbb{N}$ be the number of particles of the k-th species, and set $\mathbf{N} = (N_1, \dots , N_S)$. The total number of particles is $N = \sum_{k=1}^{S} N_k$. The Hilbert space $\mathcal{H}_{\mathbf{N},\Lambda}$ for $\mathbf{N}$ particles confined to an open set $\Lambda \subset \mathbb{R}^3$ is the subspace of $\mathrm{L}^2(\Lambda)^{\otimes N}$ carrying the permutation symmetry appropriate to the given statistics. The Hamiltonian is

$$H_{\mathbf{N},\Lambda} = -\sum_{i=1}^{N} \frac{\Delta_{\Lambda,i}}{2m_i} + \sum_{\substack{i,j=1 \\ i<j}}^{N} \frac{q_i q_j}{|x_i - x_j|} =: T_{\mathbf{N},\Lambda} + V_{\mathbf{N}} ,$$

where $(m_i, q_i) = (M_k, Q_k)$ if the i-th particle belongs to the k-th species. Here Δ_Λ is the Dirichlet Laplacian on Λ. If $\Lambda = \mathbb{R}^3$, the index Λ is omitted. Variable particle numbers are accounted for by means of the Fock space and the Hamiltonian

$$\mathcal{H}_\Lambda = \mathcal{F}(\mathrm{L}^2(\Lambda)) = \bigoplus_{\mathbf{N}} \mathcal{H}_{\mathbf{N},\Lambda} , \qquad H_\Lambda = \bigoplus_{\mathbf{N}} H_{\mathbf{N},\Lambda} .$$

For bounded Λ, the grand canonical partition function and the (finite volume) pressure are given by

$$\Xi(\beta, \boldsymbol{\mu}, \Lambda) = \mathrm{tr}_{\mathcal{H}_\Lambda} \mathrm{e}^{-\beta(H_\Lambda - \boldsymbol{\mu}\cdot\mathbf{N})} = \sum_{\mathbf{N}} \mathrm{tr}_{\mathcal{H}_{\mathbf{N},\Lambda}} \mathrm{e}^{-\beta(H_{\mathbf{N},\Lambda} - \boldsymbol{\mu}\cdot\mathbf{N})} ,$$
$$p(\beta, \boldsymbol{\mu}, \Lambda) = (\beta|\Lambda|)^{-1} \log \Xi(\beta, \boldsymbol{\mu}, \Lambda) ,$$

where $\beta > 0$ is the inverse temperature and $\boldsymbol{\mu} = (\mu_1, \ldots , \mu_S) \in \mathbb{R}^S$ are the chemical potentials of the various species. The existence of the thermodynamic limit

$$p(\beta, \boldsymbol{\mu}) = \lim_{\Lambda\to\infty} p(\beta, \boldsymbol{\mu}, \Lambda)$$

for suitable sequences $\{\Lambda\}$ (e.g. sequences of balls) has been proven by Lieb and Lebowitz [13]. They also proved that

$$p(\beta, \boldsymbol{\mu}) = p(\beta, \boldsymbol{\mu} + \lambda\mathbf{Q}) \qquad (\lambda \in \mathbb{R}) , \tag{3}$$

which expresses charge neutrality.

A basic version of the result [2, 7] states that for suitable values of the chemical potentials $\boldsymbol{\mu}_0$ and for low enough temperature β^{-1} the pressure of the S species is to good accuracy that of a classical free gas of specific 'molecules'. In this picture, molecules are non-interacting particles with no internal degrees of freedom. The types of molecules which actually occur are determined by the neutral ground states of $H - \boldsymbol{\mu}_0 \cdot \mathbf{N}$, as we shall explain shortly. Let $E_{\mathbf{N}}$ and $E(\boldsymbol{\mu})$ be the ground state energies of $H_{\mathbf{N}}$, resp. of $H - \boldsymbol{\mu} \cdot \mathbf{N}$ except for the vacuum, i.e., let

$$E_{\mathbf{N}} = \inf\{(\Psi, H_{\mathbf{N}}\Psi) \mid \Psi \in \mathcal{H}_{\mathbf{N}}, \|\Psi\| = 1\} ,$$
$$E(\boldsymbol{\mu}) = \inf_{\mathbf{N}\neq\mathbf{0}} (E_{\mathbf{N}} - \boldsymbol{\mu} \cdot \mathbf{N}) .$$

Our assumption (A) on the chemical potentials $\boldsymbol{\mu}_0$ embodies the symmetry (3): There is $\lambda_0 \in \mathbb{R}$ such that

$$\boldsymbol{\mu}_0' = \boldsymbol{\mu}_0 + \lambda_0\mathbf{Q}$$

enjoys the following two properties.

1) For some $\sigma > 0$ and all $\mathbf{N}$,

$$H_{\mathbf{N}} - \boldsymbol{\mu}_0' \cdot \mathbf{N} \geq \sigma N .$$

A first consequence is that $E(\boldsymbol{\mu}_0') > 0$ and that the set of 'ground states',

$$\mathcal{G} = \{\mathbf{N} \neq \mathbf{0} \mid E_{\mathbf{N}} - \boldsymbol{\mu}_0' \cdot \mathbf{N} = E(\boldsymbol{\mu}_0')\} ,$$

is non-empty and finite. In the center of mass frame for $\mathbf{N} \in \mathcal{G}$ the ground state energy $E_{\mathbf{N}}$ of $H_{\mathbf{N}}$ is a discrete eigenvalue. We shall henceforth count $\mathbf{N} \in \mathcal{G}$ repeatedly, according to the multiplicity of this eigenvalue.

2) Either $\mathbf{Q} \cdot \mathbf{N} = 0$ for all $\mathbf{N} \in \mathcal{G}$ (neutral case) or there are $\mathbf{N}_+, \mathbf{N}_- \in \mathcal{G}$ with $\pm\mathbf{Q} \cdot \mathbf{N}_\pm > 0$ (charged case).

The pressure of an ideal classical gas of molecules of composition $\mathbf{N}$, internal energy $E_{\mathbf{N}}$ and chemical potential μ is

$$p_{\mathbf{N}}(\beta, \mu) = \frac{1}{\beta}\Big(\frac{\mathbf{M} \cdot \mathbf{N}}{2\pi\beta}\Big)^{3/2} \mathrm{e}^{-\beta(E_{\mathbf{N}} - \mu)} .$$

Consider an ideal mixture of such gases with compositions $\mathbf{N} \in \mathcal{G}$. This notion is defined in thermodynamics by the additivity of partial pressures:

$$p_{\mathcal{G}}(\beta, \boldsymbol{\mu}) = \sum_{\mathbf{N} \in \mathcal{G}} p_{\mathbf{N}}(\beta, \boldsymbol{\mu} \cdot \mathbf{N}) .$$

The chemical potentials on the r.h.s. correspond to chemical equilibrium among the molecules $\mathbf{N} \in \mathcal{G}$. The pressure $p_{\mathcal{G}}$ may not satisfy (3), i.e., it may be related to a non-neutral ensemble. This can happen because the molecules, although possibly charged, do not interact in this picture. One enforces (3) by setting

$$p^0_{\mathcal{G}}(\beta, \boldsymbol{\mu}) = \inf_{\lambda \in \mathbb{R}} p_{\mathcal{G}}(\beta, \boldsymbol{\mu} + \lambda\mathbf{Q}) .$$

Theorem 3. [2, 7] *Suppose assumption (A) holds. Then*

$$p(\beta, \boldsymbol{\mu}) = p^0_{\mathcal{G}}(\beta, \boldsymbol{\mu})(1 + \mathrm{O}(\mathrm{e}^{-\varepsilon\beta})) \tag{4}$$

for some $\varepsilon > 0$ in the limit $(\beta, \boldsymbol{\mu}) \to (+\infty, \boldsymbol{\mu}_0)$.

In order to prove (4) as an upper bound, the inequality (1) can be used in the form of the following lemma.

Lemma 4. [9] *There is a simplex $\varDelta$ such that*

$$p(\beta, \boldsymbol{\mu}) \leq p(\beta, \boldsymbol{\mu} + \mathrm{O}(l^{-1}), l\varDelta)(1 + \mathrm{O}(l^{-1})) , \qquad (l \to +\infty) \tag{5}$$

uniformly in $\beta > 0$ and $\boldsymbol{\mu} \in \mathbb{R}^S$.

In rough terms, (1) yields a lower bound on H_Λ in terms of $H_{l\varDelta}$, which translates into the upper bound (5) for the corresponding pressures. Thereby, the last term in (1) is absorbed into a readjustment of the chemical potentials $\boldsymbol{\mu}$ by $\mathrm{O}(l^{-1})$ in (5). The factor $1 + \mathrm{O}(l^{-1})$ can be understood as coming from the Dirichlet boundary conditions on $l\Delta$.

We make use of the above lemma for $l = \mathrm{e}^{\gamma\beta}$ with $\gamma > 0$ small enough. Then the simplex $l\Delta$ most likely does not contain anything, but if it does, then most likely a molecule $\mathrm{N} \in \mathcal{G}$. This situation gives raise to the pressure $p_{\mathcal{G}}(\beta, \boldsymbol{\mu})$.

3. The continuity of the free energy. The canonical partition function and the (finite volume) free energy density for a Coulomb systems of S species are

$$Z(\boldsymbol{N}, \Lambda) = \mathrm{tr}_{\mathcal{H}_{\mathbf{N},\Lambda}} \mathrm{e}^{-H_{\mathbf{N},\Lambda}} ,$$
$$f(\boldsymbol{N}, \Lambda) = -|\Lambda|^{-1} \log Z(\boldsymbol{N}, \Lambda) .$$

where we set $\beta = 1$. The thermodynamic limit for the free energy

$$f_S(\boldsymbol{\rho}) = \lim_{\Lambda \to \infty} f(\boldsymbol{N}, \Lambda)$$

exists [13] for neutral systems $\boldsymbol{N} \cdot \boldsymbol{Q} = 0$ with $\lim_{\Lambda\to\infty} \boldsymbol{N}/|\Lambda| = \boldsymbol{\rho}$. The limiting densities $\boldsymbol{\rho}$ are those in

$$P_S = \{\boldsymbol{\rho} = (\rho_1, \ldots, \rho_S) \mid \boldsymbol{\rho} \cdot \mathbf{Q} = 0,\ \rho_i \geq 0,\ i = 1, \ldots, S\} .$$

The function $f_S(\boldsymbol{\rho})$ is convex on P_S [13] and hence continuous on its interior $\mathring{P}_S$. At points in ∂P_S convexity only implies upper semicontinuity. Nevertheless one has:

Theorem 5. [10] *$f_S(\boldsymbol{\rho})$ is continuous on P_S.*

The lower semicontinuity of f_S at points $\boldsymbol{\rho}_0 \in \partial P_S$ of the form $\boldsymbol{\rho}_0 = (\boldsymbol{\rho}_0', \mathbf{0})$ with $\boldsymbol{\rho}_0' \in \mathring{P}_{S'}$ and $0 \leq S' < S$ is the statement

$$\varliminf_{\boldsymbol{\rho} \to \boldsymbol{\rho}_0} f_S(\boldsymbol{\rho}) \geq f_{S'}(\boldsymbol{\rho}_0') . \tag{6}$$

Since $p_S(\boldsymbol{\mu})$ is the Legendre transform of $f_S(\boldsymbol{\rho})$, i.e., $p_S(\boldsymbol{\mu}) = \sup_{\boldsymbol{\rho} \in P_S} [\boldsymbol{\rho} \cdot \boldsymbol{\mu} - f_S(\boldsymbol{\rho})]$, the bound (6) would follow from

$$\varlimsup_{\boldsymbol{\mu} \to (\boldsymbol{\mu}_0', -\infty)} p_S(\boldsymbol{\mu}) \leq p_{S'}(\boldsymbol{\mu}_0') .$$

This, however, follows from (5) and fact that a corresponding statement holds in finite volume.

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