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Stability of Matter. I

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The stability problem of a system of charged point particles is discussed, and a number of relevant theorems are proven. The total energy of a system of N particles has a negative lower bound proportional to $N^{\frac{5}{3}}$ when no assumption is made on the statistics of the particles. When all particles belong to a fixed number of fermion species, a lower bound exists proportional to N.

1. INTRODUCTION

IN a recent paper, Fisher and Ruelle[1] raised the question: Is a quantum-mechanical system of electrical point charges stable? By stability they mean: There exists a lower bound for the total energy proportional to the total number of particles. In this and a following paper we address ourselves to this problem, by proving with rigorous analysis a number of theorems which are relevant to it.

The question of why matter is stable was very much the center of attention of physicists during the years after the discovery by Rutherford that matter consists of positive and negative point particles interacting by Coulomb forces, and before the establishment of wave mechanics. The origin of quantum theory, starting with Planck's work, is intimately bound up with this question. Planck's quantization of the radiation oscillators and Bohr's quantization of orbits in atoms served to stop the energy in matter from disappearing into the bottomless sink of the classical radiation field. In 1925 wave mechanics provided a quantitative solution to this problem. It became clear that an atom with a nuclear charge Ze and Z electrons of charge $-e$ could not have an energy state lower than $-Z^3\text{Ry}$, where $\text{Ry} = me^4/2\hbar^2$ is the natural atomic energy unit, the Rydberg, formed from the fundamental constants m, e, and $\hbar$.

This solved the problem of stability for single atoms. However, matter in bulk consists of a very large number of particles, positively and negatively charged, attracting and repelling each other by the Coulomb force. The effects of the Coulomb force are manifold and subtle, and often cooperative. They include such diverse phenomena as chemical binding, metallic cohesion, Van der Waals forces, superconductivity, superfluidity, and (in all likelihood) biology. The stability problem for matter in bulk is not a simple one. We need to understand why all these subtle effects have in common a saturation property, so that the binding energy per particle remains always bounded.

The empirical stability of matter does not depend on non-Coulombian forces (nuclear forces, magnetic dipole interactions, retardation and relativistic effects, radiative corrections). These contribute very small corrections to the binding energies of atoms and molecules. We are therefore justified in adopting the point of view that "matter" is a collection of point charges, interacting only through Coulomb forces, and subject to the laws of nonrelativistic quantum mechanics. If stability for this mathematical model is understood, stability for real matter is understood too.

We now give a formal definition of stability. Let the Hamiltonian operator of $N \geq 2$ charged particles be

$$H_N = \sum_{j=1}^{N}\left(-\frac{\hbar^2}{2m_j}\Delta_j\right) + \sum_{1\leq i<j\leq N}\sum \frac{e_i e_j}{|\mathbf{r}_i - \mathbf{r}_j|}. \quad (1.1)$$

Here we use the standard notation; the charges e_j may have either sign. We write

$$E_{\min}(N, e, m) = \operatorname{Inf}(\psi, H_N\psi), \quad (1.2)$$

where the infimum is taken with respect to all N-particle wavefunctions $\psi = \psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ normalized according to $(\psi, \psi) = 1$, all values of the masses satisfying

$$0 < m_j \leq m, \quad (1.3)$$

and all values of the charges satisfying

$$-e \leq e_j \leq e. \quad (1.4)$$

If there is a numerical constant A such that for all N

$$E_{\min} > -AN\,\text{Ry}, \quad (\text{Ry} = me^4/2\hbar^2), \quad (1.5)$$

we say that the system is *stable*.

In this definition, we have not mentioned the

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[1] M. E. Fisher and D. Ruelle, J. Math. Phys. 7, 260 (1966).

statistics of the particles. Fisher and Ruelle in their paper[1] conjecture stability "with perhaps the restriction that either the positive or the negative particles obey Fermi statistics." The complete statement of stability or instability therefore involves a specification of the statistics of the particles. In that case the constant A may depend on the number and kind (in the sense of statistics) of different particle species.

The recent consideration of the stability problem[1] arose in connection with the need to establish a mathematically rigorous basis for statistical mechanics. Statistical mechanics makes physical sense only if thermodynamic quantities such as the energy, entropy, etc. are extensive, i.e., proportional (asymptotically for a large system) to the number of particles. Thus, stability in the sense (1.5) is necessary for the definition of a finite free energy per particle. The investigations of Ruelle[2] and Fisher[3] were restricted to models with short-range forces only. Thus, our investigation of the stability problem for Coulomb systems may be regarded as a necessary first step in establishing a rigorous statistical mechanics based on Coulomb forces alone, a challenging and difficult task.

2. STATEMENT OF RESULTS

Quite simple arguments suffice to give lower bounds for the energy of a system of charged particles, provided we do not require these bounds to be good for large N. We begin by stating two theorems of this nature. They are superseded by later theorems, and are only interesting because of the simplicity of their proofs.

Theorem 1: Under the hypotheses (1.3) and (1.4) we have

$$E_{\min} \geq -\tfrac{1}{8}N^2(N-1)\text{ Ry}. \tag{2.1}$$

This is the result of Fisher and Ruelle.[1] For the sake of completeness, we reproduce their proof.

The following theorem, whose proof is slightly more difficult, is a refinement of Theorem 1 for $N > 5$, and it holds under the same hypotheses.

Theorem 2:

$$E_{\min} > -[N(N-1)/\sqrt{2}]\text{ Ry}. \tag{2.2}$$

Both of these theorems give lower bounds which are far too low (except for small values of N). Our first nontrivial result is a further improvement which comes much closer to the truth.

Theorem 3:

$$E_{\min} > -AN^{\frac{5}{3}}\text{ Ry}, \tag{2.3}$$

where $A < 52$ is an absolute constant.

Again, we assume inequalities (1.3) and (1.4) of the Introduction, but no assumption is made on particle statistics.

In connection with these theorems the question arises, what is the best possible result of this type? We believe that it is

$$E_{\min} > -AN^{\frac{7}{5}}\text{ Ry}. \tag{2.4}$$

To prove that the exponent $\frac{7}{5}$ cannot be decreased it is sufficient to exhibit states ψ_N of N particles such that for some constant A'

$$(\psi_N, H_N\psi_N) < -A'N^{\frac{7}{5}}\text{ Ry}. \tag{2.5}$$

Because the inequality (2.5) states an upper bound for the energy, conventional variational techniques are adequate for proving it. The result (2.5) is suggested by both a simple heuristic argument and by a detailed calculation based on the work of Foldy[4] and others.[5] Since we are interested in lower bounds for which new techniques must be used, we do not discuss the derivation of (2.5) in this paper but refer the interested reader to the lectures one of us held at the Summer Physics Institute of Brandeis University in 1966.[6] We find later that an improvement from (2.3) to (2.4) would necessitate going in an essential way beyond the techniques of the present work.

While (2.5) indicates that a Coulomb system without any restriction on particle statistics is unstable, the following result shows the importance of the exclusion principle for stability.

Theorem 4: Suppose that N particles whose masses and charges satisfy (1.3) and (1.4) belong to $q \geq 1$ distinct species of fermions. Then

$$E_{\min} > -Aq^{\frac{2}{3}}N\text{ Ry}, \tag{2.6}$$

where $A < 500$ is an absolute constant. Briefly, a system whose particles belong to a fixed number of Fermion species is stable.

In counting the number of species, each spin state of a type of particle must be counted separately, for the antisymmetry of the spatial wavefunction holds only

[2] D. Ruelle, Helv. Phys. Acta. **36,** 183; **36,** 789 (1963).
[3] M. E. Fisher, Arch. Ratl. Mech. Anal. **17,** 377 (1964).

[4] L. L. Foldy, Phys. Rev. **124,** 649 (1961).
[5] M. Girardeau and G. Arnowitt, Phys. Rev. **113,** 755 (1959); M. Girardeau, *ibid.* **127,** 1809 (1962); J. M. Stephen, Proc. Phys. Soc. (London) **79,** 994 (1962); W. H. Bassichis and L. L. Foldy, Phys. Rev. **133,** A935 (1964); W. H. Bassichis, *ibid.* **134,** A543 (1964). Another paper concerned with the stability problem, with a point of view closer to ours is: E. Teller, Rev. Mod. Phys. **34,** 627 (1962).
[6] F. J. Dyson (to be published).

between particles of the same type and spin quantum number. Note that the constants A appearing in (2.3), (2.4), (2.6), and (2.7) below are not the same.

Theorem 4 falls short in two ways of what we need in a theorem establishing the stability of matter. First, it ought not require that all particles be fermions. The statistics of the nuclei are irrelevant to stability. Therefore the hypothesis that only particles of one sign of charge (say negative) are fermions should be sufficient. Second, it is an empirical fact that all chemical binding and cohesive energies are determined by the Rydberg constant $\mathrm{Ry} = me^4/2\hbar^2$ formed with the electron mass and not the nuclear mass. Stability should be independent of the nuclear mass and should persist even if the nuclear mass is taken infinite. Both of these defects are removed in our final theorem.

Theorem 5: Let N negatively charged particles belong to q different fermion species. Let their masses and charges be subject to (1.3) and (1.4), respectively. Let an arbitrary number of positively charged particles be subject to the sole restriction (1.4) on their charges, their statistics and their masses being arbitrary. Then

$$E_{\min} > -Aq^{\frac{2}{3}} N\,\mathrm{Ry}, \tag{2.7}$$

where A is an absolute constant.

In this theorem there are no unnecessary hypotheses. However, its proof is longer and more difficult than those of the others. In this paper we prove only Theorems 1–4 and delay Theorem 5 to a separate paper. It turns out that the proof of Theorem 5 requires all the preliminary results needed for the proofs of the earlier theorems, and a number of additional ones besides. Because of its fundamental significance, it would be desirable to simplify the proof of Theorem 5. We hope that this is possible by using ideas different from ours.

We may remark that the dependence of Theorems 4 and 5 on the number q of fermion species is probably not the best possible. The results stated should hold with the exponent $\frac{2}{3}$ replaced by $\frac{2}{5}$. For some discussion of this point the reader is referred to Ref. 6.

3. PROOFS OF THEOREMS 1 AND 2

The following simple argument is due to Fisher and Ruelle.[1] Write the Hamiltonian (1.1) in the form

$$\begin{aligned} H_N &= \sum_{1\le i<j\le N}\sum \left[-\frac{\hbar^2}{2m_i(N-1)}\Delta_i - \frac{\hbar^2}{2m_j(N-1)}\Delta_j + \frac{e_ie_j}{|\mathbf{r}_i-\mathbf{r}_j|}\right] \\ &= \sum_{1\le i<j\le N}\sum H_{ij}. \end{aligned} \tag{3.1}$$

The operator H_{ij} is the Hamiltonian of a two-particle system with charges e_i, e_j and masses $m_i(N-1)$, $m_j(N-1)$. We have then

$$E_{\min} = \mathrm{Inf}\,(\psi, H_N\psi) \ge \sum_{1\le i<j\le N}\sum \mathrm{Inf}\,(\psi, H_{ij}\psi), \tag{3.2}$$

$$\mathrm{Inf}\,(\psi, H_{ij}\psi) = \begin{cases} -\dfrac{(N-1)m_im_j}{m_i+m_j}\dfrac{e_i^2e_j^2}{2\hbar^2} & (e_ie_j<0), \\ 0 & (e_ie_j\ge 0). \end{cases} \tag{3.3}$$

Among the pairs (i,j) there are at most $\frac{1}{4}N^2$ for which $e_ie_j<0$, and for these

$$\frac{(N-1)m_im_j}{m_i+m_j}\frac{e_i^2e_j^2}{2\hbar^2} \le \frac{(N-1)me^4}{4\hbar^2} = \frac{N-1}{2}\,\mathrm{Ry}. \tag{3.4}$$

This proves Theorem 1.

The proof of Theorem 2 is slightly more complicated. We now write

$$H_N = \sum_{1\le i<j\le N}\sum H_{ij} + \sum_{1\le i<j\le N}\sum H'_{ij}, \tag{3.5}$$

where

$$H_{ij} = -\frac{\hbar^2}{2m_i(N-1)}\Delta_i - \frac{\hbar^2}{2m_j(N-1)}\Delta_j + \frac{e_ie_j}{|\mathbf{r}_i-\mathbf{r}_j|}e^{-\mu|\mathbf{r}_i-\mathbf{r}_j|} \tag{3.6}$$

and

$$H'_{ij} = (e_ie_j/|\mathbf{r}_i-\mathbf{r}_j|)(1-e^{-\mu|\mathbf{r}_i-\mathbf{r}_j|}), \tag{3.7}$$

and μ is a positive number. We need a lemma which asserts that a particle in a Yukawa potential cannot have negative energy if the range of the potential is short enough.

Lemma 1: The one-particle Hamiltonian

$$H = -(\hbar^2/2m)\Delta - (e^2/r)e^{-\mu r} \tag{3.8}$$

is nonnegative if

$$\mu\hbar^2/me^2 \ge \sqrt{2}. \tag{3.9}$$

Thus if we choose

$$\mu = (N-1)me^2/\sqrt{2}\hbar^2 \tag{3.10}$$

all H_{ij} are nonnegative operators. For the second sum in (3.5) we write

$$\sum_{1\le i<j\le N}\sum H'_{ij} = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{e_ie_j}{|\mathbf{r}_i-\mathbf{r}_j|} \times (1-e^{-\mu|\mathbf{r}_i-\mathbf{r}_j|}) - \tfrac{1}{2}\mu\sum_{j=1}^{N}e_j^2. \tag{3.11}$$

By Fourier transformation the double sum may be written in the manifestly positive form

$$\frac{1}{2\pi^2}\int d^3k\left(\frac{1}{k^2}-\frac{1}{k^2+\mu^2}\right)\left|\sum_{j=1}^{N}e_je^{i\mathbf{k}\cdot\mathbf{r}_j}\right|^2 > 0. \tag{3.12}$$

Hence we have from (3.10)

$$E_{\min} > -\tfrac{1}{2}\mu N e^2 = -[N(N-1)/\sqrt{2}]\ \mathrm{Ry}. \quad (3.13)$$

It remains to prove Lemma 1. We write the energy in momentum representation

$$(\psi, H\psi) = \frac{\hbar^2}{2m}\int d^3k k^2 |\tilde{\psi}(\mathbf{k})|^2 - \frac{e^2}{2\pi^2}\int d^3k \int d^3k' \frac{\tilde{\psi}^*(\mathbf{k})\tilde{\psi}(\mathbf{k}')}{\mu^2 + |\mathbf{k}-\mathbf{k}'|^2}, \quad (3.14)$$

where $\tilde{\psi}(\mathbf{k})$ is the Fourier transform of the wave-function. By the Schwarz inequality we have

$$\left| \int d^3k \int d^3k' \frac{\tilde{\psi}^*(\mathbf{k})\tilde{\psi}(\mathbf{k}')}{\mu^2 + |\mathbf{k}-\mathbf{k}'|^2} \right| \le \int d^3k k^2 |\tilde{\psi}(\mathbf{k})|^2 J^{\frac{1}{2}} \quad (3.15)$$

with

$$J = \int d^3k \int d^3k' \frac{1}{|\mathbf{k}|^2 |\mathbf{k}'|^2 (\mu^2 + |\mathbf{k}-\mathbf{k}'|^2)^2} = 2\pi^4/\mu^2. \quad (3.16)$$

Therefore,

$$(\psi, H\psi) \ge \left(\frac{\hbar^2}{2m} - \frac{e^2}{2\pi^2} J^{\frac{1}{2}}\right) \int d^3k k^2 |\tilde{\psi}(\mathbf{k})|^2 \ge 0, \quad (3.17)$$

when the condition

$$\hbar^2/2m \ge (e^2/2\pi^2) J^{\frac{1}{2}}, \quad (3.18)$$

which is the same as (3.9), is fulfilled. This proves Lemma 1 and Theorem 2.

4. A THEOREM OF ELECTROSTATICS

We begin to work toward the proof of Theorems 3–5 by a simple consideration of electrostatics. We obtain a lower bound on the Coulomb energy of an arbitrary finite system of point charges. The resulting inequality is one of the essential tools for all that follows.

Let $\mathbf{r}_i$ $(i = 1, 2, \cdots, N)$ be points in space at which there are charges e_i. Let a_i be arbitrary positive numbers and let S_i be the spheres $|\mathbf{r} - \mathbf{r}_i| = a_i$. Suppose that each of the charges e_i is distributed uniformly over the corresponding surface S_i. This results in a surface distribution of charges, where the element of surface $d\sigma$ carries the charge $e_i d\sigma/4\pi a_i^2$ if $d\sigma$ is on S_i. If $\mathbf{E} = \mathbf{E}(\mathbf{x})$ is the electric field at the point $\mathbf{x}$, produced by this charge distribution, we have for the total energy

$$\frac{1}{8\pi}\int d^3x |\mathbf{E}|^2 = \frac{1}{2}\sum_{i=1}^{N} \frac{e_i}{4\pi a_i^2}\int_{S_i} d\sigma_x \times \sum_{j=1}^{N} \frac{e_j}{4\pi a_j^2}\int_{S_j} d\sigma_y \frac{1}{|\mathbf{x}-\mathbf{y}|}. \quad (4.1)$$

The double surface integral depends only on the distances $|\mathbf{r}_i - \mathbf{r}_j|$ between the centers of the spheres S_i and S_j, and on their radii a_i and a_j. For two spheres S_a and S_b, of radii a and b, respectively, whose centers are at a distance r, we write

$$\int_{S_a} \frac{d\sigma_x}{4\pi a^2}\int_{S_b} \frac{d\sigma_y}{4\pi b^2} \frac{1}{|\mathbf{x}-\mathbf{y}|} = \frac{1}{r} - \Delta(r, a, b). \quad (4.2)$$

This defines the function Δ. One finds

$$\Delta(r, a, b) = \begin{cases} \dfrac{1}{r} - \min\left(\dfrac{1}{a}, \dfrac{1}{b}\right) & (0 < r \le |a-b|), \\ \dfrac{(a+b-r)^2}{4abr} & (|a-b| \le r \le a+b), \\ 0 & (a+b \le r). \end{cases} \quad (4.3)$$

Δ is positive and monotone decreasing with r in the interval $(0, a+b)$, zero beyond it.

Let us write

$$W(\mathbf{r}, e) = \sum_{1\le i<j\le N}\sum \frac{e_i e_j}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (4.4)$$

$$U(\mathbf{r}, e, a) = -\sum_{1\le j\le N} \frac{e_j^2}{2a_j} + \sum_{1\le i<j\le N}\sum e_i e_j \Delta(|\mathbf{r}_i - \mathbf{r}_j|, a_i, a_j). \quad (4.5)$$

Theorem 6: $W(\mathbf{r}, e) > U(\mathbf{r}, e, a)$.

The proof consists in merely observing that the total electrostatic field energy (4.1) is positive, and then rewriting the right-hand side in terms of the notation (4.2). Note that whenever

$$a_i + a_j \le |\mathbf{r}_i - \mathbf{r}_j| \quad (1 \le i < j \le N), \quad (4.6)$$

we have

$$U(\mathbf{r}, e, a) = -\sum_{j=1}^{N} \frac{e_j^2}{2a_j}, \quad (4.7)$$

and the inequality $W > U$ is specially simple. The inequality in this form was used by Onsager in a little known paper[7] in which he established an additive lower bound for the Coulomb energy of a system in which the particles are assumed to possess hard cores. Indeed, if it is required that

$$|\mathbf{r}_i - \mathbf{r}_j| \ge 2a \quad (1 \le i < j \le N) \quad (4.8)$$

for some fixed positive a, one has

$$W > -N(e^2/2a) \quad (e = \max |e_i|). \quad (4.9)$$

This observation was also made by Fisher and Ruelle.[1]

In our work where there are no *a priori* given hard

[7] L. Onsager, J. Phys. Chem. 43, 189 (1939).

cores it is essential to keep the a_j variable. Indeed, the power of Theorem 6 lies largely in the freedom with which the a_j may be chosen.

One useful choice is $a_j = \frac{1}{2}R_j$, where

$$R_j = \min_{(1\le i\le N, i\ne j)} |\mathbf{r}_i - \mathbf{r}_j| \,. \tag{4.10}$$

Then evidently (4.6) is fulfilled. Thus we have

Theorem 7:

$$W > -\sum_{j=1}^{N} \frac{e_j^2}{R_j}. \tag{4.11}$$

In this paper we use Theorem 6 only in the form of Theorem 7. The right-hand side of (4.11) may be interpreted physically as the potential energy of a fictitious system in which each particle is attracted by a Coulomb force *to its nearest neighbor alone*. The fictitious system always has a potential energy lower than the real Coulomb system, and—what is most essential—the number of terms out of which this fictitious potential energy is made up is N and not of the order of N^2 as for the true energy.

5. PROOF OF THEOREM 3

Let $\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N$ be N distinct points in space. For a fixed j we write $R_{j1}, R_{j2}, \cdots, R_{jN-1}$ for the $N-1$ distances $|\mathbf{r}_j - \mathbf{r}_1|$, $|\mathbf{r}_j - \mathbf{r}_2|, \cdots, |\mathbf{r}_j - \mathbf{r}_N|$ arranged in increasing order. Thus R_{j1} [the same as R_j defined by (4.10) above] is the distance between $\mathbf{r}_j$ and its nearest neighbor among the other points, R_{j2} is the distance between it and its second nearest neighbor, and so on. Conventionally we define $R_{jl} = \infty$ for $l \ge N$. The R_{jl} are well-defined functions of the N variable points $R_{jl} = R_{jl}(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$.

Suppose we consider a quantum-mechanical system of N particles in a state described by the wavefunction $\psi = \psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ normalized in the usual way

$$(\psi, \psi) = \int \cdots \int d^{3N}r \, |\psi|^2 = 1. \tag{5.1}$$

Let us introduce the following quantities:

$$K_l = \frac{1}{N} \int \cdots \int d^{3N}r \, |\psi|^2 \sum_{j=1}^{N} R_{jl}^{-1} \quad (l = 1, 2, \cdots). \tag{5.2}$$

By definition of the R_{jl} we have

$$K_1 \ge K_2 \ge K_3 \ge \cdots \ge 0, \tag{5.3}$$

and $K_l = 0$ for $l \ge N$. The K_l have the dimension of an inverse distance; K_l^{-1} is a measure of the typical linear dimension of regions which contain $l+1$ (but no more) particles.

The quantity K_1 is particularly important in connection with the inequality (4.11). From it we immediately see the following fact: If the charges of a finite system of particles satisfy (1.4), then the total Coulomb energy satisfies the inequality

$$(\psi, W\psi) > -Ne^2K_1. \tag{5.4}$$

On the other hand, if the masses satisfy (1.3) we have for the kinetic energy

$$(\psi, T\psi) = \sum_{j=1}^{N} \frac{\hbar^2}{2m_j} \int \cdots \int d^{3N}r \, |\nabla_j \psi|^2 \ge N \frac{\hbar^2}{2m} t, \tag{5.5}$$

where

$$t = \frac{1}{N} \sum_{j=1}^{N} \int \cdots \int d^{3N}r \, |\nabla_j \psi|^2. \tag{5.6}$$

Thus the total energy satisfies

$$(\psi, H_N\psi) > N[(\hbar^2/2m)t - e^2K_1]. \tag{5.7}$$

Our aim is to derive an inequality involving both t and K_1 which allows the establishment of a lower bound on the right-hand side of (5.7) independent of both.

We begin by deriving an upper bound on the cumulative sum

$$\sum_{l=1}^{k} K_l \tag{5.8}$$

in terms of K_{k+1} and t. By definition, the sum (5.8) may be written out in detail as follows:

$$\frac{1}{N} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\ne i}}^{N} \int d^3r_i \int d^3r_j \sum_P \int_{\text{in}} d^3r_{\alpha_1} \cdots \int_{\text{in}} d^3r_{\alpha_k} \int_{\text{out}} d^3r_{\beta_1} \cdots \int_{\text{out}} d^3r_{\beta_{N-2-k}} \sum_{l=1}^{k} \frac{|\psi|^2}{|r_{\alpha_l} - r_i|}. \tag{5.9}$$

P is a partition of the set of $N-2$ integers $\{1, 2, \cdots, i-1, i+1, \cdots, j-1, j+1, \cdots, N\}$ into two sets $\{\alpha_1, \cdots, \alpha_k\}$ and $\{\beta_1, \cdots, \beta_{N-2-k}\}$, one containing k integers, the other $N-2-k$ integers (k being fixed). The sum over P runs over all such partitions. The phrase "in" under the integration signs means that the domain of integration is

$$|\mathbf{r}_{\alpha_l} - \mathbf{r}_i| < |\mathbf{r}_j - \mathbf{r}_i| \quad (l = 1, 2, \cdots, k), \tag{5.10}$$

while "out" means the opposite

$$|\mathbf{r}_{\beta_l} - \mathbf{r}_i| \ge |\mathbf{r}_j - \mathbf{r}_i| \quad (l = 1, 2, \cdots, N-2-k). \tag{5.11}$$

In other words: $\mathbf{r}_j$ is the $(k+1)$st nearest neighbor, and $\mathbf{r}_{\alpha_1}, \mathbf{r}_{\alpha_2}, \cdots, \mathbf{r}_{\alpha_k}$ are (in some order) the first, second, $\cdots$, (k)th nearest neighbors of the point $\mathbf{r}_i$. We now make use of the following.

Lemma 2: For any positive λ, and any complex valued function $\Psi(\mathbf{r})$, having continuous derivatives and defined in the sphere Ω: $|\mathbf{r}| \leq b$,

$$\int_\Omega d^3r \frac{|\Psi|^2}{|\mathbf{r}|} < \left(\frac{1}{\lambda} + \frac{3}{2b}\right) \int_\Omega d^3r\, |\Psi|^2 + \frac{\lambda}{4} \int_\Omega d^3r\, |\nabla\Psi|^2. \tag{5.12}$$

The proof of Lemma 2 is given later. The inequality (5.12) is applied to the integration over the variable $\mathbf{r}_{\alpha_l}$ (to be carried out first). The sphere Ω is given by (5.10), with the radius $b = |\mathbf{r}_j - \mathbf{r}_i|$ and center $\mathbf{r}_i$. It follows that an upper bound for (5.8) is obtained if we replace the integrand in (5.9) by

$$|\psi|^2\left(\frac{1}{\lambda} + \frac{3}{2}\frac{1}{|\mathbf{r}_j - \mathbf{r}_i|}\right) + \frac{\lambda}{4} |\nabla_{\alpha_l}\psi|^2. \tag{5.13}$$

For the first two terms the sum over l in (5.9) gives merely k equal integrals, so that for these one obtains

$$(k/\lambda) + \tfrac{3}{2}kK_{k+1}. \tag{5.14}$$

The gradient term may be rewritten

$$\frac{\lambda}{4N}\sum_{i=1}^{N} \int \cdots \int d^{3N}r \sum_\alpha{}' |\nabla_\alpha\psi|^2, \tag{5.15}$$

where the prime on the summation sign indicates that only those values of α are to be included in the sum for which $\mathbf{r}_\alpha$ is the (l)th nearest neighbor of $\mathbf{r}_i$ with $1 \leq l \leq k$. (The set of these values of α is a function of the integration variables $\mathbf{r}_1, \cdots, \mathbf{r}_N$, of course.) This, in turn, may be written

$$\frac{\lambda}{4N}\sum_{\alpha=1}^{N} \int \cdots \int d^{3N}r M_{\alpha k} |\nabla_\alpha\psi|^2, \tag{5.16}$$

where $M_{\alpha k} = M_{\alpha k}(\mathbf{r}_1, \cdots, \mathbf{r}_N)$ is the number of those $\mathbf{r}_i$ to which $\mathbf{r}_\alpha$ is the (l)th nearest neighbor with $1 \leq l \leq k$.

Lemma 3: For any finite set of points $\{\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N\}$ and $\alpha = 1, 2, \cdots, N$,

$$M_{\alpha k} < (4\pi/\omega)k < 15k, \tag{5.17}$$

where

$$\omega = 2\pi(1 - \cos\tfrac{1}{6}\pi) = \pi(2 - \sqrt{3}) \tag{5.18}$$

is the solid angle inside a circular cone of half-angle $\frac{1}{6}\pi$.

This Lemma is a purely geometrical fact which is proved later. Since trivially $M_{\alpha k} \leq N - 1$, we have now the upper bound for (5.16)

$$\tfrac{1}{4}\lambda t \min\{N - 1, (4\pi/\omega)k\} \tag{5.19}$$

in the notation (5.6). Thus we have obtained the following inequalities

$$\sum_{l=1}^{k} K_l < \frac{3k}{2} K_{k+1} + \frac{k}{\lambda} + \frac{\lambda t}{4} \min\left\{N - 1, \frac{4\pi}{\omega}k\right\} \quad (k = 1, 2, \cdots, N-1). \tag{5.20}$$

For $k = N - 1$ one has to set $K_N = 0$ (the proof makes use of Lemma 2 with Ω all space and $b = \infty$).

Lemma 4: Let the sequence of nonnegative numbers $x_1, x_2, \cdots$ satisfy

$$\sum_{l=1}^{k} x_l < a_k x_{k+1} + b_k \quad (k = 1, 2, \cdots), \tag{5.21}$$

where the coefficients a_k and b_k are nonnegative. Then

$$x_1 \leq A_k x_{k+1} + B_k \quad (k = 1, 2, \cdots), \tag{5.22}$$

where

$$A_k = a_k \prod_{j=1}^{k-1} \frac{a_j}{1 + a_j} \tag{5.23}$$

and

$$B_k = \sum_{l=1}^{k-1} \frac{b_l}{1 + a_l} \prod_{j=1}^{l-1} \frac{a_j}{1 + a_j} + b_k \prod_{j=1}^{k-1} \frac{a_j}{1 + a_j}. \tag{5.24}$$

In the last two equations empty sums are interpreted as zero and empty products as unity. The proof is given later.

We use Lemma 4 to eliminate $K_2, K_3, \cdots, K_k$ from (5.20) and obtain a single inequality which involves only K_1, K_{k+1}, and t. Indeed, (5.20) is precisely of the form (5.21) with

$$a_k = \tfrac{3}{2}k \tag{5.25}$$

and

$$b_k = (k/\lambda) + \tfrac{1}{4}\lambda t \min\{N - 1, (4\pi/\omega)k\}. \tag{5.26}$$

We have then

$$A_k = \prod_{j=1}^{k} \frac{3j}{3j - 1} = \frac{k!\,\Gamma(\frac{2}{3})}{\Gamma(k + \frac{2}{3})}. \tag{5.27}$$

A simple upper bound on A_k is obtained by noting

$$[3j/(3j - 1)]^3 < (3j + 1)/(3j - 2), \tag{5.28}$$

so that

$$A_k < (3k + 1)^{\frac{1}{3}}. \tag{5.29}$$

In particular

$$A_{N-1} < (3N)^{\frac{1}{3}}. \tag{5.30}$$

The computation of B_k is more complicated due to the two different analytic expressions involved in (5.26). We temporarily ignore this complication and set simply

$$b_k = k[(1/\lambda) + (\pi/\omega)\lambda t]. \tag{5.31}$$

(The inequality will be somewhat worse but the calculation is easier.) One finds with (5.25) and (5.31) the identity

$$B_k = 2(A_k - 1)[(1/\lambda) + (\pi/\omega)\lambda t]. \tag{5.32}$$

In particular, using (5.30)

$$B_{N-1} < (3N)^{\frac{1}{3}}[(2/\lambda) + (2\pi/\omega)\lambda t]. \tag{5.33}$$

We now write down the inequality which follows from (5.20) by Lemma 4 for the case $k = N - 1$

$$K_1 < (3N)^{\frac{1}{3}}[(2/\lambda) + (2\pi/\omega)\lambda t], \tag{5.34}$$

or equivalently (since λ is arbitrary)

$$K_1 < 4(3N)^{\frac{1}{3}}(\pi t/\omega)^{\frac{1}{2}}. \tag{5.35}$$

We are now ready to complete the proof of Theorem 3. From (5.7) and (5.35) we have

$$(\psi, H_N\psi) > N(\hbar^2/2m)t - 4e^2N(3N)^{\frac{1}{3}}[(\pi/\omega)t]^{\frac{1}{2}} \geq -AN^{\frac{5}{3}}\,\mathrm{Ry} \tag{5.36}$$

with

$$A = (16\pi/\omega)3^{\frac{2}{3}} = 124.2\cdots. \tag{5.37}$$

The last inequality in (5.36) arises by minimizing with respect to t.

A lower value of A can be obtained by using (5.26) instead of (5.31) to compute B_{N-1}. We find $A < 52$. However, the exponent $\frac{5}{3}$ cannot be improved. The latter originates in the factor $\frac{3}{2}$ in (5.25) and that goes back to the factor $\frac{3}{2}$ on the right-hand side of (5.12) in Lemma 2. The inequality in (5.12) can be made to approach equality with arbitrary precision, as the example $\Psi = \text{const}$ and

$$\int_\Omega d^3r\,\frac{|\Psi|^2}{|\mathbf{r}|} = \frac{3}{2b}\int_\Omega d^3r\,|\Psi|^2 \tag{5.38}$$

shows. It is clear that no constant larger than $\frac{3}{2}$ would do.

It is also easy to see that as long as we use not the true Coulomb energy W but rather the lower estimate given by Theorem 7, it is impossible to improve on the exponent $\frac{5}{3}$ of Theorem 3. For we can exhibit a sequence of states ψ_N such that

$$(\psi_N, [T + U]\psi_N) \sim -AN^{\frac{5}{3}}\,\mathrm{Ry} \tag{5.39}$$

as $N \to \infty$. Take wavefunctions of the form

$$\psi_N(\mathbf{r}_1, \cdots, \mathbf{r}_N) = \prod_{j=1}^{N} u_\Lambda(\mathbf{r}_j), \tag{5.40}$$

where $u_\Lambda(\mathbf{r})$ is a smooth wave packet of spatial extent Λ. The energy is about

$$N\left\{\frac{\hbar^2}{2m}\frac{1}{\Lambda^2} - e^2\frac{N^{\frac{1}{3}}}{\Lambda}\right\}, \tag{5.41}$$

because in the absence of correlations the nearest-neighbor distance is about the mean interparticle distance $\Lambda N^{-(\frac{1}{3})}$. If N is taken large and $\Lambda = \Lambda(N)$ is taken to minimize (5.41) one obtains (5.39). Therefore *a significant improvement over our Theorem 3 can be achieved only by giving up the use of Theorem 7.*

6. PROOFS OF LEMMAS 2, 3, AND 4

In order to complete the proof of Theorem 3 we now have to prove the three lemmas used in the last section.

We begin with Lemma 2. Suppose first that Ω is an arbitrary region and $V(r)$ an arbitrary potential. The ground-state energy ϵ of a particle of mass $(2\hbar^2/\lambda)$ in this potential is defined by

$$\epsilon = \mathrm{Inf}\left\{\int_\Omega d_3r(\tfrac{1}{4}\lambda\,|\nabla\Psi|^2 + V\,|\Psi|^2)\Big/\int_\Omega d_3r\,|\Psi|^2\right\}, \tag{6.1}$$

where the infimum is taken over all wavefunctions Ψ defined in Ω. No boundary condition is imposed on Ψ, but the minimizing Ψ satisfies the "natural" condition

$$(\mathbf{n}\cdot\nabla)\Psi = 0 \tag{6.2}$$

on the boundary of Ω. The eigenvalue equation for ϵ is

$$-\tfrac{1}{4}\lambda\nabla^2\Psi + V\Psi = \epsilon\Psi. \tag{6.3}$$

Since the minimizing Ψ is positive and nonzero in Ω, we may introduce the vector

$$\boldsymbol{\omega} = -(\nabla\Psi/\Psi),$$

so that (6.3) becomes

$$\epsilon = V + \tfrac{1}{4}\lambda(\operatorname{div}\boldsymbol{\omega} - \boldsymbol{\omega}^2). \tag{6.4}$$

Taking the gradient of (6.4), we find

$$(\boldsymbol{\omega}\cdot\nabla)\boldsymbol{\omega} = \tfrac{1}{2}\nabla^2\boldsymbol{\omega} + (2/\lambda)\nabla V, \tag{6.5}$$

an equation identical with the Navier–Stokes equation for steady flow of a fluid with velocity $\boldsymbol{\omega}$ and with kinematical viscosity equal to $\frac{1}{2}$. We do not pursue this peculiar hydrodynamical analogy any further (see note added in proof). Integrating (6.4) over the volume Ω, we obtain

$$\epsilon = \langle V\rangle_{\mathrm{av}} - \tfrac{1}{4}\lambda\langle\boldsymbol{\omega}^2\rangle_{\mathrm{av}}, \tag{6.6}$$

where $\langle\ \rangle_{\mathrm{av}}$ denotes an average over Ω, and the term in $(\operatorname{div}\boldsymbol{\omega})$ has vanished by virtue of (6.2).

We apply this analysis to the special case of a Coulomb potential

$$V(r) = -r^{-1}$$

in a spherical shell Ω defined by $a \leq |r| \leq b$. In this case

$$\langle V\rangle_{\mathrm{av}} = -\tfrac{3}{2}[(b^2 - a^2)/(b^3 - a^3)] > -3/2b. \tag{6.7}$$

The conclusion (5.12) of Lemma 2 states that

$$\epsilon > -(3/2b) - (1/\lambda) \tag{6.8}$$

for the spherical region $|r| < b$. If (6.8) holds for the shell $a \leq |r| \leq b$, then Lemma 2 follows by taking the limit $a \to 0$. By (6.6) and (6.7), we have only to prove

$$\langle \boldsymbol{\omega}^2 \rangle_{\text{av}} \leq (4/\lambda^2) \tag{6.9}$$

for the spherical shell Ω.

For a spherically symmetrical Ω, the ground-state Ψ is spherically symmetric, and the vector $\boldsymbol{\omega}$ is parallel to r. We denote by ω the component of the vector $\boldsymbol{\omega}$ in the radial direction. Then (6.5) becomes

$$\omega'' + 2\omega'[(1/r) - \omega] + (2/r^2)[(2/\lambda) - \omega] = 0, \tag{6.10}$$

where the prime denotes differentiation with respect to r, and the boundary condition (6.2) gives

$$\omega(a) = \omega(b) = 0. \tag{6.11}$$

If $\omega(r)$ were ever negative in $a \leq r \leq b$, there would be at least one minimum with

$$\omega'' \geq 0, \quad \omega' = 0, \quad \omega < 0,$$

which contradicts (6.10). If $\omega(r)$ were ever greater than $(2/\lambda)$, there would be at least one maximum with

$$\omega'' \leq 0, \quad \omega' = 0, \quad \omega > (2/\lambda),$$

again contradicting (6.10). Therefore

$$0 \leq \omega(r) \leq (2/\lambda) \quad \text{for} \quad a \leq |r| \leq b, \tag{6.12}$$

which proves (6.9) and also Lemma 2.

Lemma 3 deals with a geometrical property of a finite set of points in space. Let this set be $\{\mathbf{r}_0, \mathbf{r}_1, \cdots, \mathbf{r}_n\}$. We distinguish a point, $\mathbf{r}_0$ say, and attach an *index* to each of the rest of them. The index of $\mathbf{r}_i$ is said to be the integer l if $\mathbf{r}_0$ is the (l)th nearest neighbor of $\mathbf{r}_i$ in the given set. Let now $k \geq 1$ be fixed, and define a certain subset, say $\{\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_m\}$, consisting of all those points whose indices do not exceed k. We want to prove

$$m \leq (4\pi/\omega)k, \tag{6.13}$$

with ω defined in (5.18).

Let C_θ be the circular cone with vertex at $\mathbf{r}_0$, half-angle $\frac{1}{6}\pi$ and axis pointing in the direction θ. Let $\nu = \nu(\theta)$ be the number of points among $\{\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_m\}$ which are inside C_θ. We have

$$\int d\Omega_\theta \nu(\theta) = m\omega, \tag{6.14}$$

where the integration is over the solid angle element formed by varying θ. Thus (6.13) follows if we show

$$\nu(\theta) \leq k. \tag{6.15}$$

Let now θ be fixed, and suppose for the sake of definiteness that out of $\{\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_m\}$ the first ν points are inside C_θ. If $\nu = 0$ or 1, (6.15) is true trivially, so we may suppose $\nu \geq 2$. We choose the notation so that

$$|r_0 - \mathbf{r}_1| \leq |\mathbf{r}_0 - \mathbf{r}_2| \leq \cdots \leq |\mathbf{r}_0 - \mathbf{r}_\nu|. \tag{6.16}$$

Take an i $(1 \leq i \leq \nu - 1)$ and consider the triangle $(\mathbf{r}_0, \mathbf{r}_i, \mathbf{r}_\nu)$. Since the angle at $\mathbf{r}_0$ is $\leq \frac{1}{3}\pi$, the largest angle of this triangle must be either at $\mathbf{r}_i$ or at $\mathbf{r}_\nu$. But the latter is excluded because $|\mathbf{r}_0 - \mathbf{r}_i| \leq |r_0 - \mathbf{r}_\nu|$ and in a triangle the largest side occurs opposite the largest angle. Thus the angle at $\mathbf{r}_i$ is largest and so, by the same principle,

$$|\mathbf{r}_\nu - \mathbf{r}_i| \leq |\mathbf{r}_\nu - \mathbf{r}_0|. \tag{6.17}$$

Since this is true of $i = 1, 2, \cdots, \nu - 1$, $\mathbf{r}_0$ cannot be less than the (ν)th nearest neighbor of $\mathbf{r}_\nu$ or, in other words, the index of $\mathbf{r}_\nu$ is at least ν. By assumption this index does not exceed k, therefore $\nu \leq k$ which is what was to be shown. This completes the proof of Lemma 3.

We may remark that the numerical factor $4\pi/\omega = 8 + 4\sqrt{3} = 14.928\cdots$ in Lemma 3 is close to the best possible (if indeed not the best). To see this we display a set of $n = 12k + 1$ points such that $12k$ of them possess the index k. Choose one point $\mathbf{r}_0$ at the center of a regular icosahedron and the rest of them, $\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n$ in groups of k very close to the 12 vertices. Since the edge of an icosahedron exceeds the distance of its center from its vertices, the center $\mathbf{r}_0$ is the (k)th nearest neighbor to all $12k$ points. Thus the best constant of Lemma 3 must be ≥ 12.

To prove Lemma 4 we choose a fixed $k \geq 2$ (the case $k = 1$ is trivial), and define coefficients h_l as follows

$$\begin{cases} h_l = \dfrac{1}{1 + a_l} \displaystyle\prod_{j=1}^{l-1} \dfrac{a_j}{1 + a_j} & (l = 1, 2, \cdots, k - 1), \\ h_k = \displaystyle\prod_{j=1}^{k-1} \dfrac{a_j}{1 + a_j}. \end{cases} \tag{6.18}$$

These quantities satisfy

$$\sum_{j=1}^{k} h_j = 1,$$
$$\sum_{j=l}^{k} h_j = a_{l-1}h_{l-1} \quad (l = 2, 3, \cdots, k). \tag{6.19}$$

Now multiply the first k of the inequalities (5.21) by $h_1, h_2, \cdots, h_k$ respectively and add (this is valid because $h_l \geq 0$). The inequality which results is just (5.22) with A_k and B_k given by (5.23) and (5.24).

7. PROOF OF THEOREM 4

We now assume all particles are fermions and that they fall into $q \geq 1$ groups so that the exclusion principle holds between particles of the same group. No assumption is made about the number in each group except that the total number is $N \geq q + 1$.

We make use of the antisymmetry of the wavefunction of identical fermions only by the application of the following inequality.

Lemma 5: Let $\Psi = \Psi(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_\nu)$ be a function of $\nu \geq 2$ space points having continuous first derivatives, antisymmetric with respect to interchange of any two points, and defined with all points in a sphere Ω of radius λ. Then

$$\int_\Omega d^{3\nu}x \sum_{i=1}^{\nu} |\nabla_i \Psi|^2 \geq (\nu - 1) \frac{\xi^2}{\lambda^2} \int_\Omega d^{3\nu}x\, |\Psi|^2, \quad (7.1)$$

where $\xi = 2.082$ is the smallest positive root of the equation

$$(d^2/dx^2)(\sin x/x) = 0. \quad (7.2)$$

For simplicity take $\nu = 2$ (the proof for $\nu \geq 3$ is analogous). Expand

$$\Psi = \Psi(\mathbf{x}, \mathbf{y}) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} C_{n,m} u_n(\mathbf{x}) u_m(\mathbf{y}) \quad (7.3)$$

in terms of the complete orthonormal set of eigenfunctions $\{u_n(\mathbf{x})\}$ defined by the eigenvalue problem

$$-\Delta_x u_n(\mathbf{x}) = \epsilon_n u_n(\mathbf{x}) \quad (7.4)$$

with the boundary conditions

$$\frac{\partial}{\partial r} u_n(\mathbf{x}) = 0 \quad \text{for} \quad r = |\mathbf{x}| = \lambda. \quad (7.5)$$

One finds

$$\int_\Omega d^3x \int_\Omega d^3y\, |\nabla_x \Psi|^2 = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \epsilon_n |C_{n,m}|^2 = \frac{1}{2} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} (\epsilon_n + \epsilon_m) |C_{n\,m}|^2 \quad (7.6)$$

because the antisymmetry of Ψ implies $C_{n,m} = -C_{m,n}$. Also

$$\int_\Omega d^3x \int_\Omega d^3y\, |\Psi|^2 = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} |C_{n,m}|^2. \quad (7.7)$$

The ratio of (7.6) to (7.7) is smallest when $C_{n,m} \neq 0$ only for those two values $n \neq m$ for which ϵ_n and ϵ_m are the two lowest eigenvalues. There is one s-state eigenvalue $\epsilon_0 = 0$ with $u_0(\mathbf{x}) = (\frac{4}{3}\pi\lambda^3)^{-\frac{1}{2}}$, and three degenerate p-state eigenvalues

$$\epsilon_1 = \epsilon_2 = \epsilon_3 = \xi^2/\lambda^2. \quad (7.8)$$

The remaining ϵ_j all lie higher than (7.8). This completes the proof of Lemma 5.

The proof of Theorem 4 is based on an inequality which is important in its own right. It involves only t and K_{p-1} for some $p \geq q + 1$. It depends purely on the antisymmetry of the wavefunction and has nothing to do with the Coulomb problem as such.

Theorem 8: For a system of $N \geq q + 1$ fermions belonging to $q \geq 1$ species

$$(43/\xi^2)[p/(p - q)]t \geq K_{p-1}^2 \quad (7.9)$$

for $q + 1 \leq p \leq N$.

The proof of Theorem 8 is based on Lemma 5. Before proving it we show how Theorem 4 is derived from Theorem 8. Since for $q = 1$ the physical content of Theorem 4 is vacuous, we may assume $q \geq 2$. From (5.20) and Lemma 4 we derive, using (5.29) and (5.32),

$$K_1 < (3p)^{\frac{1}{3}}[K_{p-1} + (2/\lambda) + (2\pi/\omega)\lambda t]. \quad (7.10)$$

The inequality (7.9) may be rewritten in the alternate form

$$\mu \frac{43}{8\xi^2} \frac{p}{p - q} t - K_{p-1} + \frac{2}{\mu} \geq 0, \quad (7.11)$$

where μ is an arbitrary positive number. From (7.10) and (7.11) we eliminate K_{p-1}, obtaining

$$K_1 < (3p)^{\frac{1}{3}}\left[\left(\frac{2\pi}{\omega}\lambda + \frac{43}{8\xi^2}\frac{p}{p - q}\mu\right)t + 2\left(\frac{1}{\lambda} + \frac{1}{\mu}\right)\right]. \quad (7.12)$$

Comparing with (5.34) we observe that (7.12) is a weaker inequality when $p > N$. Thus we may ignore the restriction $p \leq N$ given in Theorem 8 and choose

$$p = 2q \quad (7.13)$$

for any $N \geq q + 1$. Finally, λ and μ are chosen to minimize the right-hand side of (7.12). This results in the following.

Corollary to Theorem 8: Under the conditions given in the theorem,

$$K_1 < Aq^{\frac{1}{3}}t^{\frac{1}{2}}, \quad (7.14)$$

with the constant

$$A = 2 \cdot 6^{\frac{1}{3}}\left[\left(\frac{4\pi}{\omega}\right)^{\frac{1}{2}} + \left(\frac{43}{2\xi^2}\right)^{\frac{1}{2}}\right] = 22.2\cdots. \quad (7.15)$$

The proof of Theorem 4 is now completed by using (7.14) in (5.7)

$$(\psi, H_N\psi) > N[(\hbar^2/2m)t - e^2K_1] > N[(\hbar^2/2m)t - Aq^{\frac{1}{3}}e^2t^{\frac{1}{2}}] \geq -A^2q^{\frac{2}{3}}N\,\text{Ry}, \quad (7.16)$$

with $A^2 < 500$ by (7.15).

8. PROOF OF THEOREM 8

We begin by introducing an arbitrary length λ and writing

$$t = \left(\frac{4\pi\lambda^3}{3}\right)^{-1} \int d^{3N}r \, \frac{1}{N} \sum_{j=1}^{N} |\nabla_j \psi|^2 \int_{|r_j - y| \le \lambda} d^3y. \quad (8.1)$$

If the order of the integrations over the $\mathbf{r}_j$ and over $\mathbf{y}$ is interchanged, this becomes

$$t = \left(\frac{4\pi\lambda^3}{3}\right)^{-1} \frac{1}{N} \int d^3y \sum_{P} \int_{\text{out}} d^3r_{j_1} \cdots \int_{\text{out}} d^3r_{j_{N-\nu}} \times \int_{\text{in}} d^3r_{i_1} \cdots \int_{\text{in}} d^3r_{i_\nu} [|\nabla_{i_1}\psi|^2 + \cdots + |\nabla_{i_\nu}\psi|^2]. \quad (8.2)$$

The summation is over all partitions P of the set of subscripts $\{1, 2, \cdots, N\}$ into two parts $\{i_1, i_2, \cdots, i_\nu\}$ and $\{j_1, j_2, \cdots, j_{N-\nu}\}$. The phrase "in" under an integral sign signifies that the corresponding integration variable is restricted to lie inside the sphere of radius λ around the center $\mathbf{y}$, while "out" means the opposite restriction.

We now drop all terms from the sum over P which do not satisfy

$$p \le \nu \le N, \quad (8.3)$$

where p is an arbitrary integer satisfying

$$q + 1 \le p \le N. \quad (8.4)$$

Consider now a particular P and the particles labeled $i_1, i_2, \cdots, i_\nu$ which are inside the sphere of radius λ around the center $\mathbf{y}$. Let $\nu_1, \nu_2, \cdots, \nu_q$ be the numbers among them which belong to the first, second, $\cdots$, (q)th species respectively. We apply Lemma 5 to the integration over the ν_1 variables belonging to the first species, then over the ν_2 variables belonging to the second species, and so on. Since

$$\sum_{s=1}^{q} (\nu_s - 1) = \nu - q \ge \frac{p - q}{p} \nu \quad (8.5)$$

under the restriction (8.3), we obtain

$$t \ge \left(\frac{4\pi\lambda^3}{3}\right)^{-1} \frac{1}{N} \frac{\xi^2}{\lambda^2} {\sum_{P}}' \frac{p-q}{p} \nu \int d^3y \int_{\text{out}} d^3r_{j_1} \cdots \int_{\text{out}} d^3r_{j_{N-\nu}} \int_{\text{in}} d^3r_{i_1} \cdots \int_{\text{in}} d^3r_{i_\nu} |\psi|^2. \quad (8.6)$$

The prime on the summation sign stands for the restriction of the sum to terms P for which $\nu = \nu(P)$ satisfies (8.3). We now restore the original order of the integration variables. This gives

$$t \ge \left(\frac{4\pi\lambda^3}{3}\right)^{-1} \frac{1}{N} \frac{\xi^2}{\lambda^2} \frac{p-q}{p} \int d^{3N}r \, |\psi|^2 \sum_{\nu=p}^{N} \nu \int_{\Omega_\nu} d^3y. \quad (8.7)$$

Here $\Omega_\nu = \Omega_\nu(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ is the set of points $\mathbf{y}$ such that the inequality $|\mathbf{r}_i - \mathbf{y}| \le \lambda$ is true for exactly ν (and not more) values of the subscript i. We find it convenient to rewrite (8.7) somewhat differently

$$\sum_{\nu=p}^{N} \nu \int_{\Omega_\nu} d^3y = \sum_{i=1}^{N} \int_{\Xi_i} d^3y. \quad (8.8)$$

Ξ_i is a set of points $\mathbf{y}$, defined by the condition that $|\mathbf{r}_i - \mathbf{y}| \le \lambda$, and *at least* $p - 1$ *more* inequalities of the same type $|\mathbf{r}_j - \mathbf{y}| \le \lambda \; (j \ne i)$ hold. The identity (8.8) is verified easiest after its intuitive content is grasped in terms of simple examples.

The next step is to obtain a lower bound for the volume of Ξ_i (as a function of the $\mathbf{r}_1, \cdots, \mathbf{r}_N$). It is at this point that we introduce the $(p-1)$st nearest-neighbor distance $R_{i,p-1}$ of the point $\mathbf{r}_i$. When $R_{i,p-1} \ge \lambda$ we write

$$\int_{\Xi_i} d^3y \ge 0. \quad (8.9)$$

Let then $R_{i,p-1} < \lambda$. There are precisely $p - 1$ values of $j \; (j \ne i)$ such that

$$|\mathbf{r}_j - \mathbf{r}_i| \le R_{i,p-1}. \quad (8.10)$$

Consider the set Ξ_i' of $\mathbf{y}$ satisfying

$$|\mathbf{y} - \mathbf{r}_i| \le \lambda - R_{i,p-1}. \quad (8.11)$$

Ξ_i' is a sphere of volume

$$\int_{\Xi_i'} d^3y = \frac{4\pi}{3} (\lambda - R_{i,p-1})^3. \quad (8.12)$$

For any $\mathbf{y}$ inside it and any j satisfying (8.11) one has $|\mathbf{y} - \mathbf{r}_j| \le \lambda$, which shows that Ξ_i' is a subset of Ξ_i. So we have

$$\int_{\Xi_i} d^2y \ge \frac{4\pi}{3} (\lambda - R_{i,p-1})^3. \quad (8.13)$$

We now take (8.13) and (8.9) into (8.8) and (8.7). This gives

$$t \ge \frac{\xi^2}{\lambda^2} \frac{p-q}{p} \frac{1}{N} \int d^{3N}r \, |\psi|^2 \sum_{i=1}^{N} \max\left\{0, \left(1 - \frac{R_{i\,p-1}}{\lambda}\right)^3\right\}. \quad (8.14)$$

This inequality holds for any positive λ. We average it over all values of λ in the interval $0 \le \lambda \le a$. We have

$$\begin{aligned} \frac{1}{a} \int_0^a \frac{d\lambda}{\lambda^2} \max\left\{0, \left(1 - \frac{R}{\lambda}\right)^3\right\} &= \frac{1}{4aR}\left(1 - \frac{R}{a}\right) \max\left\{0, \left(1 - \frac{R}{a}\right)^3\right\} \\ &\ge (1/4aR) - (1/a^2). \end{aligned} \quad (8.15)$$

Therefore (8.14) implies

$$t \geq \xi^2 \frac{p-q}{p}\left(\frac{K_{p-1}}{4a} - \frac{1}{a^2}\right). \quad (8.16)$$

The best value of a is $8(K_{p-1})^{-1}$, yielding

$$t \geq \frac{\xi^2}{64}\frac{p-q}{p} K_{p-1}^2. \quad (8.17)$$

This completes the proof of Theorem 8, except that 64 appears instead of the coefficient 43 on the left side of (7.9).

We have succeeded in deducing (8.17) with the coefficient 43, starting from (8.14). This requires only elementary but complicated manipulations which we do not present here.[8] In mathematical terms the problem is the following. Given some probability distribution function $F(t)$ on the positive real axis [F is nondecreasing and $F(0) = 0$, $F(\infty) = 1$], such that

$$\int_0^x (x-t)^3 \, dF(t) \leq C^2 x^5 \quad (8.18)$$

for all positive x, where C is a constant. Write

$$K = \int_0^\infty \frac{1}{t} \, dF(t). \quad (8.19)$$

What is the best possible inequality of the type

$$K^2 \leq \alpha C^2? \quad (8.20)$$

The argument above shows $\alpha \leq 64$. Our more elaborate argument gives $\alpha \leq 43$. It is easy to see that the best α cannot be less than 40. For if $F(t) = \min\{1, 10C^2t^2\}$, then $K^2 = 40C^2$. To determine the best α is an amusing problem, but it would give only a trivial numerical improvement of Theorems 8 and 4.

9. SMOOTH BACKGROUND CHARGE

Theorem 4 can be generalized by adding a smooth external charge distribution to the N fermions. The particles now interact not only with each other but also with the field produced by this background charge. Let $\rho(\mathbf{x})$ be the charge density producing the external field. The Hamiltonian is now

$$\bar{H}_N = \sum_{j=1}^N \left(-\frac{\hbar^2}{2m_j}\Delta_j\right) + \sum\sum_{1\leq i<j\leq N} \frac{e_ie_j}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{i=1}^N e_i \int d_3x \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{r}_i|} + \frac{1}{2}\int d^3x \int d^3y \frac{\rho(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}. \quad (9.1)$$

The last term is a C number, the self-energy of the background charge. We assume that it is finite.

[8] For details, see Ref. 6.

Theorem 9: Suppose N particles satisfy the conditions of Theorem 4 and are subject to an external field generated by a smooth charge density with finite self-energy. Then

$$E_{\min} > -A(2q)^{\frac{2}{3}} N \text{ Ry}, \quad (9.2)$$

where A is the same constant as in Theorem 4.

To prove this we consider a fictitious system consisting of $2N$ particles, N of them having the given masses m_i and charges e_i, and the other N of them having the same masses m_i but opposite charges $-e_i$. The total number of species is $2q$. Let H'_{2N} denote the Hamiltonian of this system, which includes the kinetic energy and the Coulomb energy due to the interactions between all $2N$ charges. Consider now the energy of this system in a state Ψ defined by

$$\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_{2N}) = \psi(\mathbf{r}_1, \cdots, \mathbf{r}_N)\psi(\mathbf{r}_{N+1}, \cdots, \mathbf{r}_{2N}). \quad (9.3)$$

It is

$$(\Psi, H'_{2N}\Psi) = 2(\psi, H_N\psi) - \int d^{6N}r \, |\psi(\mathbf{r}_1, \cdots, \mathbf{r}_N)|^2 \times |\psi(\mathbf{r}_{N+1}, \cdots, \mathbf{r}_{2N})|^2 \sum_{i=1}^N \sum_{j=N+1}^{2N} \frac{e_ie_j}{|\mathbf{r}_i - \mathbf{r}_j|}. \quad (9.4)$$

Here by H_N we mean the Hamiltonian (1.1), i.e., the energy of the first N particles alone. Theorem 4 asserts that

$$(\Psi, H'_{2N}\Psi) > -A2N(2q)^{\frac{2}{3}} \text{ Ry}. \quad (9.5)$$

We compare this with the expectation value of the operator $\bar{H}_N$ given by (9.1) in the state ψ.

$$(\psi, \bar{H}_N\psi) = (\psi, H_N\psi) + \int d^{3N}r \, |\psi(\mathbf{r}_1, \cdots, \mathbf{r}_N)|^2 \int d_3x \times \sum_{i=1}^N \frac{e_i\rho(\mathbf{x})}{|\mathbf{r}_i - \mathbf{x}|} + \frac{1}{2}\int d^3x \int d^3y \frac{\rho(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}. \quad (9.6)$$

Therefore we have

$$(\psi, \bar{H}_N\psi) - \tfrac{1}{2}(\Psi, H'_{2N}\Psi) = \frac{1}{2}\int d^3x \int d^3y \frac{\rho'(\mathbf{x})\rho'(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}, \quad (9.7)$$

where

$$\rho'(\mathbf{x}) = \rho(\mathbf{x}) + \int d^{3N}r \, |\psi|^2 \sum_{i=1}^N e_i \delta(\mathbf{r}_i - \mathbf{x}). \quad (9.8)$$

The integral on the right-hand side of (9.7) is nonnegative. Therefore

$$(\psi, \bar{H}_N\psi) \geq \tfrac{1}{2}\Psi, H(_{2N}'\Psi), \quad (9.9)$$

and comparing this with (9.5) the conclusion of Theorem 9 follows. Equality can occur in (9.9) only when $\rho' = 0$ identically, that is when the given background charge density exactly cancels the charge density $\int d^{3N}r\, |\psi|^2 \sum_i e_i \delta(\mathbf{r}_i - \mathbf{x})$ of the particles.

In this proof it is essential that we included the last term in (9.1), the self-energy of the background charge, in the definition of the Hamiltonian $\bar{H}_N$. Thus it is impossible to think of $\rho(\mathbf{x})$ as the (singular) charge density of a certain number of fixed point charges, for in that case the self-energy is infinite and Theorem 9 is vacuous. This consideration shows that our Theorem 5 is a significantly deeper result than Theorem 9, because it asserts the stability of a system of charged fermions in the field of fixed point charges where the energy, by definition, does not contain any self-energy term.

Note added in proof: For a deeper discussion of (6.5) see E. Nelson, Phys. Rev. **150**, 1079 (1966).

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Translational Invariance Properties of a One-Dimensional Fluid with Forces of Finite Extent

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The translational invariance properties of a one-dimensional fluid with finite range forces are investigated. For N particles in the interval $[0, L]$, with a two-body interaction potential $w(x) = 0$ for $x \geq R$, we find the following: (a) If $w(x)$ has a hard core of diameter d and $R \leq 2d$, each n-particle distribution function $D_n(x_1, \cdots, x_n)$ is translationally invariant if and only if $L > 2(N - n)R$ and $x_1, \cdots, x_n$ lie in $[(N - n)R, L - (N - n)R]$. (b) For arbitrary finite values of R, with or without a hard core, the above conditions are sufficient for translational invariance of the D_n. These conditions hold for all temperatures.

I. INTRODUCTION

In a recent paper[1] (referred to as I), translational invariance properties for a finite one-dimensional hard-core fluid were established. It was found that, for densities less than half the close packing density, there exists a *central* region in which the one-, two-, $\cdots$, N-particle distribution functions are translationally invariant. It is the main purpose of this paper to extend these results to one-dimensional systems with arbitrary forces of finite extent, R.

In I, use was made of the fact that, for systems with nearest-neighbor interactions, the n-particle distribution functions, D_n, are expressible in terms of the configurational partition function. For pure hard cores (no attractive forces), this function is well known, and its precise form was used explicitly throughout the investigation of paper I. In order to extend the investigation to a general class of potentials of finite extent, we employ a method which expresses derivatives of distribution functions in terms of other distribution functions. These expressions are in the form of recursion relations which lead to the translational invariance properties of the n-particle distribution functions. The bulk of this paper deals with the derivation of these recursion relations. Once obtained, the translational invariance properties are immediately established using mathematical induction.

The main result is that, for N particles contained in the interval $[0, L]$, where $L > 2(N - n)R$, there exist *central* regions, $[(N - n)R, L - (N - n)R]$, in which the functions D_n for $n = 1, \cdots, N$ are translationally invariant. It is rigorously established that, for nearest-neighbor potentials, these translational invariance properties *do not* hold outside the *central* regions and evidence that this is also true for potentials of arbitrary extent is presented. An interesting

[1] H. S. Leff and M. H. Coopersmith, J. Math. Phys. **8**, 306 (1967).