

INEQUALITIES FOR POTENTIALS OF PARTICLE SYSTEMS¹

BY

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1. Let x_1, \dots, x_n be points in \mathbf{R}^3 . Suppose that a (positive or negative) charge e_i is placed at each x_i . The total energy of the system of charges is $V = \sum_{1 \leq i < j \leq n} e_i e_j |x_i - x_j|^{-1}$. V may be negative. We are interested in finding lower bounds for V . If the charges approach a smooth distribution f , then V approaches

$$(1/2) \iint f(x) |x - y|^{-1} f(y) \geq 0.$$

As a tool in attacking the general case, it is useful to consider an intermediate situation in which the negative charges are replaced by a smooth distribution f , but the positive charges remain discrete, say positive charges z_1, \dots, z_m at points y_1, \dots, y_m . We may write the energy V in this case as

$$P(f; z_1, \dots, z_m; y_1, \dots, y_m).$$

It is convenient to make a slight generalization and replace both the positive and negative charges by measures μ_1, \dots, μ_m and ν respectively, while still omitting the self energies of the μ_i . Then V can be written as $P(\nu; \mu_1, \dots, \mu_m)$. In Section 2 we prove a decomposition theorem for P and deduce a simple inequality for our original discrete energy V . In Section 3 a version of the no binding theorem [7], [13] is obtained.

2. For any bounded signed measures μ and ν on \mathbf{R}^3 , let

$$\langle \mu, \nu \rangle = \int |x - y|^{-1} \mu(dx) \nu(dy),$$

provided that the double integral has a well defined finite or infinite value. Define the potential of μ by $\text{Pot } \mu(y) = \int |x - y|^{-1} \mu(dx)$. Then of course

$$\langle \mu, \nu \rangle = \int (\text{Pot } \mu) d\nu = \int (\text{Pot } \nu) d\mu.$$

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If μ has a density f we will sometimes write $\text{Pot } f$ instead of $\text{Pot } \mu$. Suppose ν, μ_1, \dots, μ_m are bounded nonnegative measures with $\langle \mu_i, \nu \rangle$ finite for each i . Let

$$(2.1) \quad P(\nu; \mu_1, \dots, \mu_m) = \left(\frac{1}{2}\right)\langle \nu, \nu \rangle - \sum_{i=1}^m \langle \mu_i, \nu \rangle + \sum_{1 \leq i < j \leq m} \langle \mu_i, \mu_j \rangle.$$

If ν has a density f we may write $P(\nu; \mu_1, \dots, \mu_m)$ as $P(f; \mu_1, \dots, \mu_m)$.

THEOREM 1. *Let ν and $\mu_i, i = 1, \dots, m$, be bounded nonnegative measures on \mathbf{R}^3 . Suppose that $\text{Pot } \nu$ is finite ν -almost everywhere. Then there exist nonnegative measures $\nu_i, i = 1, \dots, m + 1$, such that:*

$$(2.2) \quad \sum_{i=1}^{m+1} \nu_i = \nu,$$

$$(2.3) \quad \text{Pot } \nu_i \leq \text{Pot } \mu_i \text{ on } \mathbf{R}^3, \quad i = 1, \dots, m,$$

$$(2.4) \quad \nu_i(\mathbf{R}^3) \leq \mu_i(\mathbf{R}^3), \quad i = 1, \dots, m,$$

$$(2.5) \quad \text{Pot } \nu_i = \text{Pot } \mu_i, \quad \nu_j\text{-almost everywhere,}$$

for $j = i + 1, \dots, m + 1, \quad i = 1, \dots, m$.

In proving Theorem 1 we need only the following known fact from potential theory: [10], [12], [9], [5]:

THEOREM 2. *Let μ and ν be bounded nonnegative measures on \mathbf{R}^3 . Suppose that $\text{Pot } \nu$ is finite ν -almost everywhere. Then there exists a nonnegative measure λ , such that:*

$$(2.6) \quad \lambda \leq \nu, \quad \lambda(\mathbf{R}^3) \leq \mu(\mathbf{R}^3),$$

$$(2.7) \quad \text{Pot } \lambda \leq \text{Pot } \mu \text{ on } \mathbf{R}^3,$$

$$(2.8) \quad \text{Pot } \lambda = \text{Pot } \mu, \quad (\nu - \lambda)\text{-almost everywhere.}$$

One might say loosely that λ screens μ , as far as $\nu - \lambda$ is concerned.

Proof of Theorem 2. As in [9, Section 2], let σ be the measure, $0 \leq \sigma \leq \nu$, such that $(\text{Pot } \sigma) dm$ is the réduite of $(\text{Pot } (\nu - \mu)) dm$, where m is Lebesgue measure on \mathbf{R}^3 . Since the value of a potential at a point is the limit of its mean values over balls shrinking to the point, the equation $(\text{Pot } \sigma) dm \geq (\text{Pot } (\nu - \mu)) dm$ implies $\text{Pot } \mu \geq \text{Pot } \lambda$ on \mathbf{R}^3 , if we define $\lambda = \nu - \sigma$. Thus (2.7) holds. As a consequence of (2.7), or by proposition 4 of [9], $\lambda(\mathbf{R}^3) \leq \mu(\mathbf{R}^3)$. Thus (2.6) holds.

Since $\text{Pot } \sigma$ is finite σ -almost everywhere, Lusin's theorem implies that there exists a pairwise disjoint sequence of compact sets K_n such that $\mathbf{R}^3 - \bigcup_{n=1}^{\infty} K_n$ is σ -null and such that $\text{Pot } \sigma$ is continuous on each K_n . Define the measure σ_n by $\sigma_n(A) = \sigma(A \cap K_n)$. Since potentials are lower semicontinuous, each $\text{Pot } \sigma_n$ is continuous on K_n and hence on \mathbf{R}^3 by the theorem of Evans and Vasilescu.

Let a_n be the supremum of $\text{Pot } \sigma_n$ on \mathbf{R}^3 , $b_n = (2^n(1 + a_n))^{-1}$, $\gamma = \sum_{n=1}^{\infty} b_n \sigma_n$. Then γ is bounded, $\sigma \ll \gamma$, $\gamma \ll \sigma$, and $\text{Pot } \gamma$ is continuous and bounded on \mathbf{R}^3 . Let $f = \text{Pot } \gamma$.

By Proposition 6 of [9] there exists a sequence g_n of superharmonic functions such that $0 \leq g_n \leq f$ and $\int g_n d(v - \mu) \rightarrow \int f d\sigma$ as $n \rightarrow \infty$. Let γ_n be the measure such that $g_n = \text{Pot } \gamma_n$. We have

$$\int g_n d(v - \mu) = \int \text{Pot } (v - \mu) d\gamma_n \leq \int \text{Pot } \sigma d\gamma_n = \int g_n d\sigma \leq \int f d\sigma.$$

Thus $\int g_n d\sigma \rightarrow \int f d\sigma$ as $n \rightarrow \infty$. Hence $g_n \rightarrow f$ in $\mathcal{L}^1(\sigma)$. By choosing a subsequence and relabelling, we may assume $g_n \rightarrow f$ σ -almost everywhere, hence $g_n \rightarrow f$ γ -almost everywhere.

Fix $x \in \mathbf{R}^3$ and $\varepsilon > 0$. Since $f(x) = \text{Pot } \gamma(x) < \infty$, there exists $\delta > 0$ such that if B is any Borel set with $\gamma(\mathbf{R}^3 - B) < \delta$ then $\text{Pot } \gamma_B(x) \geq f(x) - \varepsilon$, where γ_B is the measure defined by $\gamma_B(A) = \gamma(A \cap B)$. Choose B compact and $N > 0$ such that $\gamma(\mathbf{R}^3 - B) < \delta$ and $g_n \geq f - \varepsilon$ everywhere on B for all $n \geq N$. By the domination principle $g_n(x) \geq \text{Pot } \gamma_B(x) - \varepsilon \geq f(x) - 2\varepsilon$ for $n \geq N$.

Hence $g_n \rightarrow f$ pointwise everywhere on \mathbf{R}^3 . Therefore $\int g_n d(v - \mu) \rightarrow \int f d(v - \mu)$, so that $\int f d(v - \mu) = \int f d\sigma$, or $\int f d\lambda = \int f d\mu$, or $\int (\text{Pot } \mu - \text{Pot } \lambda) d\gamma = 0$. Hence $\text{Pot } \mu = \text{Pot } \lambda$ γ -almost everywhere, so (2.8) holds and Theorem 2 is proved.

Other versions of Theorem 2 are given in [10], [12 Theorem 6], [5 Theorem 2.1], [2]. Theorem 2 actually holds for a wide class of potential kernels, including of course the classical kernel on \mathbf{R}^N , $N \geq 3$. We restrict ourselves to \mathbf{R}^3 for the sake of simplicity.

The work of Rost [12] gives a probabilistic interpretation for the measure λ of Theorem 2, in terms of the filling scheme stopping time. The filling scheme was used originally by Chacon and Ornstein in their proof of the ratio ergodic theorem [1].

Proof of Theorem 1. Follows at once by induction from Theorem 2.

Now let ν_i , $i = 1, \dots, m + 1$ be any system of nonnegative measures satisfying (2.2)–(2.5). Suppose $\langle \mu_i, \nu \rangle$ is finite for $i = 1, \dots, m$. Clearly, for any l , $1 < l \leq m$,

$$(2.9) \quad P(\nu; \mu_1, \dots, \mu_m) = P\left(\sum_{i=1}^l \nu_i; \mu_1, \dots, \mu_l\right) + P\left(\sum_{i=l+1}^m \nu_i; \mu_{l+1}, \dots, \mu_m\right) + Q,$$

where the remainder term Q is nonnegative. We have

$$(2.10) \quad Q = \sum_{i=1}^l \sum_{j=l+1}^m (\langle \mu_i, \mu_j \rangle - \langle \nu_i, \mu_j \rangle) + \frac{1}{2} \langle \nu_{m+1}, \nu_{m+1} \rangle.$$

Iterating (2.9), we have in particular,

$$(2.11) \quad P(\nu; \mu_1, \dots, \mu_m) \geq \sum_{i=1}^m P(\nu_i; \mu_i) \geq - \sum_{i=1}^m \langle \mu_i, \nu_i \rangle.$$

As an application of (2.11), consider negative charges $-q_1, \dots, -q_n$ at points x_1, \dots, x_n , together with positive charges z_1, \dots, z_m at points y_1, \dots, y_m . The total energy is

$$(2.12) \quad V = \sum_{1 \leq i < j \leq n} q_i q_j |x_i - x_j|^{-1} - \sum_{i=1}^n \sum_{j=1}^m q_i z_j |x_i - y_j|^{-1} + \sum_{1 \leq i < j \leq m} z_i z_j |y_i - y_j|^{-1}.$$

Suppose $z_j \leq z$ for $j = 1, \dots, m$. Let $R_i = \inf \{ |x_i - y_j| : j = 1, \dots, m \}$.

PROPOSITION 1. $V \geq -\sum_{i=1}^n q_i^2/R_i - \sum_{i=1}^n 2q_i z/R_i$. In particular if $q_i = 1 = z$, $R_i \geq R$, $i = 1, \dots, n$, we have

$$(2.13) \quad V \geq -3n/R.$$

Proof. For $i = 1, \dots, n$, let γ_i denote the measure of total mass q_i uniformly distributed on the surface of the sphere with centre x_i and radius $R_i/2$. Let μ_j be the measure with mass z_j concentrated at y_j . Clearly $\text{Pot } \gamma_i(y) \leq q_i |y - x_i|^{-1}$ for all y in \mathbf{R}^3 , with equality holding when $|y - x_i| \geq R_i/2$. Hence $\langle \gamma_i, \gamma_j \rangle \leq q_i q_j |x_i - x_j|^{-1}$ and $\langle \gamma_i, \mu_j \rangle = q_i z_j |x_i - y_j|^{-1}$. Thus

$$(2.14) \quad V \geq \sum_{1 \leq i < j \leq n} \langle \gamma_i, \gamma_j \rangle - \sum_{i=1}^n \sum_{j=1}^m \langle \gamma_i, \mu_j \rangle + \sum_{1 \leq i < j \leq m} \langle \mu_i, \mu_j \rangle.$$

Let $v = \sum_{i=1}^n \gamma_i$. Since $\langle \gamma_i, \gamma_i \rangle = 2q_i^2 R_i^{-1}$, we can rewrite (2.14) as

$$(2.15) \quad V \geq -\sum_{i=1}^n q_i^2/R_i + P(v; \mu_1, \dots, \mu_m).$$

By (2.11), for some $v_i \geq 0$, $i = 1, \dots, m$, with $\sum_{i=1}^m v_i \leq v$, we have

$$(2.16) \quad P(v; \mu_1, \dots, \mu_m) \geq -\sum_{i=1}^m \langle \mu_i, v_i \rangle.$$

Let $g(x) = \sup \{ \text{Pot } \mu_j(x) : j = 1, \dots, m \}$. Clearly $g(x) \leq 2zR_i^{-1}$ when x is in the support of γ_i . We have

$$\begin{aligned} & \sum_{i=1}^m \langle \mu_i, v_i \rangle \\ &= \sum_{i=1}^m \int \text{Pot } \mu_i \, dv_i \leq \sum_{i=1}^m \int g \, dv_i \leq \int g \, dv = \sum_{i=1}^n \int g \, d\gamma_i \leq \sum_{i=1}^n 2q_i z R_i^{-1}. \end{aligned}$$

This proves Proposition 1.

The constant 3 in (2.13) is not sharp, as a slight change in the proof shows. On the other hand the best constant cannot be less than 1.5, by a trivial example. It would be of interest to find the best possible value.

Proposition 1 may be compared to an inequality of Onsager [11]. In the notation of Proposition 1, if we let $S_j = \inf \{|x_i - y_j| : i = 1, \dots, n\}$, Onsager's inequality reads

$$(2.17) \quad V \geq - \sum_{i=1}^n q_i^2/R_i - \sum_{j=1}^m z_j^2/S_j.$$

A more general inequality is given in [3, Theorem 6].

If we let $q_i = 1 = z_j$, $R_i \geq R$, $S_j \geq R$ for all i and j , (2.17) becomes

$$(2.18) \quad V \geq -(m + n)/R.$$

The bound in (2.18) depends on $m + n$ rather than n as in (2.13), but the constant is smaller.

The proof of (2.17) is similar to that of Proposition 1, except that (2.11) is not used. Instead, the positivity of the self-energy plays a similar role. This positivity may be expressed as follows: if μ and ν are bounded nonnegative measures with $\langle \mu, \nu \rangle$ finite, then

$$(2.19) \quad \langle \mu - \nu, \mu - \nu \rangle \geq 0.$$

We note that (2.11) implies (2.19). Indeed, fix integral $m > 0$, and let $\mu_i = \mu/m$, $i = 1, \dots, m$. Without loss of generality we may assume that $\langle \mu, \mu \rangle$ and $\langle \nu, \nu \rangle$ are finite. Let ν_i be as in Theorem 1. By (2.11) and (2.3),

$$(2.20) \quad P(\nu; \mu_1, \dots, \mu_m) \geq - \sum_{i=1}^m \langle \mu_i, \nu_i \rangle \geq - \sum_{i=1}^m \langle \mu_i, \mu_i \rangle = - \left(\frac{1}{m}\right) \langle \mu, \mu \rangle.$$

But $\langle \mu - \nu, \mu - \nu \rangle = 2P(\nu; \mu_1, \dots, \mu_m) + \sum_{i=1}^m \langle \mu_i, \mu_i \rangle$, so

$$\langle \mu - \nu, \nu - \mu \rangle \geq -(1/m) \langle \mu, \mu \rangle.$$

Letting $m \rightarrow \infty$ proves (2.19). Thus one may regard (2.11) as an extension of (2.19).

3. Let \mathcal{L} be a space of Lebesgue integrable functions $f \geq 0$ on \mathbf{R}^3 with $\int f < \infty$. (We shall not distinguish functions that differ on a null set.) Suppose \mathcal{L} is closed under addition, and such that if f is in \mathcal{L} , g measurable, and $0 \leq g \leq f$ then g is in \mathcal{L} . As a consequence \mathcal{L} is also closed under multiplication by nonnegative numbers.

Let $\Phi: \mathcal{L} \rightarrow [0, \infty)$ be a nonnegative functional with the property that

$$\Phi(f_1 + f_2) \geq \Phi(f_1) + \Phi(f_2) \quad \text{for all } f_1, f_2 \text{ in } \mathcal{L}.$$

Clearly then $\Phi(0) = 0$ and $\Phi(g) \leq \Phi(f)$ whenever f, g are in \mathcal{L} with $g \leq f$.

We shall assume also that $\langle f, f \rangle$ is finite for all f in \mathcal{L} .

Let μ_1, \dots, μ_m be nonnegative bounded measures with compact support such that $\langle \mu_i, \mu_j \rangle$ is finite for $i \neq j$. For any number $a \geq 0$, let

$$(3.1) \quad F(a; \mu_1, \dots, \mu_m) = \inf \left\{ \Phi(f) + P(f; \mu_1, \dots, \mu_m) : f \in \mathcal{L}, \int f = a \right\}.$$

We will write $F(a) = F(a; \mu_1, \dots, \mu_m)$. Clearly $-\infty \leq F < \infty$. We note:

$$(3.2) \quad F \text{ is nondecreasing on } [z, \infty), \text{ where } z = \sum_{i=1}^m \mu_i(\mathbf{R}^3).$$

To see this, fix $a \geq z$, and $b \geq a$. Let f be in \mathcal{L} with $\int f = b$. f is the density of a measure ν . Let $\nu_i, i = 1, \dots, m + 1$ be the measures of Theorem 1. By (2.4) we can find some $c, 0 \leq c \leq 1$, such that $\sum_{i=1}^m \nu_i(\mathbf{R}^3) + c\nu_{m+1}(\mathbf{R}^3) = a$. Let g be the density of $\sum_{i=1}^m \nu_i + c\nu_{m+1}$. Then $g \leq f$ so $g \in \mathcal{L}$. We have $\int g = a$. Consider (2.9) and (2.10) with ν_{m+1} replaced by $c\nu_{m+1}$ and ν replaced by $\sum_{i=1}^m \nu_i + c\nu_{m+1}$. We see at once that

$$P(f; \mu_1, \dots, \mu_m) = P(g; \mu_1, \dots, \mu_m) + (1 - c^2)^{1/2} \langle \nu_{m+1}, \nu_{m+1} \rangle,$$

and hence that $\Phi(f) + P(f; \mu_1, \dots, \mu_m) \geq \Phi(g) + P(g; \mu_1, \dots, \mu_m)$. Hence

$$\Phi(f) + P(f; \mu_1, \dots, \mu_m) \geq F(a),$$

and thus $F(b) \geq F(a)$. This proves (3.2).

In the Thomas-Fermi case (see (3.4) below), (3.2) is proved in [7].

Now fix $l, 1 \leq l \leq m$. For any $a \geq 0$, let

$$F_1(a) = F(a; \mu_1, \dots, \mu_l), \quad F_2(a) = F(a; \mu_{l+1}, \dots, \mu_m).$$

Let $z_1 = \sum_{i=1}^l \mu_i(\mathbf{R}^3), z_2 = \sum_{i=l+1}^m \mu_i(\mathbf{R}^3)$.

PROPOSITION 2. For any $a \geq 0$,

$$(3.3) \quad F(a) \geq \inf \{F_1(x_1) + F_2(x_2) : 0 \leq x_1 \leq z_1, 0 \leq x_2 \leq z_2, x_1 + x_2 \leq a\}.$$

Proof. Let f be in \mathcal{L} with $\int f = a$. Let $\nu_i, i = 1, \dots, m + 1$, be the measures of Theorem 1. Let f_1 be the density of $\sum_{i=1}^l \nu_i, f_2$ the density of $\sum_{i=l+1}^m \nu_i$. Let $\int f_1 = x_1, \int f_2 = x_2$. By (2.4), $x_1 \leq z_1$, and $x_2 \leq z_2$. By (2.2), $x_1 + x_2 \leq a$. By (2.9),

$$P(f; \mu_1, \dots, \mu_m) \geq P(f_1; \mu_1, \dots, \mu_l) + P(f_2; \mu_{l+1}, \dots, \mu_m).$$

Thus

$$\begin{aligned} \Phi(f) + P(f; \mu_1, \dots, \mu_m) &\geq \Phi(f_1) + P(f_1; \mu_1, \dots, \mu_l) \\ &\quad + \Phi(f_2) + P(f_2; \mu_{l+1}, \dots, \mu_m), \end{aligned}$$

so

$$\Phi(f) + P(f; \mu_1, \dots, \mu_m) \geq F_1(x_1) + F_2(x_2).$$

Then (3.3) follows at once, so Proposition 2 is proved.

If we take

$$(3.4) \quad \mathcal{L} = \left\{ f : f \text{ measurable, } f \geq 0, \int f^{5/3} \text{ and } \int f \text{ finite} \right\}, \quad \Phi(f) = c \int f^{5/3},$$

then all the assumptions of this section are satisfied. Hölder's inequality gives

$$(3.5) \quad \text{Pot } f \leq (\text{constant}) \left[\int f^{5/3} \right]^{1/2} \left[\int f \right]^{1/6} \text{ on } \mathbf{R}^3.$$

By completing a square, (3.5) implies

$$(3.6) \quad F(a) \geq \sum_{1 \leq i < j \leq m} \langle \mu_i, \mu_j \rangle - (\text{constant})z^2 a^{1/3},$$

for all a in $[0, \infty)$.

Considering $f = \alpha \chi_B$, where B is a large ball, gives

$$(3.7) \quad F(a) \leq \sum_{1 \leq i < j \leq m} \langle \mu_i, \mu_j \rangle.$$

(3.6) and (3.7) show F is continuous at 0. Since Φ and P are convex in f , F is convex on $[0, \infty)$, and hence F is continuous on $(0, \infty)$. Thus F is continuous on $[0, \infty)$. Since F is convex and bounded above, F is nonincreasing on $[0, \infty)$. Thus, by (3.2), F is constant on $[z, \infty)$.

Since F_1 and F_2 in (3.3) are now continuous, one can rewrite (3.3) as

$$(3.8) \quad F(a) \geq F_1(a_1) + F_2(a_2),$$

where a_1 and a_2 are chosen to minimize $F(x_1) + F(x_2)$, $0 \leq x_1 \leq z_1$, $0 \leq x_2 \leq z_2$, $0 \leq x_1 + x_2 \leq a$. (If $a = z$ then $a_1 = z_1$, $a_2 = z_2$ by monotonicity.)

If we assume (3.4), and in addition assume that the measures μ_i are point measures, we are dealing with the Thomas-Fermi atomic model. The μ_i are nuclei, f is the electronic charge density, $P(f; \mu_1, \dots, \mu_m)$ is the classical electrostatic energy, and $\Phi(f)$ is an approximation to the kinetic energy of the electrons. Then $F(a)$ is an approximation to the lowest energy level under the constraint that the total electronic charge is a . See [6], [7], [8], [13]. Proposition 2 is a version of the no binding theorem [7], [13] for the Thomas-Fermi model. Many other properties of this model, in addition to those mentioned here, are given in [7].

One reason for interest in the no binding theorem is that it was used by Lieb and Thirring, together with their estimate for the average kinetic energy of a system of fermions, to give an elegant proof of the stability of matter [8]. A discussion of the relations between the stability theorem of Lieb and Thirring and the original stability theorem of Dyson and Lenard [3], [4] is given in [8].

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