THE STABILITY OF MANY-PARTICLE SYSTEMS

Michael E. FISHER* and David RUELLE

Institut des Hautes Etudes Scientifiques

Bures-sur-Yvette (S. et O.) France

Abstract

It is shown that a quantal or classical system of N particles of distinct species α, $\beta = 1, 2, \ldots \mu$ interacting through pair potentials $\varphi_{\alpha\beta}(\underset{\sim}{r})$ are stable, in the sense that the total energy is always bounded below by $-\underset{\wedge}{N}B$, provided $\varphi_{\alpha\beta}(\underset{\sim}{r})$ exceeds some $\varphi_{\alpha\beta}^{(2)}(r)$ whose Fourier transform $\hat{\varphi}_{\alpha\beta}(p)$ corresponds to a positive semidefinite $\mu \times \mu$ matrix for all p.

This result is applied to discuss "charged" systems and stability is proved for Coulomb interactions if the charges are somewhat smeared rather than concentrated at points. For a large class of potentials it is shown that classical instability implies quantum instability in the case of bosons and, in three or more dimensions, also of fermions. Quantum systems with Coulomb interactions (point charges) are discussed and it is shown in particular that their stability cannot depend on the ratios between the masses of the particles.

*On leave from Wheatstone Physics Laboratory, King's College, London W.C.2, England

[12]

I. INTRODUCTION

Consider a classical system of N particles in a ν-dimensional space with total potential energy $U_N = U_N(\underset{\sim}{r}_1 \dots \underset{\sim}{r}_N)$, where $\underset{\sim}{r}_i$ is the position vector of the i-th particle. In order that the system behave thermodynamically in the limit $N \to \infty$ it is natural to ask that the total configurational energy satisfy the <u>stability condition</u>

$$U_N(\underset{\sim}{r}_1 \dots \underset{\sim}{r}_N) \geqslant -NB \tag{I.1}$$

for all sets of $\underset{\sim}{r}_i$, where B is a fixed bound. (Otherwise the energy per particle in the thermodynamic limit might not be bounded below). With the aid of this condition, a further condition on the potentials at large particle separations and suitable restrictions on the shapes of domain'containing the system, one can prove rigorously the existence of the thermodynamic limit for the canonical and grandcanonical partition functions for both classical and quantum·mechanical systems[1-3].

Suppose the particles interact only through a pair potential $\varphi(\underset{\sim}{r})$ so that

$$U_N = \sum_{i<j} \varphi(\underset{\sim}{r}_j - \underset{\sim}{r}_i) \tag{I.2}$$

It has then been shown[1-3] that stability is assured if the following conditions are satisfied :

(A) The pair potential can be decomposed as

$$\varphi(\underset{\sim}{r}) = \varphi^{(1)}(\underset{\sim}{r}) + \varphi^{(2)}(\underset{\sim}{r}) \tag{I.3}$$

where $\varphi^{(1)}(\underset{\sim}{r})$ may take the value $+\infty$ but is nonnegative, that is

$$\varphi^{(1)}(\underset{\sim}{r}) \geqslant 0 \tag{I.4}$$

and

$$\varphi^{(2)}(\underset{\sim}{r}) = \int d\underset{\sim}{p} \; e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}} \; \hat{\varphi}^{(2)}(\underset{\sim}{p}) \tag{I.5}$$

where the Fourier transform $\hat{\varphi}^{(2)}(\underset{\sim}{p})$ is (absolutely) integrable and satisfies

$$\hat{\varphi}^{(2)}(\underset{\sim}{p}) \geqslant 0 \tag{I.6}$$

so that, in other words, $\varphi^{(2)}(\underset{\sim}{r})$ is of <u>positive type</u>.

With the aid of this theorem one can show[3-4] that the following simple conditions are sufficient for stability, namely,

$$\text{(B)} \quad \text{for} \quad r < a_1 \qquad \varphi(\underset{\sim}{r}) \geqslant C/r^{\nu+\varepsilon}, \tag{I.7}$$

$$\text{for} \quad a_1 \leqslant r \leqslant a_2 \qquad \varphi(\underset{\sim}{r}) \geqslant -w, \tag{I.8}$$

$$\text{for} \quad r > a_2 \qquad \varphi(\underset{\sim}{r}) \geqslant -C'/r^{\nu+\varepsilon'}, \tag{I.9}$$

where a_1, a_2, C, ε, w, C' and ε' are positive constants.

More recently Dobrushin[5] has shown by an independent method that the following closely related but more general conditions, are also sufficient for stability, namely

(C) there are monotonic decreasing functions $\xi(r)$ and $\eta(r)$ such that

$$\text{for} \quad r < a_1 \qquad \varphi(r) \geqslant \xi(r) , \tag{I.10}$$

$$\text{while} \quad \int_0^{a_1} \xi(r)\, r^{\nu-1}\, dr = +\infty , \tag{I.11}$$

$$\text{for} \quad a_1 < r < a_2 \qquad \varphi(r) \geqslant -w ,$$

$$\text{for} \quad r > a_2 \qquad \varphi(r) \geqslant -\eta(r) , \tag{I.12}$$

$$\text{while} \quad \int_{a_2}^{\infty} \eta(r)\, r^{\nu-1}\, dr < \infty , \tag{I.13}$$

Dobrushin's proof is rather involved (and proceeds through a complicated inequality) so in Appendix A we present a proof of the sufficiency of conditions (C) which shows that they are, in fact, encompassed by the conditions (A) .

Our main purpose in this paper, however, is to extend the conditions (A) to systems in which species of different particles interact with one another or in which the pair potentials depend on some internal, for example orientational, coordinates. The principal result is to replace the nonnegativity of the Fourier transform $\hat{\varphi}(\underset{\sim}{p})$, Equ.(I.6) , by the positive semidefiniteness of a corresponding <u>stability matrix</u> $\Phi(\underset{\sim}{p}) = \hat{\varphi}_{\alpha\beta}(\underset{\sim}{p})$. This theorem is applied to the discussion of charged systems interacting through Coulomb and more general forces. We show that such a system is stable if the charges are slightly "smeared" by some not too singular distribution, for example by a Yukawa type function, or if the potential is cut off in some more drastic way at small r .

For quantum mechanical systems it seems likely that when account is taken of kinetic energy T_N , stability in the sense

$$\langle \mathcal{H}_N \rangle = \langle (T_N + U_N) \rangle \geqslant -NB , \tag{I.14}$$

would be attained with purely Coulomb interactions. We have been unable to solve this challenging problem but we make some remarks on the relation between the stability of classical and quantal systems. We also show that the long range part of the Coulomb potential does not cause instability and that stability cannot depend on the mass ratios of the differently charged species (as might perhaps be suggested by the "observed stability" of a system of hydrogen or deuterium atoms and the large ratio of nucleon to electron mass).

II. MULTISPECIES SYSTEMS.

Consider a system of N particles made up of μ different species with N_1 particles of species $1, \ldots N_\alpha$ particles of species α, etc, so that

$$N_1 + N_2 + \ldots + N_\mu = N \tag{II.2}$$

Let the position of the ith particle of species α be $\underset{\sim}{r}_{i(\alpha)}$, $\{ i(\alpha) = 1, 2, \ldots N_\alpha \}$ and suppose that the total configurational energy is given by

$$U_N(\underset{\sim}{r}_{1(\alpha)} \cdots \underset{\sim}{r}_{N_\mu(\mu)}) \quad \sum_{\alpha=1}^{\mu} \sum_{i(\alpha)<j(\alpha)} \varphi_{\alpha\alpha}(\underset{\sim}{r}_{j(\alpha)} - \underset{\sim}{r}_{i(\alpha)}) + \sum_{\alpha<\beta}^{\mu} \sum_{i(\alpha)} \sum_{j(\beta)} \varphi_{\alpha\beta}(\underset{\sim}{r}_{j(\beta)} - \underset{\sim}{r}_{i(\alpha)}) \tag{II.2}$$

in which $\varphi_{\alpha\beta}(r)$ is the interaction potential between a particle of species α and one of species β and may take the value $+\infty$ as well as

We will not assume that the functions $\varphi_{\alpha\beta}(\underset{\sim}{r})$ are rotationally symmetric. For instance we may suppose that the particles are asymmetric molecules but that the orientation of each one in space is held fixed as their positions vary. (Each different orientation may be considered as a distinct species.) It is obvious, however, that we should require

$$\varphi_{\alpha\beta}(\underset{\sim}{r}) = \varphi_{\beta\alpha}(-\underset{\sim}{r}) \qquad \text{(II.3)}$$

for all α, β and $\underset{\sim}{r}$. Then we have

<u>Theorem I.</u> <u>Let</u> $\varphi_{\alpha\beta}(\underset{\sim}{r}) = \varphi_{\alpha\beta}^{(1)}(\underset{\sim}{r}) + \varphi_{\alpha\beta}^{(2)}(r)$ <u>be a decomposition of the potentials respecting</u> (2.3) i.e. <u>such that</u>

$$\varphi_{\alpha\beta}^{(2)}(r) = \varphi_{\beta\alpha}^{(2)}(-r) \quad \text{for all } \alpha, \beta, \underset{\sim}{r}, \qquad \text{(II.4)}$$

<u>and suppose</u>

$$\varphi_{\alpha\beta}^{(2)}(r) = \int d\underset{\sim}{p}\, e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}}\, \hat{\varphi}_{\alpha\beta}^{(2)}(\underset{\sim}{p}) \qquad \text{(II.5)}$$

<u>where the Fourier transform</u> $\hat{\varphi}_{\alpha\beta}^{(2)}(\underset{\sim}{p})$ <u>is absolutely integrable.</u>

<u>If</u> $\varphi_{\alpha\beta}^{(1)}(\underset{\sim}{r}) \geq 0$ <u>for all</u> α, β, $\underset{\sim}{r}$ <u>and if the</u> $\mu \times \mu$ <u>matrix</u> $\underset{\sim}{\Phi}(p) = \left[\hat{\varphi}_{\alpha\beta}^{(2)}(\underset{\sim}{p})\right]$ <u>has no negative eigenvalues for any value of</u> $\underset{\sim}{p}$ <u>then the total potential energy, defined in</u> (II.2), <u>satisfies</u>

$$U_N(\underset{\sim}{r}_{1(\alpha)} \cdots \underset{\sim}{r}_{N_\mu(\mu)}) \geq -1/2 \sum_{\alpha=1} N_\alpha\, \varphi_{\alpha\alpha}^{(2)}(\underset{\sim}{0}). \qquad \text{(II.6)}$$

To prove this theorem notice firstly that the matrix $\underset{\sim}{\Phi}$ is Hermitean because

$$\hat{\varphi}_{\alpha\beta}^{(2)}(\underset{\sim}{p}) = (2\pi)^{-\nu} \int d\underset{\sim}{r}\, e^{-i\underset{\sim}{p}\underset{\sim}{r}}\, \varphi_{\alpha\beta}^{(2)}(\underset{\sim}{r})$$

and so by (II.4)

$$= (2\pi)^{-\nu} \int d\underset{\sim}{r}\, e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}}\, \varphi_{\beta\alpha}^{(2)}(-\underset{\sim}{r})$$

$$= (2\pi)^{-\nu} \int d\underset{\sim}{r}\, e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}}\, \varphi_{\beta\alpha}^{(2)}(\underset{\sim}{r}) = \hat{\varphi}_{\beta\alpha}^{(2)}(\underset{\sim}{p})^{*} . \tag{II.7}$$

Thus Φ has real eigenvalues and the statement that these are never negative is equivalent to the assertion that the Hermitean quadratic form $\underset{\sim}{x}^{+}\underset{\sim}{\Phi}\,\underset{\sim}{x}$, where $\underset{\sim}{x}$ is a $\mu \times 1$ column vector, is positive semidefinite. Secondly by (II.5) and the absolute integrability of $\hat{\varphi}_{\alpha\alpha}^{(2)}(\underset{\sim}{p})$ it follows that $\varphi_{\alpha\alpha}^{(2)}(\underset{\sim}{0})$ is finite for each α .

By definition (2.2) and the assumed positivity of the potentials $\varphi_{\alpha\beta}^{(1)}(\underset{\sim}{r})$ we have

$$U_N \geqslant \sum_{\alpha=1}^{\mu} \sum_{i(\alpha)<j(\alpha)} \varphi_{\alpha\alpha}^{(2)}(\underset{\sim}{r}_{j(\alpha)} - \underset{\sim}{r}_{i(\alpha)})$$

$$+ \sum_{\alpha<\beta}^{\mu} \sum_{i(\alpha)} \sum_{j(\beta)} \varphi_{\alpha\beta}^{(2)}(\underset{\sim}{r}_{j(\beta)} - \underset{\sim}{r}_{i(\alpha)})$$

$$\geqslant 1/2\, W_N - 1/2 \sum_{\alpha=1}^{\mu} N_\alpha\, \varphi_{\alpha\alpha}^{(2)}(\underset{\sim}{0}) \tag{II.8}$$

where

$$W_N = \sum_{\alpha=1}^{\mu} \sum_{\beta=1}^{\mu} \sum_{i(\alpha)=1}^{N} \sum_{j(\beta)=1}^{N} \varphi_{\alpha\beta}^{(2)}(r_{j(\beta)} - r_{i(\alpha)}) . \tag{II.9}$$

Introducing the Fourier transform through (II.5) yields

$$W_N = \sum_{\alpha=1}^{\mu} \sum_{\beta=1}^{\mu} \sum_{i(\alpha)} \sum_{j(\beta)} \int d\underset{\sim}{p} \exp\left[i\underset{\sim}{p}\cdot(\underset{\sim}{r}_{j(\beta)} - \underset{\sim}{r}_{i(\alpha)})\right] \hat{\varphi}_{\alpha\beta}^{(2)}(\underset{\sim}{p})$$

$$= \int d\underset{\sim}{p} \sum_{\alpha=1}^{\mu} \sum_{\beta=1}^{\mu} \left[\sum_{i(\alpha)} \exp(i\underset{\sim}{p}\cdot\underset{\sim}{r}_{i(\alpha)})\right]^{*} \hat{\varphi}_{\alpha\beta}^{(2)}(\underset{\sim}{p}) \left[\sum_{j(\beta)} \exp(i\underset{\sim}{p}\cdot\underset{\sim}{r}_{j(\beta)})\right]$$

On defining the column vector

$$\hat{\underset{\sim}{n}}(\underset{\sim}{p}) = \left[\sum_{i(\alpha)=1}^{N} \exp(i\underset{\sim}{p}\cdot\underset{\sim}{r}_{i(\alpha)})\right] \tag{II.10}$$

this may be written simply as

$$W_N = \int d\underset{\sim}{p}\ \hat{\underset{\sim}{n}}(\underset{\sim}{p})^{\dagger}\ \underset{\sim}{\Phi}(\underset{\sim}{p})\ \hat{\underset{\sim}{n}}(\underset{\sim}{p}) \ . \tag{II.11}$$

Since the integrand is a nonnegative quadratic form for all $\underset{\sim}{p}$ we have $W_N \geqslant 0$ and the theorem is proved.

<u>Remarks</u>. The theorem may obviously be extended to the case where, in addition to two-body potentials, U_N contains non-negative many body potentials. The theorem applies even when $N_\alpha = 1$ (all α) so that each particle belongs to a distinct species ; but in that case the "self interaction" potential $\varphi_{\alpha\alpha}(r)$ may be chosen arbitrarily.

<u>III. CHARGED SYSTEMS.</u>

Suppose the particles of the system are "charged" so that each particle of species α carries a charge q_α and the interactions are given by

$$\varphi_{\alpha\beta}(\underset{\sim}{r}) = q_\alpha\ q_\beta\ \chi(\underset{\sim}{r}) \tag{III.1}$$

where $\chi(\underset{\sim}{r})$ is a fixed "shape factor" satisfying

$$\chi(\underset{\sim}{r}) = \chi(-\underset{\sim}{r}) \qquad \chi(-\underset{\sim}{r}) \longrightarrow 0 \quad \text{as} \quad r \longrightarrow \infty \,. \tag{III.2}$$

We have principally in mind, of course, Coulomb systems for which $\chi(r) = 1/r$, screened Coulomb or Yukawa systems with $\chi(\underset{\sim}{r}) = e^{-\kappa r}/r$, etc.

The charges q_α may be positive, negative or zero. (Complex charges $q_\alpha = q'_\alpha + iq''_\alpha$ may be included equally if the interactions are taken proportional to $1/2\,(q^*_\alpha q_\beta + q_\alpha q^*_\beta) = (q'_\alpha q'_\beta + q''_\alpha q''_\beta.)$

To test the stability of such a system consider the stability matrix

$$\underset{\sim}{\Phi}(\underset{\sim}{p}) = \left[q_\alpha q_\beta \hat{\chi}(\underset{\sim}{p}) \right] \tag{III.3}$$

where $\hat{\chi}(\underset{\sim}{p})$ is the Fourier transform of $\chi(\underset{\sim}{r})$. Since the rows of the matrix are proportional to one another it may be factorized as

$$\underset{\sim}{\Phi} = \hat{\chi}(p)\, \underset{\sim}{q}\, \underset{\sim}{q}^\dagger \qquad \text{where} \qquad \underset{\sim}{q} = \left[q_\alpha \right] . \tag{III.4}$$

It follows that $\underset{\sim}{\Phi}$ has one eigenvalue

$$\lambda_1(\underset{\sim}{p}) = \hat{\chi}(\underset{\sim}{p}) \textstyle\sum_{\alpha=1}^{\mu} |q_\alpha|^2 \quad \text{and} \quad \mu-1 \quad \text{zero eigenvalues} \,.$$

Consequently the conditions of Theorem I will be satisfied (with $\varphi^{(1)}_{ij} \equiv 0$) if

$$\hat{\chi}(\underset{\sim}{p}) = (2\pi)^{-\nu} \int d\underset{\sim}{r}\; e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}}\, \chi(\underset{\sim}{r}) \geqslant 0 \quad \text{all } \underset{\sim}{p} \tag{III.5}$$

and

$$\chi(\underset{\sim}{0}) = \int d\underset{\sim}{p}\; \hat{\chi}(p) < \infty \,. \tag{III.6}$$

In that case we have

$$U_N \geqslant -1/2\; \chi(\underset{\sim}{0}) \textstyle\sum_{\alpha=1}^{N_\mu} |q_\alpha|^2 \,. \tag{III.7}$$

For the Coulomb and Yukawa potentials in ν dimensions we have

$$\hat{\chi}(p) = C_\nu / p^2 \quad , \quad C_\nu / (p^2 + \kappa^2) \quad , \tag{III.8}$$

respectively, where the C_ν are constants $(C_3 = 1/2\pi^2)$. When we try to apply the above result we find that (III.5) is satisfied but that for $\nu \geq 2$ the condition (III.6) is violated owing to a divergence of the integral at the upper limit $(p \to \infty)$[6]. This corresponds, of course, simply to the divergence of the potential itself as $r \to 0$. Accordingly let us suppose more generally (and more realistically !) that the charges are distributed rather than concentrated at points. If $\rho_\alpha(\underset{\sim}{r})$ is the charge density of a particle of the α species with respect to its position as origin, the interaction between particles becomes

$$\varphi_{\alpha\beta}(\underset{\sim}{r}) = \int d\underset{\sim}{x}_\alpha \int d\underset{\sim}{x}_\beta \; \rho_\alpha(\underset{\sim}{x}_\alpha) \; \rho_\beta(\underset{\sim}{x}_\beta) \; \chi(\underset{\sim}{r} + \underset{\sim}{x}_\beta - \underset{\sim}{x}_\alpha) \; . \tag{III.9}$$

We assume that the charge distributions of the particles are not perturbed by their mutual interaction but rather are "frozen" so that, in particular, Van der Waals or dispersion forces cannot arize. Permanent charges (ions) and dipoles are, however, adequately represented.

Introducing the Fourier transforms of the densities by

$$\hat{\rho}_\alpha(\underset{\sim}{p}) = \int d\underset{\sim}{r} \; e^{-i\underset{\sim}{p}\cdot\underset{\sim}{r}} \; \rho_\alpha(\underset{\sim}{r}) \tag{III.10}$$

and noting that $\hat{\rho}_\alpha(-\underset{\sim}{p}) = \hat{\rho}_\alpha(\underset{\sim}{p})^*$ since $\rho_\alpha(r)$ is real, gives

$$\hat{\rho}_{\alpha\beta}(\underset{\sim}{p}) = \rho_\alpha(\underset{\sim}{p}) \; \rho_\beta(\underset{\sim}{p})^* \; \hat{\chi}(\underset{\sim}{p}) \quad . \tag{III.11}$$

We thus, as before, find that the matrix $\underset{\sim}{\Phi}$ has only the single nonzero eigenvalue $\lambda_1(\underset{\sim}{p}) = \hat{\chi}(\underset{\sim}{p}) \; \Sigma_\alpha \; |\hat{\rho}_\alpha(\underset{\sim}{p})|^2$. For stability we require, again that $\hat{\chi}(p)$ is nonnegative but also, in place of (III.6) , that

$$\varphi_{\alpha\alpha}(0) = \int dp \; | \hat{\rho}_\alpha (p) |^2 \; \hat{\chi}(p) < \infty \tag{III.12}$$

which justifies (III.11) . From Theorem I we then obtain

$$U_N \geqslant - \sum_{\alpha=1}^{\mu} N_\alpha E_\alpha \tag{III.13}$$

where

$$E_\alpha = 1/2 \; \varphi_{\alpha\alpha}(0) = 1/2 \int dx \int dx' \; \rho_\alpha(x) \; \rho_\alpha(x') \; \chi(x' - x) \; . \tag{III.14}$$

Evidently E_α is just the self-energy of the charge distribution $\rho_\alpha(r)$ (which might even have zero total charge). Notice that if $\chi(r)$ is spherically symmetric and $\rho_\alpha(r)$ and $\rho_\beta(r)$ differ only by a rotation then $E_\alpha = E_\beta$. Furthermore if we add some positive potentials to the charge interactions, (III.13) remains unmodified. Accordingly we have proved the following result.

Theorem II. Suppose $U_N = U_N^{(1)} + U_N^{(2)}$ where $U_N^{(1)}$ is positive and $U_N^{(2)}$ is the potential energy of N_1 particles of species 1 with charge distribution $\rho_1(r), \ldots, N_\mu$ particles of species μ with charge distribution $\rho_\mu(r)$, where point charges q and q' interact with a pair potential $q\, q' \; \chi(r) = q\, q' \; \chi(-r)$ tending to zero as $r \to \infty$.
(If $\chi(r)$ is spherically symmetric the distributions $\rho_\alpha(r)$ may be identified up to a rotation.) Then

$$U_N (r_1 \ldots r_N) \geqslant - \sum_{\alpha=1}^{\mu} N_\alpha E_\alpha \tag{III.15}$$

provided the self-energy of a particle of species α ,

$$E_\alpha = 1/2 \int dx \int dx' \; \rho_\alpha(x) \; \rho_\alpha(x') \quad (x' - x) \quad ,$$

$$= 1/2 \int dp \; | \hat{\rho}_\alpha(p) |^2 \; \hat{\chi}(p) \quad , \tag{III.16}$$

<u>where</u> $\hat{\rho}_\alpha(\underset{\sim}{p})$ <u>and</u> $\hat{\chi}(\underset{\sim}{p})$ <u>are the Fourier transforms of</u> $\rho_\alpha(r)$ <u>and</u> $\chi(r)$ <u>is finite for all</u> α .

<u>Remark.</u> For pure Coulomb forces another derivation of the theorem is as follows[7-8]. Let $\phi(R)$ be the (total) electrostatic potential due to a charge distribution $\rho(\underset{\sim}{R})$. Then it is well known that the electrostatic self-energy of $\rho(\underset{\sim}{R})$ may be expressed in terms of the electric field $\mathcal{E} = \nabla\phi$ since

$$1/2 \int d\underset{\sim}{R} \int d\underset{\sim}{R}' \frac{\rho(\underset{\sim}{R})\ \ \rho(\underset{\sim}{R}')}{|\underset{\sim}{R}' - \underset{\sim}{R}|} = 1/2 \int d\underset{\sim}{R}\ \rho(\underset{\sim}{R})\ \phi(\underset{\sim}{R}) \qquad \text{(III.17)}$$

and so by Poisson's equation (taking $\nu = 3$)

$$= -(1/8\pi) \int d\underset{\sim}{R} \left[\nabla^2 \phi(R)\right] \phi(R) = (1/8\pi) \int d\underset{\sim}{R} \left[\nabla\phi(R)\right]^2 ,$$

$$= (1/8\pi) \int d\underset{\sim}{R}\ \mathcal{E}^2 \quad . \qquad \text{(III.18)}$$

Now if $\phi_i(R)$ is the electrostatic field due to a distribution of charge $\rho_i(\underset{\sim}{R} - \underset{\sim}{r}_i)$ centred at $\underset{\sim}{r}_i$ we may write, distinguishing between all particles,

$$U_N^{(2)} = \Sigma_{i<j}\ \varphi_{ij}^{(2)}\ (\underset{\sim}{r}_j - \underset{\sim}{r}_i) = 1/2\ \Sigma_i\ \Sigma_j\ \varphi_{ij}^{(2)}\ (\underset{\sim}{r}_j - \underset{\sim}{r}_i) - 1/2\ \Sigma_i\ \varphi_{ii}^{(2)}\ (\underset{\sim}{0})$$

$$= 1/2 \int d\underset{\sim}{R} \int d\underset{\sim}{R}' \left[\Sigma_i\ \rho_i(\underset{\sim}{R} - \underset{\sim}{r}_i)\right] \left[\Sigma_j\ \rho_j(\underset{\sim}{R} - \underset{\sim}{r}_j)\right] / |\underset{\sim}{R}' - \underset{\sim}{R}|$$

$$- \sum_{i=1}^{N} 1/2 \int d\underset{\sim}{x} \int d\underset{\sim}{x}'\ \rho_i(\underset{\sim}{x})\ \rho_i(\underset{\sim}{x}') / |\underset{\sim}{x}' - \underset{\sim}{x}| \qquad \text{(III.18)}$$

and so by (III.17)

$$U_N^{(2)} = (1/8\pi) \int d\underline{R} \left[\nabla \Sigma_i \phi_i(R)\right]^2 - \Sigma_{i=1}^N (1/8\pi) \int d\underline{x} \left[\nabla \phi_i(x)\right]^2$$

$$\geqslant - \Sigma_{i=1}^N (1/8\pi) \int d\underline{x} \left[\nabla \phi_i(\underline{x})\right]^2 \quad . \tag{III.19}$$

This is just (III.15) with another expression for the electrostatic selfenergy namely

$$E_i = (1/8\pi) \int dx \left[\nabla \phi_i(\underline{x})\right]^2 \quad . \tag{III.20}$$

Applications

The condition that the self-energy (III.16) be finite means physically that the density $\rho_\alpha(\underline{r})$ must be sufficiently "smooth" in relation to the shape factor $\chi(\underline{r})$. It may none-the-less be quite singular. As an example consider the Coulomb potential in three dimensions. We will show that stability is assured if the charge is distributed over the surface of a sphere so that

$$\rho_\alpha(\underline{r}) = \sigma(\theta,\psi)\, \delta\,(r - a) \tag{III.21}$$

where r, θ and ψ are polar coordinates, provided the surface density is bounded, say by σ_o. For by (III.16)

$$|E_\alpha| \leqslant 1/2 \int d\underline{x} \int d\underline{x}' \;\; \delta(x - a) \;|\sigma(\theta,\psi)|\; \delta(x' - a)\; |\sigma(\theta',\psi')| \cdot |x'-x|^{-1}$$

$$\leqslant 1/2\;\; \sigma_o \int d\underline{x}\;\; \delta(x - a)\;\; \phi_o(\underline{x}) \quad , \tag{III.22}$$

where $\phi_o(\underline{x})$ is simply the potential due to a uniform surface distribution of total charge $4\pi a^2\sigma_o$ on a sphere of radius a. This has the finite value $4\pi a^2\sigma_o/a$ <u>on</u> the sphere so that

$$E_\alpha \leqslant 8\,\pi^2\,\sigma_o^2\, a^3 \tag{III.23}$$

With a surface distribution such as (III.21) one may, for example, reproduce outside the sphere the field of a point dipole.

By the same argument it is clear that the stability will be obtained for any volume distribution of bounded density, vanishing outside a bounded region. In fact one may even allow singular distributions, such as the Yukawa or its square, provided the divergence is not worse than $1/|\underset{\sim}{r} - \underset{\sim}{r}_0|^{\delta}$ with $\delta < 5/2$ (or, in ν dimensions, $\delta < 1/2\nu + 1$) . This may be seen by studying the Fourier transforms for large p . On the other hand it is easily seen that a linear distribution of charge does not suffice for stability.

Let us further establish stability for truncated Coulomb interactions defined (for $\nu = 3$) such that

$$\varphi_{\alpha\beta}(r) \geqslant \sup\,(q_\alpha\, q_\beta\, /|\underset{\sim}{r}|\ ,\ -\ |q_\alpha\, q_\beta|/\, a) \qquad \text{(III.24)}$$

for all α , β , $\underset{\sim}{r}$ and some fixed a . A simple example is provided by supposing the particles have hard cores of diameter a in addition to pure Coulomb interactions[7] . Consider the Coulomb interaction $\varphi_{\alpha\beta}{}^{(2)}(\underset{\sim}{r})$ between two charges q_α and q_β each distributed uniformely through a sphere of diameter a (and hence radius $1/2\ a$) . Since the convolution of two distributions vanishing outside a sphere of radius $1/2\ a$, vanishes outside a sphere of radius a this interaction satisfies

$$\varphi_{\alpha\beta}{}^{(2)}(\underset{\sim}{r}) = |q_\alpha\, q_\beta|/|\underset{\sim}{r}|\ , \qquad \text{for } |\underset{\sim}{r}| \geqslant a \qquad \text{(III.25)}$$

and

$$|\varphi_{\alpha\beta}{}^{(2)}(r)| \geqslant |q_\alpha\, q_\beta|/\, a\ , \qquad \text{for } |\underset{\sim}{r}| \geqslant a\ . \qquad \text{(III.26)}$$

Thus we have a stable potential always lying below the truncated Coulomb potential (III.24) which is hence also stable.

Finally consider a system of point dipoles interacting through the usual dipole-dipole (or tensor) forces, namely,

$$\varphi_{\alpha\beta}(\underset{\sim}{r}\ ;\ \underset{\sim}{m}_\alpha\ ,\ \underset{\sim}{m}_\beta) = \frac{\underset{\sim}{m}_\alpha \cdot \underset{\sim}{m}_\beta}{r^3} - 3\ \frac{(\underset{\sim}{m}_\alpha \cdot \underset{\sim}{r})(\underset{\sim}{m}_\beta \cdot \underset{\sim}{r})}{r^5} \qquad \text{(III.27)}$$

where $\underset{\sim}{m}_\alpha$ and $\underset{\sim}{m}_\beta$ are the dipole moments. The Fourier transform is

$$\hat{\varphi}_{\alpha\beta}(\underset{\sim}{p}\ ;\ \underset{\sim}{m}_\alpha\ ,\ \underset{\sim}{m}_\beta) = C_3(\underset{\sim}{m}_\alpha \cdot \underset{\sim}{p})\ /|\underset{\sim}{p}|^2 \quad , \qquad \text{(III.29)}$$

so that, as before, the stability matrix $\underset{\sim}{\Phi}$ will be non-negative definite for all $\underset{\sim}{m}_\alpha$, $\underset{\sim}{m}_\beta$. As it stands, however, the self-energy is divergent but we may clearly obtain a stable system if the dipole moment $\underset{\sim}{m}_\alpha$ is distributed with some density $\underset{\sim}{\mu}_\alpha(\underset{\sim}{r})$. The smoothness conditions on $\mu_\alpha(\underset{\sim}{r})$ are, however, more stringent than on the charge density as is natural since a distribution $\rho_\alpha(\underset{\sim}{r})$ proportional to the divergence of $\underset{\sim}{\mu}(\underset{\sim}{r})$ will have the same electrostatic field. A Yukawa distribution of dipole moments would yield stability but a surface distribution on a sphere would not.

IV. QUANTUM MECHANICAL SYSTEMS.

For the stability of a quantum mechanical system of N particles of masses m_i it is sufficient to require only that

$$\langle \mathcal{H}_N \rangle = \sum_{i=1}^{N} (\hbar^2 / m_i) \int |\nabla_i \Psi_N|^2 \, d\underset{\sim}{r}_1 \cdots d\underset{\sim}{r}_N$$

$$+ \int U_N(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_N) \, |\Psi_N|^2 \, d\underset{\sim}{r}_1 \cdots d\underset{\sim}{r}_N \, , \qquad \text{(IV.1)}$$

$$\geqslant - NB \quad ,$$

for fixed B and all N-body functions $\Psi_N = \Psi_N(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_N)$ in the domain of $\mathcal{H}_N$. (We assume the wave function vanishes on the boundary of the domain and on any hard cores[2].) Since the kinetic energy is evidently positive for any Ψ_N the stability of a classical system, that is the assertion $U_N \geqslant - N B$ for all $\underset{\sim}{r}_i$ and N , implies the stability of the corresponding quantal systems. It is of interest to enquire, however, into potentials that might be stable for quantum systems of given statistics while being unstable for classical systems or for different statistics. In particular the experimentaly observed stability of systems of electrons and protons (hydrogen) or electrons and deuterons (deuterium) suggest strongly that a charged quantum mechanical system should be stable even with <u>pure</u> Coulomb forces. We take this specific question up in Section 5 and consider firstly the converse general problem of establishing instability.

For a classical system of identical particles, one may show that certain potentials are <u>catastrophically unstable</u> in the sense that for N indefinitely large there are sets of configurations for which

$$U_N(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_N) \leqslant - w^* \, N^{1+\eta} \qquad \text{(IV.2)}$$

where w^* and η are positive constants, and that the grand canonical partition function does not exist (the series being divergent). In particular for pair interactions this is so if[9] :

(D) $\varphi(\underset{\sim}{r})$ is finite valued and piecewise continuous [10],

and for some k and configuration $\underset{\sim}{r}_i$ one has

$$\sum_{i=1}^{k} \sum_{j=1}^{k} \varphi(\underset{\sim}{r}_j - \underset{\sim}{r}_i) < 0 \quad . \tag{IV.3}$$

It is quite straightforward to generalize the proof of this result [9] to a multi-species system provided that N_α / N remains bounded below for all α as $N = \sum_\alpha N_\alpha \longrightarrow \infty$.

For a quantum mechanical system we may prove,

Theorem III. If the potential energy of a quantum mechanical system of N identical particles is the sum of pairwise interactions with potential $\varphi(\underset{\sim}{r})$ which is (i) bounded for large $|\underset{\sim}{r}|$, (ii) finite valued upper semi--continuous [11], and (iii) which for some k and $\underset{\sim}{r}_i^o$ (i=1,2,...k) satisfies

$$\sum_{i=1}^{k} \sum_{j=1}^{k} \varphi(\underset{\sim}{r}_j^o - \underset{\sim}{r}_i^o) = - U_o < 0 \quad , \tag{IV.4}$$

then for a sufficiently large domain there is a $w^* > 0$ and an N^* such that the ground state energy satisfies

$$E_o(N) \leqslant - w^* N^2 \quad \text{for} \quad N \geqslant N^* \quad , \tag{IV.5}$$

provided either (a) the particles obey Bose-Einstein or Boltzmann statistics (and ν is arbitrary) or (b) they obey Fermi-Dirac statistics and $\nu \geqslant 3$ (or $\nu = 2$ and U_o is sufficiently large).

Remarks. When the conditions of the theorem are satisfied it is evident that the canonical free energy per particle cannot approach a finite thermodynamic limit since, in a diagonal representation, the canonical partition function contains a term $\exp\left[-\beta E_o(N)\right] = \exp(\beta W^* N^2)$. For the same reason the grand canonical partition function does not exist.

Notice that for Bose-Einstein and Boltzmann statistics the theorem is as strong as in the classical case. For fermions on the other hand the theorem proves instability for all U_o only in three or more dimensions. In two dimensions the system will be unstable if U_o is sufficiently large (or more generally if (IV.4) holds as an inequality over a sufficiently large region of configuration space) but might perhaps be stable otherwise. Indeed the arguments in the proof, which depend on the way the total kinetic energy of a system confined in a domain increases with N , suggest that one and two-dimensional Fermi-Dirac systems probably are stable for certain forces that would be classically unstable. We have however, not established any such counterexamples.

Theorem III is proved by constructing a trial wavefunction Ψ_N , and hence a variational upper bound for $E_o(N)$, which corresponds to superimposing closely many replicas of the configuration satisfying (IV.4) . As in the classical case there are no obstacles to generalizing the results to multispecies systems if N_α / N is bounded below. The proof occupies the remainder of this section ; the reader uninterested in the technical details is advised to proceed directly to section 5 .

<u>Proof</u>. We first observe, following the classical argument [9], that the function

$$U(\underset{\sim}{r}_1 \cdots \underset{\sim}{r}_k \,;\, \underset{\sim}{r}'_1 \cdots \underset{\sim}{r}'_k) = \sum_{i=1}^{k} \sum_{j=1}^{k} \varphi(\underset{\sim}{r}'_j - \underset{\sim}{r}_i) \qquad \text{(IV.6)}$$

is upper semicontinuous in the space of the $2k\nu$ coordinates $\underset{\sim}{r}_1 = (x_{1,1}, \dots x_{\nu,1})$ to $\underset{\sim}{r}'_k = (x'_{1,k}, \dots x'_{\nu,k})$. Consequently there exists a positive length d and a set of k cubes Γ_i° of edge d_j namely

$$\Gamma_i^\circ \;: \qquad 0 \leqslant x_\gamma - x^\circ_{\gamma,i} \leq d \;, \; (\gamma = 1,2,\dots \nu) \quad , \tag{IV.7}$$

such that

$$U(\underset{\sim}{r}_1, \cdot \;, \underset{\sim}{r}'_k) < -1/2\, U_\circ \qquad \text{for} \quad \underset{\sim}{r}_i \in \Gamma_i^\circ \text{ and } \underset{\sim}{r}'_j \in \Gamma_j^\circ \; . \tag{IV.8}$$

Now if $N = h\,k + c$ where h is an integer and $0 \leqslant c < k$ we may write the total potential energy as

$$U_N = 1/2 \sum_{f=1}^{h} \sum_{g=1}^{h} \Big\{ \sum_{i=1}^{k} \sum_{j=1}^{k} \varphi(\underset{\sim}{r}_{gk+j} - \underset{\sim}{r}_{fk+i}) \Big\} - 1/2\, h\,k\, \varphi(\underset{\sim}{0})$$

$$+ \sum_{j=1}^{c} \sum_{i=1}^{N} \varphi(\underset{\sim}{r}_i - \underset{\sim}{r}_{hk+j}) - c\, \varphi(\underset{\sim}{0}) \quad . \tag{IV.9}$$

If the coordinates of k of the first $h\,k$ particles lie within each cube Γ_i° , that is

$$0 \leqslant x_{\gamma, fk+i} - x^\circ_{\gamma,i} \leqslant d \qquad \text{all } \gamma, f, i, \tag{IV. 10}$$

then we have by (IV.6) and (IV.8)

$$U_N \leqslant -1/4\, h^2\, U_\circ - 1/2\, h\,k\, \varphi(0) + Y_{N,c} - c\, \varphi(0) \tag{IV. 11}$$

where $Y_{N,c}$ denotes the penultimate term in (IV.9) . Since $\varphi(r)$ is bounded for large $|\underset{\sim}{r}|$ there is a distance a_2 and a fixed η such that

$$|\varphi(\underset{\sim}{r})| < \eta \quad , \qquad \text{for} \quad |\underset{\sim}{r}| \geqslant a_2 \quad . \tag{IV. 12}$$

The k cubes Γ_i^o are fixed and so in a sufficiently large domain we can find c further similar cubes Γ_j^1 $(j=1,\dots c)$ such that if $\underset{\sim}{r}$ is in cube Γ_j^1 and $\underset{\sim}{r}'$ is in any other cube then $|\underset{\sim}{r}' - \underset{\sim}{r}| > a_2$, i.e. the mutual distances exceed a_2. Let Γ_j^1 be defined by $0 \leqslant x_\gamma - x'_{\gamma,j} \leqslant d$ for all γ. If we impose

$$0 \leqslant x_{\gamma,hk+j} - x^1_{\gamma,j} \leqslant d \qquad \text{all } \gamma,\ j=1,\dots c, \tag{IV.13}$$

we therefore have

$$Y_{N,c} \leqslant N c \eta < N k \eta \quad . \tag{IV.14}$$

Thus under conditions (IV.10) and (IV.13) we may write (for $N \gg k$)

$$U_N \leqslant -(N-k)^2 (U_o / 4k^2) + N(1/2\,|\varphi(0)| + k\eta) + 1/2\, k\,|\varphi(\underset{\sim}{0})| \quad , \tag{IV.15}$$

which in fact restablishes instability for the classical case under slightly wider conditions.

Let $\xi_\gamma = x_\gamma - x^o_{\gamma,i}$ or $x_\gamma - x^1_{\gamma,j}$ and consider the single particle wave function which vanishes outside the cube Γ: $0 \leqslant \xi_\gamma \leqslant d$ (all γ) but is given internally by

$$\psi_{l_1\dots l_\nu}(\xi_1,\dots \xi_\nu) = (1/2d)^{-1/2\nu} \prod_{\gamma=1}^{\nu} \sin(l_\gamma \pi\, \xi_\gamma / d) \tag{IV.16}$$

where the l_γ are positive integers. For this wave function the kinetic energy has the expectation value

$$t_{l_1\dots l_\nu} = (\hbar^2 \pi^2 / 2 m d^2)(l_1^2 + \dots + l_\nu^2) \ . \tag{IV.17}$$

For the Bose-Einstein and Boltzmann case(s) now take as a trial wave function a product of N single particle functions $\psi_{11\dots1}$ with h functions based on each of the cubes Γ_i^o and one based on each of the Γ_j^1. For this Ψ_N we clearly have

$$\langle T_N \rangle = N (\nu \hbar^2 \pi^2 / 2 m d^2) , \tag{IV.18}$$

while $\langle U_N \rangle$ satisfies the inequality (IV.15). By the variational principle the sum of these terms exceeds the ground state energy $E_o(N)$ and so (IV.5) follows.

For the case (b) of Fermi-Dirac statistics we can allow only totally antisymmetric trial wave functions. Thus in each cube Γ_i^o take h different $\psi_{l_1 \dots l_\nu}$ and antisymmetrize the product wave function with respect to their arguments. (We may assume the cubes do not overlap.) The expectation value of U_N will clearly still satisfy (IV.15) but for the kinetic energy we have

$$\langle T_N \rangle = (\hbar^2 \pi^2 / 2 m d^2) \left[k D_\nu(h) + c \right] \tag{IV.19}$$

where

$$D_\nu(h) = \Sigma_{f=1}^h \left| \underset{\sim}{l}(f) \right|^2 \tag{IV.20}$$

in which the $\underset{\sim}{l}(f)$ are h <u>distinct</u> vectors with positive integral coordinates. This function will be a minimum when the vectors fill out, to best approximation the positive 2^ν-ant of a ν-dimensional hypersphere. Let $A_\nu L^\nu$ be the volume of such a hypersphere of radius L and let $B_\nu L^{\nu+2}$ be its moment of inertia about one axis. If we choose L so that

$$2^{-\nu} A_\nu L^\nu = h \tag{IV.21}$$

then for large h we will have

$$D_\nu(h) \approx 2^{-\nu} \; B_\nu \; L^{\nu+2} = 4\,\nu \; B_\nu \; A_\nu^{-1-(2/\nu)} h^{1+(2/\nu)} \; . \qquad \text{(IV.22)}$$

Consequently for sufficiently large N there are positive numbers ζ_1 and ζ_2 depending only on k and ν, such that

$$\zeta_2 \,(\hbar^2 / m\, d^2)\; N^{1+(2/\nu)} \leqslant \langle T_N \rangle \leqslant \zeta_1 (\hbar^2 / m\, d^2)\; N^{1+(2/\nu)} . \qquad \text{(IV.23)}$$

Hence for $\nu \geqslant 3$ the kinetic energy increases no faster than $N^{5/3}$ and so is dominated by the potential energy which diverges as N^2 thus proving the theorem. For $\nu = 2$ the kinetic energy increases as N^2 and the theorem follows only if

$$U_o \;>\; 4\, k^2 \;\; \zeta_2 \,(\hbar^2 / 2\, m\, d^2) \quad , \qquad \text{(IV.24)}$$

that is if U_o is sufficiently large. This completes the proof.

For $\nu = 1$ the method always fails. Indeed since (IV.23) will hold for any antisymmetric wave function vanishing outside a bounded domain of dimensions of order d it appears that the conditions on the potential might in general be sufficient for instability.

V. QUANTUM SYSTEMS WITH COULOMB INTERACTIONS

The Hamiltonian of a system of N point charges q_i with Coulomb interactions is given by

$$\mathcal{H}_N = T_N + U_N , \qquad (V.1)$$

$$T_N = \sum_{i=1}^{N} \left(\frac{-\hbar^2}{2m_i} \nabla_i^2\right) , \qquad (V.2)$$

$$U_N = \sum_{i<j} \frac{q_i \quad q_j}{|\underset{\sim}{r}_j - \underset{\sim}{r}_i|} , \qquad (V.3)$$

where m_i is the mass of the i-th particle. Notice that we do not enclose the particles in a box ; $\mathcal{H}_N$ acts thus in the Hilbert space of square integrable functions of 3N real variables.

We shall restrict ourselves to the case where q_i takes only the values +1 and −1 and m_i two values m_+ (if $q_i = +1$) and m_- (if $q_i = -1$) . We suppose that there are N_+ particles with charge +1 and mass m_+ and N_- particles with charge −1 and mass m_- . The remarks which we shall make could, however, be extended to the situation of different values of q_i and more than two different masses.

We first prove a <u>scaling property</u> of the Hamiltonian $\mathcal{H}_N$. Let $\lambda > 0$ and, if ψ is a square-integrable function of $\underset{\sim}{r}_1, \ldots, \underset{\sim}{r}_N$, let $\psi^{(\lambda)}$ be defined by

$$\psi^{(\lambda)} (\underset{\sim}{r}_1, \ldots, \underset{\sim}{r}_N) = \lambda^{3N/2} \quad \psi(\lambda \underset{\sim}{r}_1, \ldots, \lambda \underset{\sim}{r}_N). \qquad (V.4)$$

The transformation $\psi \longrightarrow \psi^{(\lambda)}$ conserves the scalar products (it is a unitary transformation of Hilbert space). Furthermore

$$(\lambda^{-2} T_N + \lambda^{-1} U_N) \psi^{(\lambda)} = \Big[(T_N + U_N) \psi\Big]^{(\lambda)} . \qquad (V.5)$$

From this it follows that <u>the spectrum of</u> $\mathcal{H}_N^{(\lambda)} = \lambda^{-2} T_N + \lambda^{-1} U_N$ <u>is the same as that of</u> $\mathcal{H}_N$.

Let $E_o(N)$ be the g.l.b. to the spectrum of $\mathcal{H}_N$, or "lowest eigenvalue" of $\mathcal{H}_N$. By the scaling property it is also the g.l.b. to the spectrum of $\mathcal{H}_N^{(\lambda)}$. The g.l.b. $E_o(2)$ to the spectrum of

$$\mathcal{H}_2 = -\frac{\hbar^2}{2\,m_+}\nabla_1^2 - \frac{\hbar^2}{2\,m_-}\nabla_2^2 - \frac{1}{|\underset{\sim}{r}_2 - \underset{\sim}{r}_1|} \tag{V.6}$$

is just the ground state energy of a "hydrogen atom" with masses m_+ and m_- . We now compute an upper and a lower bound of $E_0(N)$ in terms of $E_0(2)$. For simplicity we take $N_+ = N_- = N_o = 1/2\,N$.

We may obtain an upper bound to $E_0(N)$ by taking the expectation value of $\mathcal{H}_N$ for a normalized test function ψ . If we take as ψ the wave function of N_o "hydrogen atoms" formed by pairing the positive and negative charges, and if we assume that the mutual distances between these "hydrogen atoms" is large, we find

$$E_0(N) \leqslant -N_o\,E_0(2) \quad . \tag{V.7}$$

To find a lower bound to $E_0(N)$ we write

$$\mathcal{H}_N \geq \sum_{i=1}^{N_o} \frac{-\hbar^2}{2\,m_+}\nabla_i^2 + \sum_{j=1}^{N_o} \frac{-\hbar^2}{2\,m_-}\nabla_j^2 + \sum_{i=1}^{N_o}\sum_{j=1}^{N_o} \frac{-1}{|\underset{\sim}{r}_j - \underset{\sim}{r}_i|}$$

$$= \sum_i \sum_j \left[N_o^{-1}\left(-\frac{\hbar^2}{2\,m_+}\nabla_i^2 - \frac{\hbar^2}{2\,m_-}\nabla_j^2\right) - \frac{1}{|\underset{\sim}{r}_j - \underset{\sim}{r}_i|} \right)$$

$$= N_o \sum_i \sum_j \left[N_o^{-2}\left(-\frac{\hbar^2}{2\,m_+}\nabla_i^2 - \frac{\hbar^2}{2\,m_-}\nabla_j^2\right) + N_o^{-1}\cdot\frac{-1}{|\underset{\sim}{r}_j - \underset{\sim}{r}_i|} \right) \ . \tag{V.8}$$

Using the scaling property for $\mathcal{H}_2$ we see that the operator in square brackets on the r.h.s. of (V.8) is bounded below by $E_0(2)$, therefore (V.8) gives

$$E_0(N) \geqslant - N_o^3 \quad E_0(2) \quad . \tag{V.9}$$

We have thus found for $E_0(N)$ an upper bound (V.7) which is linear in the number of particles, and a lower bound (V.9) which is cubic. As discussed in Section 4 one would expect that a linear lower bound should exist, with perhaps the restriction that either the positive or the negative particles obey Fermi statistics. What we can at least show is that the existence of a linear lower bound

$$E_0(N) \geqslant - N_o \, B \tag{V.10}$$

for any one choice of the masses m_+ , m_- implies its existence for any other choice m_+' , m_-' . This statement follows readily from the relations (V.11) and (V.12) below. The identity

$$E_0 \, (N, m_+, m_-) = \lambda \, E_0(N, m_+', m_-') \quad \text{if} \quad \frac{m_+'}{m_+} = \frac{m_-'}{m_-} = \lambda \tag{V.11}$$

follows from the scaling property if one notices that the Hamiltonian for the masses m_+' , m_-' is just $\lambda \, \mathcal{H}^{(\lambda)}$.

The inequality

$$E_0 \, (N, m_+, m_-) \leqslant E_0(N, m_+', m_-') \quad \text{if} \quad m_{\pm} \geqslant m_{\pm}' \tag{V.12}$$

is obtained by remarking that to change $m_{\pm}$ to $m_{\pm}'$ amounts to adding the positive term

$$\left(\frac{\hbar^2}{m_+'} - \frac{\hbar^2}{m_+} \right) \sum_{i=1}^{N_o} (-\nabla_i^2) + \left(\frac{\hbar^2}{m_-'} - \frac{\hbar^2}{m_-} \right) \sum_{j=1}^{N_o} (-\nabla_j^2) \tag{V.13}$$

As a last remark we notice that the difficulty in proving (V.10) does not come from the long-range part of the Coulomb potential. Indeed let

$$\frac{1}{r} = \varphi_1(\underset{\sim}{r}) + \varphi_2(\underset{\sim}{r}) \ , \tag{V.14}$$

with

$$\varphi_1(\underset{\sim}{r}) = \frac{e^{-\alpha r}}{r} \ , \qquad \varphi_2(\underset{\sim}{r}) = \frac{1 - e^{-\alpha r}}{r} \ . \tag{V.15}$$

We may write

$$\mathcal{H}_N = \mathcal{H}_N^{(1)} + U_N^{(2)} \ , \tag{V.16}$$

$$\mathcal{H}_N^{(1)} = \Sigma_{i=1}^N \left(-\frac{\hbar^2}{2\, m_i} \nabla_i^2\right) + \Sigma_{i<j}\, q_i\, q_j\, \varphi_1(\underset{\sim}{r}_j - \underset{\sim}{r}_i), \tag{V.17}$$

$$U_N^{(2)} = \Sigma_{i<j}\, q_i\, q_j\, \varphi_2(\underset{\sim}{r}_j - \underset{\sim}{r}_i) \ . \tag{V.18}$$

In $\mathcal{H}_N^{(1)}$ we have removed the long-range part of the Coulomb potential, replacing $1/r$ by a Yukawa potential. Our remark is that the long-range part of the Hamiltonian, namely $U_N^{(2)}$, is bounded below by a multiple of N. This follows from theorem I if one notices that $\varphi_2(0)$ is finite and that the Fourier transform of φ_2 is non-negative, being proportional to

$$\frac{1}{p^2} - \frac{1}{p^2 + \alpha^2} = \frac{\alpha^2}{p^2\,(p^2 + \alpha^2)} \tag{V.19}$$

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APPENDIX A

The object of this appendix is to prove the following result

Theorem IV. Let $0 < a_1 < a_2$ and let $\xi(r)$, $\eta(r)$ be monotonic non-increasing non-negative functions, defined on the intervals $(0, a_1)$ and $(a_2, +\infty)$ respectively, such that

$$\int_0^{a_1} \xi(r)\ r^{\nu-1}\,dr = +\infty \tag{A.1}$$

$$\int_{a_2}^{+} \eta(r)\ r^{\nu-1}\,dr < +\infty \tag{A.2}$$

If the pair potential $\varphi(r)$ satisfies

$$\varphi(r) \geqslant \xi(r) \qquad \text{for} \quad r \leqslant a_1 \tag{A.3}$$

$$\varphi(r) \geqslant -\eta(r) \qquad \text{for} \quad r \geqslant a_2 \tag{A.4}$$

<u>and if there exists a constant</u> $w \geqslant 0$ <u>such that</u>

$$\varphi(r) \geqslant -w \qquad \text{for all} \quad r \tag{A.5}$$

<u>then there exists a constant</u> $B \geqslant 0$ <u>such that</u>

$$U(x_1, \dots, x_n) = \sum_{1 \leq i \leq j \leq n} \varphi(\underset{\sim}{r}_j - \underset{\sim}{r}_i) \geqslant -nB \tag{A.6}$$

for all $n, x_1, \dots, x_n$.

To prove the theorem we show that we may write

$$\varphi(r) = \varphi^{(1)}(r) + \varphi^{(2)}(r) \tag{A.7}$$

where $\varphi^{(1)}(r) \geqslant 0$ and $\varphi^{(2)}$ has an integrable non-negative Fourier transform $\widehat{\varphi}^{(2)}(p)$, i.e. $\varphi^{(2)}$ is of positive type [1-4]. The fact that φ admits a positive type minorant $\varphi^{(2)}$ follows from lemmas 1 and 2 below as the reader will immediately check by writing

$$\varphi^{(2)}(r) = \xi_1(r) - \eta_3(r) \tag{A.8}$$

<u>Lemma 1.</u> <u>There exists a non-negative function</u> η_3 <u>such that</u>

$$\varphi(\underset{\sim}{r}) = -\eta_3(\underset{\sim}{r}) \qquad \text{for all} \quad \underset{\sim}{r} \tag{A.9}$$

<u>and the Fourier transform of</u> η_3 <u>satisfies</u>

$$|\widehat{\eta}_3(p)| \leqslant C(p^2 + 1)^{-\nu} \tag{A.10}$$

<u>for some positive constant</u> C.

We define a function η_1 in the interval $(0, +\infty)$ as follows :

$$\eta_1(r) = \begin{cases} w & \text{if} \quad r \leqslant a_2 \\ \inf\{w, \eta(r)\} & \text{if} \quad r \geqslant a_2 \end{cases} \tag{A.11}$$

Then our hypotheses imply that

$$\varphi(r) \geqslant - \eta_1(r) \tag{A.12}$$

Given b such that $0 < b < a_2$ we introduce also a function η_2 on $(0, +\infty)$ by

$$\eta_2(r) = \begin{cases} w & \text{if} \quad r \leqslant b \\ \eta_1(r-b) & \text{if} \quad r \geqslant b \end{cases} \tag{A.13}$$

The functions η_1 and η_2 are non-negative, non increasing and integrable because

$$\int_0^\infty \eta_1(r)\, r^{\nu-1}\, dr = w\int_0^{a_2} r^{\nu-1}\, dr + \int_{a_2}^\infty \eta(r)\, r^{\nu-1}\, dr < +\infty \tag{A.14}$$

$$\int_0^\infty \eta_2(r)\, r^{\nu-1}\, dr = w\int_0^b r^{\nu-1}\, dr + \int_b^\infty \eta_1(r-b)\, r^{\nu-1}\, dr$$

$$= w\int_0^b r^{\nu-1}\, dr + \int_0^\infty \eta_1(r)\,(r+b)^{\nu-1}\, dr < +\infty\,, \tag{A.15}$$

where we have used the fact that $(r+b)^{\nu-1}/r^{\nu-1}$ tends to unity as $r \to \infty$.

From the definition (A.13) of η_2 and the monotonicity of η_1 and η_2 it follows that

$$\eta_2(r') \geqslant \eta_1(r) \qquad \text{if} \quad |r' - r| \leqslant b \quad . \tag{A.16}$$

If η_1 and η_2 are considered as functions of position vectors we therefore also have

$$\eta_2(\underset{\sim}{r}') \geqslant \eta_1(\underset{\sim}{r}) \qquad \text{if} \quad |\underset{\sim}{r}' - \underset{\sim}{r}| \leqslant b \quad . \tag{A.17}$$

Now let ψ be a non-negative function on R^ν vanishing outside a sphere of radius b centered at the origin and such that

$$\int d\underset{\sim}{r} \;\; \psi(\underset{\sim}{r}) = 1 \quad . \tag{A.18}$$

We suppose that ψ has continuous derivatives of all orders and define η_3 as

$$\eta_3(\underset{\sim}{r}) = \int d\underset{\sim}{r}' \;\; \psi(\underset{\sim}{r} - \underset{\sim}{r}') \; \eta_2(r') \quad . \tag{A.19}$$

Then, (A.16) gives

$$\eta_3(r) \geqslant \eta_1(r) \quad . \tag{A.20}$$

Furthermore the Fourier transform $\hat{\eta}_3$ of η_3 is proportional to the product of $\hat{\eta}_2$ (which is continuous and bounded) and $\hat{\psi}$ (which is continuous and decreases at infinity faster than any inverse polynomial). Therefore $\hat{\eta}_3$ is continuous and decreases faster than any inverse polynomial at infinity. Lemma 1 follows from this fact and (A.12), (A.20).

Lemma 2. There exists a (non-negative) function ξ_1 such that

$$\xi_1(r) \begin{cases} \leqslant \varphi(r) & \text{for} \quad r \leqslant a_1 \\ \end{cases} \tag{A.21}$$

and the Fourier transform of ξ_1 satisfies

$$\hat{\xi}_1(r) \geqslant C\,(p^2+1)^{-\nu} \qquad (A.22)$$

with the same constant C as in Lemma 1 .

Let $\chi(\underset{\sim}{r})$ be continuous, non-negative and satisfy $\chi(0) > 0$ and $\chi(\underset{\sim}{r}) = 0$ for $r \geqslant 1/2$. Define χ_1 as

$$\chi_1(\underset{\sim}{r}) = \int d\underset{\sim}{r}'\,\chi(\underset{\sim}{r}-\underset{\sim}{r}')\,\chi(\underset{\sim}{r}') \;. \qquad (A.23)$$

Then χ_1 is continuous, non-negative and $\chi_1(\underset{\sim}{r}) = 0$ if $r \geqslant 1$. Furthermore the Fourier transform $\hat{\chi}_1$ of χ_1 is continuous, non-negative (being proportional to the square of $\hat{\chi}$) and nonzero in some neighbourhood of the origin.

Consider the function χ_2 defined by

$$\chi_2(\underset{\sim}{r}) = \chi_1(\underset{\sim}{r}) \int d\underset{\sim}{p}\, e^{i\underset{\sim}{p}\cdot\underset{\sim}{r}}\,(p^2+1)^{-\nu} \;. \qquad (A.24)$$

Then χ_2 is continuous, non-negative (the integral in (A.24) is a K-function of the theory of Bessel functions [12]) and $\chi_2(\underset{\sim}{r}) = 0$ if $r \geqslant 1$. Dividing χ_2 by $\max_{r\leq 1} \chi_2(r)$ we obtain a function χ_3 with properties given as follows

Lemma 3. The function χ_3 is continuous, non-negative, bounded above by 1 and $\chi_3(r) = 0$ if $r \geqslant 1$. The Fourier transform of χ_3 satisfies

$$\hat{\chi}_3(p) \geqslant C'\,(p^2+1)^{-\nu} \qquad (A.25)$$

for some positive C' .

To prove (A.25) we remark that $\hat{\chi}_3$ is proportional to

$$\int d\underset{\sim}{p}' \ \hat{\chi}_1(\underset{\sim}{p}') \left[(\underset{\sim}{p} - \underset{\sim}{p}')^2 + 1 \right]^{-\nu} , \tag{A.26}$$

where $\hat{\chi}_1$ is continuous and non-negative. Since $\hat{\chi}_1(0) \neq 0$, (A.25) follows from (A.26) by restricting the integration to a small neighbourhood of the origin.

We now use Lemma 3 to prove Lemma 2. We may suppose that ξ is a strictly decreasing function of r. Then, for all sufficiently large positive integers n $(n \geqslant n_o)$, let $\alpha_n < 1$ be defined by $\xi(\alpha_n) = n$.

The step function $\xi^*(r) = n$ for $\alpha_{n+1} < r \leqslant \alpha_n$, clearly does not exceed $\xi(r)$ when $r < \alpha_{n_o}$. This step function is simply the sum of the unit step functions $\theta_n(r) = 1$ for $r \leqslant \alpha_n$ but zero otherwise. But the properties of $\chi_3(r)$ stated in Lemma 3 imply that $\chi_3(r/\alpha_n) \leqslant \theta_n(r)$. In total we thus find

$$\Sigma_{n \geqslant n_o} \chi_3(r/\alpha_n) \leqslant \xi(r) . \tag{A.27}$$

On the other hand, because of (A.1) we have

$$\Sigma_{n \geqslant n_o} \alpha_n^{\nu} = +\infty . \tag{A.28}$$

Since $\alpha_n < 1$, (A.25) yields for the Fourier transform of $\Sigma_{n_o}^{n_1} \chi_3(\alpha_n^{-1} \underset{\sim}{r})$ the inequality

$$\Sigma_{n_o}^{n_1} \alpha_n^{\nu} \ \hat{\chi}_3(\alpha_n \underset{\sim}{p}) \geqslant \left[\Sigma_{n_o}^{n_1} \alpha_n^{\nu} \right] C' \ (p^2 + 1)^{-\nu} . \tag{A.29}$$

Lemma 3 follows from (A.27), (A.28), (A.29) if we write

$$\xi_1(\underset{\sim}{r}) = \Sigma_{n_o}^{n_1} \chi_3(\alpha_n^{-1} r) \tag{A.30}$$

for n_1 sufficiently large.

FOOTNOTES AND REFERENCES

1) D. Ruelle, Helv. Phys. Acta 36, 183 (1963).

2) D. Ruelle, Helv. Phys. Acta 36, 789 (1963).

3) M.E. Fisher, Arch. Rat. Mech. Anal. 17, 377 (1964).

4) D. Ruelle, Lectures in Theoretical Physics, Vol. VI, Boulder 1963 pp. 93-95 (University of Colorado Press, 1964).

5) R.L. Dobrushin, Th. Prob. Appl. (U.S.S.R.) 9, 646 (1964).

6) For $\nu \leqslant 2$ the integral (3.6) for the pure Coulomb case would diverge also at its lower limit owing to the divergence of the potential as $r \to \infty$ in violation of (3.2). This prevents the unambiguous determination of the zero of potential energy and is the reason for restricting attention to potentials which converge to zero at infinity, however slowly.

7) The stability of an electrostatic system seems first to have been considered by L. Onsager, J. Phys. Chem. 43, 189 (1939) who supposed the particles interacted in addition with an infinite hard core (see also below).

8) A proof of stability somewhat similar to that presented here has been communicated privately (to M.E.F.) by O. Penrose.

9) D. Ruelle, Ref. 4 pp. 86-88 .

10) At a discontinuity $\varphi(\underset{\sim}{r}_0)$ should be assigned the value $\limsup \varphi(\underset{\sim}{r})$ as $\underset{\sim}{r} \to \underset{\sim}{r}_0$. More generally, see Theorem III, we only require <u>upper semi-continuity</u> which means that for any r_0 and $\epsilon > 0$ there is a $\delta > 0$ such that $\varphi(\underset{\sim}{r}) < \varphi(\underset{\sim}{r}_0) + \varepsilon$ if $|\underset{\sim}{r} - \underset{\sim}{r}_0| < \delta$.

11) See footnote 10 .

12) See Ref. 4. p. 94 of Formula 7.12 (20) in Erdelyi, Magnus, Oberhettinger, Tricomi. Higher Transcendental Functions, Vol. 2. Mc Graw-Hill, New York(1953)

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