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THE GROUND STATE ENERGY OF A CLASSICAL GAS*

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1. Introduction

In this paper we are concerned with the ground state energy of a classical gas. Suppose the gas consists of N particles in $\mathbb{R}^3$ interacting under a potential $\phi(x)$ which we assume is positive definite. The positions of the particles are described by a probability distribution function $P(x_1,\ldots,x_N)$ with one and two point functions $\rho(x)$, $\rho(x,y)$ defined by

$$\rho(x) = \sum_{i=1}^{N} \int P(x_1,\ldots,x_{i-1},x,x_{i+1},\ldots,x_N)d\hat{x}_i \ , \tag{1.1}$$

$$\rho(x,y) = \sum_{i\neq j=1}^{N} \int P(x_1,\ldots,x_{i-1},x,x_{i+1},\ldots,x_{j-1},y,x_{j+1},x_N)d\hat{x}_{i,j} \ . \tag{1.2}$$

The energy of the N particles with distribution P is then given by

$$E(P) = \frac{1}{2} \iint \rho(x,y)\ \phi(x-y)dxdy \ . \tag{1.3}$$

Now let us confine the N particles to a cube Λ in such a way that the density $N/\mathrm{Vol}\ \Lambda = \rho$ is fixed. Let E_N be the infimum of $E(P)$ taken over all P supported in Λ^N. Then we define the ground state energy of the gas at density ρ, $E(\rho)$, by

$$E(\rho) = \liminf_{N\to\infty} E_N/N \ . \tag{1.4}$$

Our first result here is to show that

$$\lim_{\rho\to\infty} [E(\rho) - \frac{1}{2} \int_{\mathbb{R}^3} \phi(x)dx] = -\frac{1}{2}\phi(0) \ , \tag{1.5}$$

for potentials $\phi \in L^1 \cap L^\infty$. The identity (1.5) was essentially proved in Lewis et al. [6]. Here we prove it in a slightly different manner which relates to our subsequent work.

Next we wish to consider a Coulomb gas so $\phi(x) = 1/|x|$. In this case the integral in (1.5) is infinite so we must subtract it off by using equal numbers of positive and negative charges. Hence our Coulomb gas consists of N negative particles described by a probability distribution $P_1(x_1,\dots,x_N)$ and N positive particles described by a probability distribution $P_2(x_1,\dots,x_N)$. Thus in this gas the negative particles are independent of the positive. Let $\rho_1(x)$, $\rho_1(x,y)$ be the one and two point functions corresponding to P_1 and $\rho_2(x)$, $\rho_2(x,y)$ be the one and two point functions corresponding to P_2. Then the energy of the Coulomb gas is given by

$$E(P_1,P_2) = \frac{1}{2}\iint \frac{\rho_1(x,y)}{|x-y|}\,dxdy + \frac{1}{2}\iint \frac{\rho_2(x,y)}{|x-y|}\,dxdy - \iint \frac{\rho_1(x)\rho_2(y)}{|x-y|}\,dxdy\ . \tag{1.6}$$

Now confine the 2N particles to a cube Λ with density $N/\mathrm{Vol}\,\Lambda = \rho$ and assume P_2 is a constant so the positive particles are assumed to form a uniform background. Let E_N be the infimum of $E(P_1,P_2)$ taken over all P_1 supported in Λ^N. Then the ground state $E(\rho)$ for the Coulomb system is defined just as in (1.4). We shall show that

$$E(\rho) \geq -1.5\,\rho^{1/3}\ . \tag{1.7}$$

The result (1.7) is already well known [9] even with a slightly better constant (1.45). Our approach is rather different and generalizes to other singular potentials. The key property of the Coulomb potential seems to be that it can be written as a sum

$$\phi(x) = \phi^{(1)}(x) + \phi^{(\infty)}(x)\ , \tag{1.8}$$

where the potential $\phi^{(1)}$ is pointwise positive and has L^1 norm $\|\phi^{(1)}\|_1 \leq$ $\leq \varepsilon^2$ for any arbitrary $\varepsilon > 0$. The potential $\phi^{(\infty)}$ is positive definite and has L^∞ norm $\|\phi^{(\infty)}\|_\infty \leq C/\varepsilon$, where C is a constant independent of ε. Evidently any function $\phi(x)$ which has the property (1.8) must be both positive and positive definite and lie in the space $L^3{}_w$. It would be of interest to know if the converse were true.

It is not possible to prove (1.7) by using the fact that the first two integrals in (1.6) are positive and just bounding the third integral. In fact if we do this and assume $\rho_1(x) = \rho$ we get the bound

$$E_N \geq - C N^{5/3} \rho^{1/3} . \tag{1.9}$$

Thus this approach gives a bound which is a factor $N^{2/3}$ larger than we want. For <u>arbitrary</u> distributions P_1, P_2 let us bound $E(P_1,P_2)$ from below by using the positivity of the first two integrals of (1.6) and applying the weak Young inequality to the third. We wish also to exhibit the factor $N^{2/3}$ which should be the price we have paid for not taking into account the first two integrals of (1.6). We have the following:

<u>Lemma 1.1</u> Let p, q, α, β satisfy the relations

$$\alpha + \beta = 1 , \qquad p\alpha + q\beta = 4/3 , \tag{1.10}$$

$$p,q \geq 1 , \tag{1.11}$$

$$p\alpha \leq 1 , \qquad q\beta \leq 1 , \tag{1.12}$$

where if an equality holds in (1.11) then strict <u>inequality</u> must hold in (1.12). Then there is a constant C, depending only on p, q such that

$$E(P_1,P_2) \geq - C N^{2/3} \|\rho_1\|_p^{p\alpha} \|\rho_2\|_q^{q\beta} . \tag{1.13}$$

Proof: Applying the weak Young inequality to the third integral of (1.6) we have

$$E(P_1,P_2) \geq - C \|\rho_1\|_r \|\rho_2\|_s , \tag{1.14}$$

where r and s are related by

$$\frac{1}{r} + \frac{1}{s} = \frac{5}{3} , \qquad r,s > 1 . \tag{1.15}$$

Since the L^1 norm of ρ_1 is N we have by Hölder's inequality that

$$\|\rho_1\|_r \leq N^{1/r - \alpha} \|\rho_1\|_p^{p\alpha} , \tag{1.16}$$

where

$$\alpha = (r-1)/(p-1)r\ , \qquad p \geq r\ . \tag{1.17}$$

Similarly we have

$$\|\rho_2\|_s \leq N^{1/s - \beta}\ \|\rho_2\|_q^{q\beta}\ , \tag{1.18}$$

with

$$\beta = (s-1)/(q-1)s\ , \qquad q \geq s\ . \tag{1.19}$$

Suppose now that p, q, α, β satisfy the conditions of the theorem. Then we may define r, s by (1.17) and (1.19). The condition (1.12) guarantees that $p \geq r$, $q \geq s$. Assume for the moment that strict inequality holds in (1.11). Hence $r,s > 1$ and from (1.10) it follows that (1.15) holds. Thus (1.13) follows from (1.14), (1.16) and (1.18). Q.E.D.

In section 3 we show that if we take into account the two positive integrals in (1.6) then just as in the simple case already discussed we may drop the factor $N^{2/3}$ in (1.13). Thus we have

Theorem 1.2 With p, q, α, β satisfying the conditions of lemma 1.1 we can find a constant C depending only on p, q such that

$$E(P_1,P_2) \geq -C\ \|\rho_1\|_p^{p\alpha}\ \|\rho_2\|_q^{q\beta}\ . \tag{1.20}$$

Two cases of theorem 1.2 are already known, and in these the constants C are much better than we obtain here. They are for $p = q = 4/3$ with $P_1 = P_2$ and for $p = 1$ which implies $q > 3/2$. In the former case the result is known as the exchange energy inequality of Lieb and Oxford [7]. In the latter the result is due to Lieb and Thirring [8] and is proved by exploiting the no binding theorem of Thomas-Fermi theory.

Let H_N be the N particle relativistic kinetic energy Hamiltonian

$$H_N = \sum_{i=1}^{N} (-\Delta_i)^{1/2}\ , \tag{1.21}$$

where Δ_i denotes the Laplacian in the x_i variable. Suppose the probability distribution P_1 is obtained from a Fermion wave function ψ so

$$P_1(x_1,\ldots,x_N) = |\psi|^2(x_1,\ldots,x_N) \ . \tag{1.22}$$

Let $\langle\psi,H_N\psi\rangle$ denote the expected value of H_N on ψ. Our final theorem in section 4 is:

Theorem 1.3 There is a constant C independent of ψ, N such that

$$C \langle\psi,H_N\psi\rangle + E(P_1,P_2) \geq 0 \ , \tag{1.23}$$

where P_1 is related to ψ by (1.22) and P_2 is arbitrary.

Theorem 1.3 can be regarded as the stability theorem for a relativistic Hamiltonian with Coulomb interaction. It cannot be proved by applying theorem 1.2 in the case of p = 1 as in the Lieb-Thirring proof of stability of matter [8].

The techniques we employ here are taken from the proof by Federbush of stability of matter [3]. In fact the key lemma 3.1 is taken from his paper [3]. As pointed out in [3] the advantage of the Federbush spproach to stability of matter is that it is more flexible than either the Dyson-Lenard approach [2,5] or that of Lieb-Thirring [8]. However the price one pays for this flexibility is that the constants obtained in the theorems are far from being optimal.

2. The Case of Fixed Density

We turn to the proof of (1.5). Our main lemma, which will also be of importance later is the following:

Lemma 2.1 Let k(x,y) be a positive definite kernel and $P(x_1,\ldots,x_N)$ be an N particle probability distribution with one and two point functions $\rho(x)$, $\rho(x,y)$. Then

$$\iint k(x,y)\,\rho(x,y)dxdy \geq \iint k(x,y)\,\rho(x)\,\rho(y)dxdy - \int k(x,x)\,\rho(x)dx \ . \tag{2.1}$$

Proof: Define numbers e_i, $1 \le i \le 2N$, by

$$e_i = 1, \quad 1 \le i \le N ; \quad e_i = -1 , \quad N+1 \le i \le 2N . \tag{2.2}$$

Since $k(x,y)$ is positive definite we have

$$\sum_{i,j=1}^{2N} e_i e_j k(x_i,x_j) \ge 0 . \tag{2.3}$$

If we integrate (2.3) against the product $P(x_1,\ldots,x_N)\ P(x_{N+1},\ldots,x_{2N})$ we obtain the inequality (2.1). Q.E.D.

Lemma 2.2 Let $E(\rho)$ be defined by (1.4). Then we have

$$E(\rho) \ge \frac{1}{2} \rho \int \phi(x)dx - \frac{1}{2} \phi(0) , \tag{2.4}$$

provided the function $\phi(x)$ is positive definite and in $L^1 \cap L^\infty$.

Proof: We take $k(x,y) = \phi(x-y)$ in lemma 2.1. Thus we have

$$E(P) \ge \frac{1}{2} \int_\Lambda \int_\Lambda \phi(x-y)\ \rho(x)\ \rho(y)dxdy - \frac{1}{2} N\ \phi(0) . \tag{2.5}$$

Let Λ_h be an h neighbourhood of Λ, so

$$\Lambda_h = \{x: d(x,\Lambda) \le h\} . \tag{2.6}$$

Then if χ_{Λ_h} is the characteristic function of Λ_h we have by the positive definiteness of Λ_h the inequality

$$[\int_\Lambda \int_\Lambda \phi(x-y)\ \rho(x)\ \rho(y)dxdy][\iint \phi(x-y)\ \chi_{\Lambda_h}(x)\ \chi_{\Lambda_h}(y)dxdy] \ge$$

$$\ge [\iint \phi(x-y)\ \chi_{\Lambda_h}(x)\ \rho(y)dxdy]^2 . \tag{2.7}$$

Hence from (2.5) we have that

$$E(P) \ge \frac{1}{2} [\iint \phi(x-y)\ \chi_{\Lambda_h}(x)\ \rho(y)dxdy]^2/[\iint \phi(x-y)\ \chi_{\Lambda_h}(x)\ \chi_{\Lambda_h}(y)dxdy]$$

$$- \frac{1}{2} N\ \phi(0) . \tag{2.8}$$

Now for any $\delta > 0$ we can choose h independent of N, Λ such that for any $y \in \Lambda$

$$\int_{\mathbb{R}^3} \phi(x)dx - \delta \leq \int_{\Lambda_h} \phi(x-y)dx \leq \int_{\mathbb{R}^3} \phi(x)dx + \delta \ . \tag{2.9}$$

By choosing δ small enough in (2.9) we see from (2.8) that for any $\eta > 0$ we have

$$E(\rho) \geq \frac{1}{2} \rho \int \phi(x)dx - \frac{1}{2} \phi(0) - \eta \ . \tag{2.10}$$

Letting $\eta \to 0$ proves the lemma. Q.E.D.

<u>Lemma 2.3</u> With $E(\rho)$ as in (1.4) we have

$$\limsup_{\rho\to\infty} [E(\rho) - \frac{1}{2} \rho \int \phi(x)dx] \leq - \frac{1}{2} \phi(0) \ . \tag{2.11}$$

<u>Proof:</u> Let $\psi_1(x), \ldots, \psi_N(x)$ be N orthonormal wave functions and form the Hartree-Fock wave function

$$\psi(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \det \psi_i(x_j) \ . \tag{2.12}$$

Then if we take $P = |\psi|^2$ it is well known that the two point function $\rho(x,y)$ is given by

$$\rho(x,y) = \rho(x)\, \rho(y) - |\sum_{i=1}^{N} \psi_i(x)\, \overline{\psi_i(y)}|^2 \ . \tag{2.13}$$

Now given the cube Λ with $N/\mathrm{Vol}\ \Lambda = \rho$ we divide Λ into N equal subcubes and define the $\psi_i(x)$ as constant functions supported on the subcubes. In this situation $\rho(x) = \rho$ and as $\rho \to \infty$ the $\psi_i(x)$ are supported on increasingly smaller cubes. Thus, using the fact that $\phi(x)$ is continuous at $x = 0$ we obtain the result (2.11). Q.E.D.

The previous three lemmas prove (1.5). The use of the Schwarz inequality in (2.7) is taken from Lewis et al. [6]. Next we state a lemma which appears trivial but is yet important.

Lemma 2.4 Suppose the potential $\phi(x)$ is pointwise positive. Then we have $E(\rho) \geq 0$.

Observe that lemma 2.2 applies for potentials which are positive definite while lemma 2.4 applies for potentials which are pointwise positive. To prove (1.7) we use both of these lemmas by writing the Coulomb potential as a sum (1.8) of a positive potential and a positive definite potential. There are many ways of doing this. We choose the following:

$$1/4\pi|x| = \int_0^\infty \frac{1}{(4\pi t)^{3/2}} \exp\left[-\frac{|x|^2}{4t}\right] dt , \tag{2.14}$$

and so we have

$$1/|x| = \phi_\lambda^{(1)}(x) + \phi_\lambda^{(\infty)}(x) , \tag{2.15}$$

where

$$\phi_\lambda^{(1)}(x) = 4\pi \int_0^\lambda \frac{1}{(4\pi t)^{3/2}} \exp\left[-\frac{|x|^2}{4t}\right] dt , \tag{2.16}$$

$$\phi_\lambda^{(\infty)}(x) = 4\pi \int_\lambda^\infty \frac{1}{(4\pi t)^{3/2}} \exp\left[-\frac{|x|^2}{4t}\right] dt . \tag{2.17}$$

Evidently we have

$$E(\rho) \geq E_\lambda^{(1)}(\rho) + E_\lambda^{(\infty)}(\rho) , \tag{2.18}$$

where $E_\lambda^{(1)}(\rho)$ is the ground state energy per particle corresponding to $\phi_\lambda^{(1)}$ and similarly $E_\lambda^{(\infty)}(\rho)$ corresponds to $\phi_\lambda^{(\infty)}$. From lemma 2.4 we have

$$E_\lambda^{(1)}(\rho) \geq -2\pi\rho\lambda , \tag{2.19}$$

since we must take into account the attraction from the background charge. From lemma 2.2 we have

$$E_\lambda^{(\infty)}(\rho) \geq -1/(4\pi\lambda)^{1/2} . \tag{2.20}$$

In (2.20) the infinite integral in (2.4) is subtracted off by means of the background charge. Thus we have

$$E(\rho) \geq -2\pi\rho\lambda - 1/(4\pi\lambda)^{1/2} . \tag{2.21}$$

If we optimize (2.21) with respect to λ for $\lambda > 0$ we obtain (1.7).

It is easy to see from the above procedure how to generalize the result (1.7) to other singular potentials. Although the method employed in [9] to obtain (1.7) also uses the splitting (1.8) this fact is not mentioned as the important principle involved.

3. The Coulomb Gas with Variable Density

Here we turn to the proof of theorem 1.2. The method is just like the proof of (1.7) except that we need to vary the parameter λ in (2.21) as ρ varies since λ is proportional to $\rho^{-2/3}$.

There are two important localization lemmas involved. The first is lemma 2.1 and this lemma is already required in the proof of the exchange energy inequality [7]. The second localization lemma is needed in the case when $P_1 \neq P_2$ and is taken from Federbush [3].

Lemma 3.1 Let $\chi_i(x)$, $i \in L$, denote the translates of an arbitrary C^∞ function with compact support over the lattice L in $\mathbb{R}^3$. Then there is a constant $C > 0$ such that the kernel

$$e^{-|x-y|} - C \sum_{i \in L} \chi_i(x)\, \chi_i(y) \tag{3.1}$$

is positive definite.

Proof: The Fourier transform of $e^{-|x|}$ is a constant times $(1+k^2)^{-2}$. Now we have

$$\iint f(x)\, e^{-|x-y|}\, \overline{f(y)}\,dx\,dy = \int |\hat{f}(k)|^2 (1+k^2)^{-2} dk . \tag{3.2}$$

Hence we need to prove that

$$\int |\hat{f}(k)|^2(1+k^2)^{-2}dk \geq C \sum_i |\langle\hat{f},\hat{\chi}_i\rangle|^2 = C \sum_i |\langle\frac{\hat{f}}{1+k^2}, (1+k^2)\hat{\chi}_i\rangle|^2 . \quad (3.3)$$

Thus it is sufficient to show that for an arbitrary function g(x) we have

$$\int |g(x)|^2dx \geq C \sum_i |\langle g, (-\Delta+1)\chi_i\rangle|^2 . \quad (3.4)$$

The inequality (3.4) however follows from the fact that the χ_i are translates of a function with compact support. Q.E.D.

Now let f(x) be a nonnegative function to be chosen later and put

$$k_\infty(x,y) = \int_0^\infty \chi[f(x)-u]\ \chi[f(y)-u]\ e^{-u|x-y|}du , \quad (3.5)$$

where $\chi(t)$ is the Heaviside function $\chi(t) = 1$ if $t > 0$, $\chi(t) = 0$ if $t \leq 0$. Observe that k_∞ is analogous to $\phi^{(\infty)}$ in (2.17) except that instead of (2.14) we are using the representation

$$1/|x| = \int_0^\infty e^{-u|x|}\ du . \quad (3.6)$$

Let $k_1(x,y)$ be given by

$$k_1(x,y) = |x-y|^{-1} - k_\infty(x,y) , \quad (3.7)$$

so k_1 like $\phi^{(1)}$ in (2.14) is pointwise positive while k_∞ like $\phi^{(\infty)}$ is positive definite. We apply lemma 2.1 to obtain

$$\begin{aligned} E(P_1,P_2) &\geq \tfrac{1}{2} \iint k_\infty(x,y)\rho_1(x)\rho_1(y)dxdy - \iint \rho_1(x)\rho_2(y)[k_\infty(x,y)+k_1(x,y)]dxdy \\ &+ \tfrac{1}{2} \iint k_\infty(x,y)\rho_2(x)\rho_2(y)dxdy - \tfrac{1}{2} \int k_\infty(x,x)\rho_1(x)dx - \tfrac{1}{2} \int k_\infty(x,x)\rho_2(x)dx = \\ &= \tfrac{1}{2} \iint k_\infty(x,y)[\rho_1(x)-\rho_2(x)][\rho_1(y)-\rho_2(y)]dxdy - \iint \rho_1(x)\rho_2(y)k_1(x,y)dxdy \\ &\quad - \tfrac{1}{2} \int f(x)[\rho_1(x)+\rho_2(x)]dx . \end{aligned} \quad (3.8)$$

Hence if we use lemma 3.1 we have

$$E(P_1,P_2) \geq I_1 - I_2 - I_3 \,, \tag{3.9}$$

where

$$I_1 = \frac{1}{2} C \iint \int_0^\infty du \; \chi[f(x)-u] \; \chi[f(y)-u]$$

$$\sum_{i\in L} \chi_i(ux) \; \chi_i(uy) du [\rho_1(x)-\rho_2(x)][\rho_1(y)-\rho_2(y)] dxdy \,, \tag{3.10}$$

$$I_2 = \iint \frac{\rho_1(x)\rho_2(y)}{|x-y|} [e^{-f(x)|x-y|} + e^{-f(y)|x-y|}] dxdy \,, \tag{3.11}$$

$$I_3 = \int f(x)[\rho_1(x)+\rho_2(x)] dx \,. \tag{3.12}$$

We define the function $f(x)$. First we assume N is large so that theorem 1.2 is not just a corollary of lemma 1.1. We put

$$\rho(x) = \rho_1(x) + \rho_2(x) \,, \tag{3.13}$$

and define $f(x)$ as the largest number λ such that

$$\int_{|x-y|<1/\lambda} \rho(y) dy \geq 2N_o \,, \tag{3.14}$$

where N_o is a number to be fixed for all large N later. Thus $f(x)$ is an average value of the one third power of the density at x.

We consider the sets

$$E_n = \{x: \; 2^{n-1} < f(x) \leq 2^n\} \,, \quad n = 0, \pm 1, \ldots \,. \tag{3.15}$$

For each $x \in E_n$ let B_x be the ball with center x and radius $2^{-(n+1)}$. Then it is evident that

$$\int_{B_x} \rho(y) dy \leq 2N_o \,, \tag{3.16}$$

$$2^{n-2} \leq f(y) \leq 2^{n+1} \,, \qquad y \in B_x \,. \tag{3.17}$$

The balls B_x cover the neighbourhood of E_n with radius $2^{-(n+2)}$ so we may choose a subcover which have finite intersection number smaller than some universal constant. Let us denote the subcover by $B_{n,i}$, $1 \le i \le \kappa(n)$. We say that a ball $B = B_{n,i}$ belongs to the set S if

$$\int_B \rho(y)dy \ge 2N_0/C_0 , \tag{3.18}$$

where C_0 is a universal constant to be given in the following lemma.

<u>Lemma 3.2</u> There is a universal constant C_0 and a constant κ such that

$$I_3 \le \kappa \sum_{B \in S} \int_B f(y)\ \rho(y)dy . \tag{3.19}$$

<u>Proof:</u> Evidently we have

$$I_3 \le \sum_{n=-\infty}^{\infty} \sum_{i=1}^{\kappa(n)} 2^{n+1} \int_{B_{n,i}} \rho(y)dy . \tag{3.20}$$

For the ball $B_{n,i}$ let $B^*_{n,i}$ be the ball concentric with $B_{n,i}$ but with radius $1/2^{n-1}$. Then from (3.14) we have

$$\int_{B^*_{n,i}} \rho(y)dy \ge 2N_0 . \tag{3.21}$$

Observe that

$$f(y) \ge 2^{n-2} , \qquad y \in B^*_{n,i} . \tag{3.22}$$

Since the sets $B_{n,i}$ have finite intersection number, $1 \le i \le \kappa(n)$, so also do the sets $B^*_{n,i}$, $1 \le i \le \kappa(n)$. Let the intersection number of the $B^*_{n,i}$ be smaller than $2^{\gamma-1}$, where γ is some universal constant, $\gamma \ge 1$. Then we may choose a universal constant C_0 such that one of two possibilities holds: Either there is a set $B_{n-1,j}$, $B_{n,j}$, ..., $B_{n+\gamma,j}$ in S which intersects $B^*_{n,i}$ or the integral of $\rho(y)$ over the set

$$B^*_{n,i} \cap \bigcup_{m=n+\gamma+1}^{\infty} \bigcup_{j=1}^{\kappa(m)} B_{m,j} \tag{3.23}$$

is larger than the integral of $\rho(y)$ over $B_{n,i}$.

We therefore conclude that

$$\sum_{i=1}^{\kappa(n)} \int_{B_{n,i}} \rho(y)dy \le A \sum_{m=n-1}^{n+\gamma} \sum_{B_{m,j}\in S} \int_{B_{m,j}} \rho(y)dy + 2^{\gamma-1} \sum_{m=n+\gamma+1}^{\infty} \sum_{j=1}^{\kappa(m)} \int_{B_{m,j}} \rho(y)dy, \qquad (3.24)$$

where A is a universal constant depending on γ.

Now if we multiply (3.24) by 2^{n+1} and sum with respect to n we have - denoting by I the right side of (3.20) - the inequality

$$I \le 16A(\gamma+1) \sum_{B\in S} \int_B f(y)\ \rho(y)dy + \frac{1}{2} I\ . \qquad (3.25)$$

The result follows from (3.25). Q.E.D.

Lemma 3.3 Let p, q, α, β satisfy the conditions of lemma 1.1. Then there is a constant $C(N_0)$ depending on N_0 and a universal constant κ such that

$$I_2 \le C(N_0)\ \|\rho_1\|_p^{p\alpha}\ \|\rho_2\|_q^{q\beta} + \kappa \sum_{B\in S} \int_B f(y)\ \rho(y)dy\ . \qquad (3.26)$$

Proof: We write the integral

$$\iint \frac{\rho_1(x)\rho_2(x)}{|x-y|} e^{-f(x)|x-y|} dxdy = \iint_{|x-y|<1/8f(x)} + \iint_{|x-y|\ge 1/8f(x)}\ . \qquad (3.27)$$

Since the sets $B_{n,i}$ cover a neighbourhood of E_n with radius $2^{-(n+2)}$ and for $x \in E_n$ we have $f(x) > 2^{n-1}$ it follows that the integral in (3.27) over $|x-y| < 1/8f(x)$ is bounded by

$$\sum_{n=-\infty}^{\infty} \sum_{i=1}^{\kappa(n)} \int_{B_{n,i}} \int_{B_{n,i}} \frac{\rho_1(x)\rho_2(y)}{|x-y|} dxdy\ . \qquad (3.28)$$

Since the sets $B_{n,i}$, $-\infty < n < \infty$, $1 \le i \le \kappa(n)$, have finite intersection number we can apply the Young inequality to each term in (3.28) just as in lemma 1.1, using the fact that

$$\int_{B_{n,i}} \rho(y)dy \le 2N_0\ . \qquad (3.29)$$

Then a further application of the Hölder inequality with exponents $1/\alpha$, $1/\beta$ yields the first term in the right side of (3.26) as a bound on (3.28).

To deal with the second integral in (3.27) we define for integers $r = 1,2,\ldots,$

$$a_r = \int f(x)\,\rho_1(x) \int_{|x-y|<r/f(x)} \rho_2(y)dy\ . \tag{3.30}$$

Evidently the second integral is bounded by

$$7a_1 + \sum_{r=1}^{\infty} a_r\, e^{-r+1}\ . \tag{3.31}$$

Let $U_{n,i}(r)$, $1 \leq i \leq \kappa(n)$, be the ball concentric with $B_{n,i}$ but with radius $(r+1)/2^{n-1}$. Then, in view of (3.15), we have that

$$a_r \leq \sum_{n=-\infty}^{\infty} 2^{n+1} \sum_{i=1}^{\kappa(n)} \int_{B_{n,i}} \rho_1(x)dx \int_{U_{n,i}(r)} \rho_2(y)dy\ . \tag{3.32}$$

Next, observe that the sets $U_{n,i}(r)$, $1 \leq i \leq \kappa(n)$, have finite intersection number smaller than a universal constant times r^3 and that $U_{n,i}$ can only intersect E_j for j which satisfy

$$2^j \geq 2^{n-1}/(r+2)\ . \tag{3.33}$$

Let the set $S_{n,i,k}$ be defined by

$$S_{n,i,k} = \{j:\ B_{k,j} \cap U_{n,i} \neq \emptyset\}\ , \tag{3.34}$$

and R be the smallest integer such that

$$2^{R-1} \geq r+2\ . \tag{3.35}$$

Then it follows from (3.33) and (3.17) that if

$$k < n - R - 1\ , \tag{3.36}$$

then $S_{n,i,k}$ is empty. Furthermore, by the finite intersection property of the sets $U_{n,i}(r)$, $1 \le i \le \kappa(n)$, it follows that any integer j, $1 \le j \le \kappa(k)$, occurs at most a universal constant times r^3 in the disjoint union

$$\bigcup_{i=1}^{\kappa(n)} S_{n,i,k} \,. \tag{3.37}$$

From (3.36) we have that

$$\int_{U_{n,i}(r)} \rho_2(y)dy \le \sum_{k=n-\ell-1}^{\infty} \sum_{j\in S_{n,i,k}} \int_{B_{k,j}} \rho_2(y)dy \,. \tag{3.38}$$

Hence for any integer m_o we have

$$a_r \le \sum_{t=-\ell-1}^{m_o-1} \sum_{n=-\infty}^{\infty} 2^{n+1} \sum_{i=1}^{\kappa(n)} \int_{B_{n,i}} \rho_1(x)dy \sum_{j\in S_{n,i,n+t}} \int_{B_{n+t,j}} \rho_2(y)dy$$

$$+ \sum_{n=-\infty}^{\infty} \sum_{i=1}^{\kappa(n)} 2^{n+2} N_o \sum_{k=m_o+n}^{\infty} \sum_{j\in S_{n,i,k}} \int_{B_{k,j}} \rho(y)dy \,, \tag{3.39}$$

where in the second sum we have used (3.29). From (3.37) we see that the second sum in (3.39) is bounded by

$$c\, r^3 N_o 2^{-m_o} \sum_{k=-\infty}^{\infty} \sum_{j=1}^{\kappa(k)} 2^{k+1} \int_{B_{k,j}} \rho(y)dy \,, \tag{3.40}$$

where c is a universal constant. Now from lemma 3.2 we have that (3.40) is bounded by

$$\kappa\, c\, r^3 N_o 2^{-m_o} \sum_{B\in S} \int_B f(y)\, \rho(y)dy \,. \tag{3.41}$$

Next we show that

$$\sum_{n=-\infty}^{\infty} 2^n \sum_{i=1}^{\kappa(n)} \int_{B_{n,i}} \rho_1(x)dx \sum_{j\in S_{n,i,n+t}} \int_{B_{n+t,j}} \rho_2(y)dy$$

$$\le C(N_o)\, r^3\, 2^{3(1-q\beta)t} \|\rho_1\|_p^{p\alpha} \|\rho_2\|_q^{q\beta} \,, \tag{3.42}$$

where the constant $C(N_0)$ depends only on N_0. To do this first observe that the cardinality of $S_{n,i,n+t}$ is bounded as

$$|S_{n,i,n+t}| \le c\, 2^{3t} r^3 , \tag{3.43}$$

for some universal constant c. Now the sum in (3.42) is bounded by

$$C(N_0) \sum_{n=-\infty}^{\infty} 2^n \sum_{i=1}^{\kappa(n)} \Big[\int_{B_{n,i}} \rho_1(x)dx\Big]^{p\alpha} \sum_{j\in S_{n,i,n+t}} \Big[\int_{B_{n+t,j}} \rho_2(y)dy\Big]^{q\beta}$$

$$\le C(N_0)\, 2^{-3\beta(q-1)t} \sum_{n=-\infty}^{\infty} \sum_{i=1}^{\kappa(n)} \Big[\int_{B_{n,i}} \rho_1(x)^p dx\Big]^{\alpha} \sum_{j\in S_{n,i,n+t}} \Big[\int_{B_{n+t,j}} \rho_2(y)^q dy\Big]^{\beta}$$

$$\le C(N_0)\, 2^{-3\beta(q-1)t} \Big[\sum_{n=-\infty}^{\infty} \sum_{i=1}^{\kappa(n)} \sum_{j\in S_{n,i,n+t}} \int_{B_{n,i}} \rho_1(x)^p dx\Big]^{\alpha}$$

$$\Big[\sum_{n=-\infty}^{\infty} \sum_{i=1}^{\kappa(n)} \sum_{j\in S_{n,i,n+t}} \int_{B_{n+t,j}} \rho_2(y)^q dy\Big]^{\beta}$$

$$\le C(N_0)\, r^3\, 2^{3(1-q\beta)t}\, \|\rho_1\|_p^{p\alpha}\, \|\rho_2\|_q^{q\beta} . \tag{3.44}$$

Now if we choose m_0 such that

$$N_0\, 2^{-m_0} \le 1 , \tag{3.45}$$

we can bound a_r as in (3.26). Then summing with respect to r as in (3.31) yields the result. Q.E.D.

<u>Lemma 3.4</u> Given a constant κ we can choose the number N_0 such that

$$I_1 - \kappa \sum_{B\in S} \int_B f(y)\rho(y)dy \ge - C(N_0)\, \|\rho_1\|_p^{p\alpha}\, \|\rho_2\|_q^{q\beta} . \tag{3.46}$$

<u>Proof:</u> We first define the lattice L of lemma 3.1. A vector $i \in L$ if $128i$ is a vector with integer components. Thus any point $x \in \mathbb{R}^3$ is less than a distance 1/128 from some point of L. Let $\phi(x)$ be a C^∞ function which is such that $0 \le \phi(x) \le 1$, $x \in \mathbb{R}^3$, and

$$\phi(x) = 1 \quad \text{if} \quad |x| \le 9/64 \; ; \qquad \phi(x) = 0 \quad \text{if} \quad |x| \ge 5/32 \; . \tag{3.47}$$

Then the functions $\chi_i(x)$ are translates of $\phi(x)$ through the lattice L.

We write I_1 in (3.10) as

$$I_1 = \sum_{n=-\infty}^{\infty} \int_{2^{n-3}}^{2^{n-2}} du \; . \tag{3.48}$$

Next consider a ball $B_{n,k}$, $1 \le k \le \kappa(n)$, which has radius $1/2^{n+1}$. Then there is a vector $i \in L$ such that $i/2^{n-2}$ is less than $1/2^{n+5}$ from the center of $B_{n,k}$. Furthermore

$$\chi_i(2^{n-2}x) = \phi(2^{n-2}x - i) = \phi(2^{n-2}[x - i/2^{n-2}]) \; . \tag{3.49}$$

Thus $\chi_i(2^{n-2}x) = 1$ if $x \in B_{n,k}$ and $\chi_i(2^{n-2}x) = 0$ if $x \notin B^*_{n,k}$, where $B^*_{n,k}$ is the ball concentric with $B_{n,k}$ but with radius $3/2^{n+2}$. One can also easily see that if

$$2^{n-2} \ge u \ge \left(\frac{1}{4} - \frac{1}{128}\right) 2^n \; , \tag{3.50}$$

then there is an $i \in L$ - which may vary with u - such that $\chi_i(ux) = 1$ if $x \in B_{n,k}$ and $\chi_i(ux) = 0$ if $x \notin B^*_{n,k}$.

Now suppose $B = B_{n,k} \in S$. Then, in view of (3.18) we can assume without loss of generality that

$$\int_B \rho_1(y)dy \ge N_o/C_o \; . \tag{3.51}$$

If we also have

$$\int_{B^*_{n,k}} \rho_2(y)dy \le N_o/2C_o \; , \tag{3.52}$$

we shall say $B \in S'$. If we fix n and let k vary, $1 \le k \le \kappa(n)$ then it is clear by the finite intersection property of the $B^*_{n,k}$ that any $i \in L$ which occurs with $\chi_i(ux) = 1$ for $x \in B_{n,k}$, occurs only finitely many times. We therefore conclude that for u satisfying (3.50) there is a universal constant C such that

$$\iint \chi[f(x)-u]\ \chi[f(y)-u] \sum_{i\in L} \chi_i(ux)\ \chi_i(uy)[\rho_1(x)-\rho_2(x)][\rho_1(y)-\rho_2(y)]dxdy$$

$$\geq c\ N_o^2\ \#\ \{B = B_{n,k} \in S'\}\ . \tag{3.53}$$

Now if we use (3.48) and choose N_o large enough we may conclude from (3.29) that

$$I_1 \geq \kappa \sum_{B\in S'} \int_B f(y)\ \rho(y)\ dy\ . \tag{3.54}$$

It remains for us to deal with $B \notin S'$. In that case we see that

$$\sum_{B\in S\setminus S'} \int_B f(y)\rho(y)dy \leq \sum_{B=B_{n,k}\in S\setminus S'} 2^{n+1} \int_{B^*_{n,k}} \rho(y)dy$$

$$\leq C(N_o) \sum_{n=-\infty}^{\infty} \sum_{k=1}^{\kappa(n)} 2^{n+1} [\int_{B^*_{n,k}} \rho_1(y)dy]^{p\alpha}[\int_{B^*_{n,k}} \rho_2(y)dy]^{q\beta}\ , \tag{3.55}$$

for some constant $C(N_o)$ depending on N_o. Now we can estimate the last sum in (3.55) just as before to obtain (3.46). Q.E.D.

Finally we observe that theorem 1.2 follows from (3.9) and the previous lemmas.

4. Stability of the Relativistic System

To prove theorem 1.3 we need an estimate which is not contained in theorem 1.2 but is proved in exactly the same manner.

Lemma 4.1 Suppose $\rho_1(x)$ is such that $\rho_1(x)^{1/2}$ is in the domain of $H_1 = (-\Delta)^{1/2}$. Then there is a constant C independent of N such that

$$E(P_1,P_2) \geq C[\int_{\mathbb{R}^3} \rho_1(x)^{4/3}dx + \langle\rho_1^{1/2},H_1\rho_1^{1/2}\rangle]\ . \tag{4.1}$$

Proof: First we show that

$$I_2 \le C(N_0)\Big[\int_{\mathbb{R}^3} \rho_1(x)^{4/3}dx + \langle \rho_1^{1/2}, H_1 \rho_1^{1/2}\rangle\Big] + \kappa \sum_{B\in S} \int_B f(y)\, \rho(y)dy \ . \quad (4.2)$$

To show (4.2) we must estimate (3.42) somewhat differently. We divide the sets $B = B_{n,i}$ into two kinds. We say $B \in A$ if

$$\int_B \rho_1(x)dx \ge 1 \ . \quad (4.3)$$

We write (3.42) as

$$\sum_{B\in A} + \sum_{B\notin A} \ . \quad (4.4)$$

Then we see that

$$\sum_{B\in A} \le C(N_0)\ 2^{3t}\ r^3 \sum_{n=-\infty}^{\infty} 2^n \sum_{i=1}^{\kappa(n)} \sum_{B_{n,i}\in A} \int_{B_{n,i}} \rho_1(x)\, dx$$

$$\le C(N_0)\ 2^{3t}\ r^3 \sum_{n=-\infty}^{\infty} 2^n \sum_{i=1}^{\kappa(n)} \sum_{B_{n,i}\in A} \Big[\int_{B_{n,i}} \rho_1(x)dx\Big]^{4/3}$$

$$\le C(N_0)\ 2^{3t}\ r^3 \int_{\mathbb{R}^3} \rho_1(x)^{4/3}dx \ , \quad (4.5)$$

on using Hölder's inequality and the finite intersection property of the balls $B_{n,i}$. We have also

$$\sum_{B\notin A} \le \sum_{n=-\infty}^{\infty} \sum_{i=1}^{\kappa(n)} \sum_{j\in S_{n,i,n+t}} 2^n \int_{B_{n+t,j}} \rho_2(y)dy$$

$$\le c\ 2^{-t}\ r^3 \sum_{n=-\infty}^{\infty} \sum_{i=1}^{\kappa(n)} 2^{n+1} \int_{B_{n,i}} \rho(y)dy \ , \quad (4.6)$$

where c is a universal constant. Hence, on using lemma 3.2, we have that

$$a_r \le C(N_0)\ r^3 \int_{\mathbb{R}^3} \rho_1(x)^{4/3}dx + \kappa\ r^4 \sum_{B\in S} \int_B f(y)\ \rho(y)dy \ , \quad (4.7)$$

where κ is a constant independent of N_0. Thus on summing (3.31) we shall get the estimate (4.2) provided we can deal with (3.28).

To do this we use the Fefferman-Phong technique [4]. Let Q_o be a large cube in $\mathbb{R}^3$ and make a dyadic decomposition of Q_o. For a function $u \in L^2(Q_o)$ and a dyadic subcube Q of Q_o let $\hat{u}(Q)$ be the projection of u onto the functions which are linear + constant on the 8 subcubes of Q and orthogonal to the functions linear + constant on all of Q. Then if $u \in L^2(Q_o)$ is orthogonal to functions linear + constant on all of Q_o we have

$$u = \sum_{Q \subset Q_o} \hat{u}(Q) \; . \tag{4.8}$$

Now from [4] we see that if u is in the domain of H_1 then there is a constant C such that

$$\langle u, H_1 u\rangle \geq C \sum_{Q \subset Q_o} (\text{diam } Q)^{-1} \; \|\hat{u}(Q)\|^2 \; . \tag{4.9}$$

For a ball $B_{n,i}$ – with radius $1/2^{n+1}$ – let $B^*_{n,i}$ be the ball concentric with $B_{n,i}$ but with radius $3/2^{n+2}$, so the balls $B^*_{n,i}$ have the finite intersection property. Suppose $B_{n,i}$ is contained in Q_o. Then $B_{n,i}$ is covered by a finite number of dyadic subcubes of Q_o, each with the same diameter $\sim 2^{-n}$ and contained in $B^*_{n,i}$. Let Q be one of these subcubes and P_Q be the projection operator onto linear + constant on Q. Then we know from [4] that

$$\int_Q [\sqrt{\rho_1}(x) - P_Q \sqrt{\rho_1}(x)]^2 \, \frac{dx}{|x-y|} \leq C \sum_{Q' \subset Q} (\text{diam } Q')^{-1} \; \|\hat{\sqrt{\rho_1}}(Q')\|^2 \; , \tag{4.10}$$

for some constant C independent of y and Q.

It is easy to see that

$$\int_Q [P_Q \sqrt{\rho_1}(x)]^2 \, \frac{dx}{|x-y|} \leq C \; (\text{diam } Q)^{-1} \int_Q \rho_1(x) dx \; , \tag{4.11}$$

with C independent of Q. Hence if $B_{n,i}$ is covered by cubes $Q_1, \ldots, Q_L$ we conclude that

$$\int_{B_{n,i}} \int_{B_{n,i}} \frac{\rho_1(x)\rho_2(y)}{|x-y|} dxdy \leq C\, 2^n \int_{B^*_{n,i}} \rho_1(x)dx \int_{B^*_{n,i}} \rho_2(y)dy +$$

$$+ C(N_o) \sum_{j=1}^{L} \sum_{Q' \subset Q_j} (\text{diam } Q')^{-1} \|\widehat{\sqrt{\rho_1}}(Q')\|^2 \, , \tag{4.12}$$

where here we have used (3.29).

Next we sum (4.12) with respect to n, i with $B_{n,i} \subset Q_o$. We may estimate the first sum just as was done in (4.7). To estimate the second sum in (4.12) observe that by the finite intersection property of the sets $B^*_{n,i}$ that any dyadic cube Q we have chosen to cover $B_{n,i}$ occurs only a finite number of times as we vary n, i. The result (4.2) then follows from (4.9).

To complete the proof of the lemma we shall replace the right side of the inequality (3.46) by

$$- C(N_o) \int_{\mathbb{R}^3} \rho_1(x)^{4/3} dx \, . \tag{4.13}$$

We easily observe that, instead of the estimate (3.55) we have

$$\sum_{B \in S \setminus S'} \int_B f(y)\rho(y)dy \leq C(N_o) \sum_{B=B_{n,k}} 2^n \left[\int_B \rho_1(y)dy\right]^{4/3} \leq C(N_o) \int_{\mathbb{R}^3} \rho_1(x)^{4/3} dx \, .$$

Q.E.D. (4.14)

Finally we complete the proof of theorem 1.3 by bounding below a fermion gas in terms of the density. Let H_N be the N particle Hamiltonian

$$H_N = \sum_{i=1}^{N} (-\Delta_i)^{1/2} \tag{4.15}$$

acting on wave functions $\psi(x_1, \ldots, x_N)$. Here Δ_i is the Laplacian in the x_i variable. The following lemma is due to Daubechies [1].

<u>Lemma 4.2</u> Let ψ be a normalized Fermion wave function in the domain of H_N and with one point function $\rho(x)$. Then there is a constant C independent of N such that

$$\langle \psi, H_N \psi \rangle \geq C \int_{\mathbb{R}^3} \rho(x)^{4/3} dx \, . \tag{4.16}$$

We are indebted to Barry Simon for the proof of the following lemma:

Lemma 4.3 Let ϕ be a normalized wave function in the domain of H_N and with one point function $\rho(x)$. Then

$$\langle\phi,H_N\phi\rangle \geq \langle\rho^{1/2},H_1\rho^{1/2}\rangle \ . \tag{4.17}$$

Proof: Let the kernel $k(x,y)$ be defined by

$$k(x,y) = \sum_{i=1}^{N} \int \bar{\phi}(x_1,\ldots,x_{i-1},x,x_{i+1},\ldots,x_N)\phi(x_1,\ldots,x_{i-1},y,x_{i+1},\ldots,x_N)d\hat{x}_i \ . \tag{4.18}$$

Then it is easy to see that $k(x,y)$ is a positive definite kernel and

$$k(x,x) = \rho(x) \ . \tag{4.19}$$

The key observation is that the operator $\exp(-H_1t)$ has positive integral kernel

$$e^{-H_1t}(x,y) \ . \tag{4.20}$$

Thus if we put

$$F_N(t) = \sum_{i=1}^{N} \langle\phi,\exp\ (-(-\Delta_i)^{1/2}t)\phi\rangle \tag{4.21}$$

and let

$$F(t) = \langle\rho^{1/2},\exp\ (-H_1t)\rho^{1/2}\rangle \ , \tag{4.22}$$

we see that

$$F_N(0) = F(0) = N \ . \tag{4.23}$$

Now for $t > 0$ we have

$$F_N(t) = \iint e^{-H_1t}(x,y)k(x,y)dxdy \leq \iint e^{-H_1t}(x,y)k(x,x)^{1/2}k(y,y)^{1/2}dxdy$$

$$= F(t) \ . \tag{4.24}$$

We conclude therefore from (4.23), (4.24) that

$$- \partial F_N/\partial t|_{t=0} \geq - \partial F/\partial t|_{t=0} . \tag{4.25}$$

However the left side of (4.25) is just the left side of (4.17) and the right side of (4.25) is just the right side of (4.17). Q.E.D.

It is now evident that theorem 1.3 follows from the previous three lemmas.

Remark: Barry Simon has noted that stability of matter follows directly from the stability of the relativistic system. The reason is that

$$(-\Delta_i)^{1/2} - 1/4 \leq -\Delta_i . \tag{4.26}$$

If we sum (4.26) with respect to i we then get

$$\sum_{i=1}^{N} -\Delta_i \geq H_N - N/4 . \tag{4.27}$$

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