Commun. Math. Phys. 118, 177–213 (1988)

Communications in
Mathematical
Physics

The Stability and Instability of Relativistic Matter

Elliott H. Lieb[1,*] and Horng-Tzer Yau[2,**]

[1] Departments of Mathematics and Physics, Princeton University, P.O. Box 708, Princeton, NJ 08544, USA

[2] School of Mathematics, The Institute for Advanced Study, Princeton, NJ 08540, USA

Abstract. We consider the quantum mechanical many-body problem of electrons and fixed nuclei interacting via Coulomb forces, but with a relativistic form for the kinetic energy, namely $p^2/2m$ is replaced by $(p^2c^2+m^2c^4)^{1/2}-mc^2$. The electrons are allowed to have q spin states ($q=2$ in nature). For one electron and one nucleus instability occurs if $z\alpha>2/\pi$, where z is the nuclear charge and α is the fine structure constant. We prove that stability occurs in the many-body case if $z\alpha\leqq 2/\pi$ and $\alpha<1/(47q)$. For small z, a better bound on α is also given. In the other direction we show that there is a critical α_c (no greater than $128/15\pi$) such that if $\alpha>\alpha_c$ then instability always occurs for *all* positive z (not necessarily integral) when the number of nuclei is large enough. Several other results of a technical nature are also given such as localization estimates and bounds for the relativistic kinetic energy.

I. Introduction

One of the early important successes of quantum mechanics was the interpretation of the stability of the hydrogen atom. The ground state energy of the hydrogen Hamiltonian is finite and thus the hydrogen atom is stable quantum mechanically, even though it is unstable classically. The Coulomb singularity $-ze^2/r$ is controlled by a new feature of Schrödinger mechanics, the uncertainty principle. While the stability of the hydrogen atom is clear and simple, a more subtle question arises when many particles are taken into account. It is convenient to distinguish two notions of stability.

Stability of the first kind: The ground state energy is finite.

Stability of the second kind: The ground state energy is bounded below by a constant times the number of particles.

---

* Work partially supported by U.S. National Science Foundation grant PHY-85-15288-A02

** The author thanks the Institute for Advanced Study for its hospitality and the U.S. National Science Foundation for support under grant DMS-8601978

The second kind of stability, now commonly known as the stability of matter, was proved in 1967 by Dyson and Lenard [10] – four decades after the invention of Schrödinger mechanics. The Dyson-Lenard analysis clearly showed that the stability of matter depends crucially on the Pauli exclusion principle. The ground state energy (call if E_f) of N fermions interacting with K infinitely massive nuclei via the Coulomb potential is bounded below by a constant time the total particle number, i.e. $E_f \geqq -C_1(N+K)$. On the other hand, if all the particles considered are bosons, Dyson and Lenard [10] showed that the ground state energy (call it E_b) satisfies $E_b \geqq -C_2(N+K)^{5/3}$. Lieb [20] showed that this 5/3 bound is indeed the correct law for infinitely massive nuclei. If the nuclei have finite mass, and are also bosons, Dyson [9] showed by a variational calculation, that the ground state energy of bosons is bounded above by $E_b \leqq -C_3(N+K)^{7/5}$. This clearly shows that bosons are stable in the first sense, but never in the second. Dyson [9] also conjectured a lower bound $E_b \geqq -C_4(N+K)^{7/5}$ and this was finally proved 20 years later by Conlon, Lieb, and Yau [4]. They also proved a related bound for bosonic jellium.

The Dyson-Lenard proof for fermions involved a sequence of inequalities such that the final bound for C_1 is 10^{14} Rydberg. New proofs were given by Federbush [12] and Lieb-Thirring [25] in the seventies. The Lieb-Thirring proof gave a much better bound on C_1 (23 Rydbergs) and related the stability problem to the semiclassical picture of Thomas-Fermi theory. These matters are reviewed in [19].

The aforementioned considerations are all based on the nonrelativistic Schrödinger equation. The kinetic energy operator is the standard $p^2/2m = -\Delta/2m$ (when $\hbar = 1$). One might wonder whether stability still prevails in the relativistic case since the kinetic energy then decreases from $p^2/2m$ to $(p^2+m^2)^{1/2} - m(\hbar = c = 1)$. Historically, Chandrasekhar [2] was one of the first to ask this question, but in the context of gravitational interaction instead of Coulomb interaction. The famous Chandrasekhar model for neutron stars or white dwarfs consists of a semiclassical relativistic kinetic energy and classical gravitational potential energy. This simple model remarkably predicted collapse (i.e. instability of the first kind) and gave a critical mass which is correct, at least approximately. Despite the success of the simple semi-relativistic Chandrasekhar theory, the kinetic energy operator,

$$T = (p^2 + m^2)^{1/2} - m\,,$$

which it employs is nonlocal and therefore violates a basic physical principle. Nevertheless it is worthwhile studying this operator for several reasons. When $m = 0$, $T = |p|$ and it has the correct inverse length scaling (like the Dirac operator). Unlike the Dirac operator it allows one to formulate a variational principle for the ground state energy and thereby to give a rigorous definition of stability without the necessity of filling the Dirac sea or invoking quantum electrodynamics. In any event, there does not exist a truly relativistic many-body quantum theory at the present time and it is our belief that the study of Schrödinger operators based on T will capture some of the essential features of "the correct theory" when it is eventually formulated.

Let us start with the Hydrogen atom by considering the one particle Hamiltonian $\tilde{H}$ defined by

$$\tilde{H}_1 = (p^2 + m^2)^{1/2} - m - \alpha z/|x|, \tag{1.1}$$

where $\alpha = e^2$ is the fine structure constant ($\hbar = c = 1$). This operator was studied independently by Weder [29] and Herbst [16]. See also Daubechies' paper [7]. Since the difference between the operator $(p^2 + m^2)^{1/2} - m$ and $|p|$ is bounded (more precisely $|p| \geqq (p^2 + m^2)^{1/2} - m \geqq |p| - m$), the stability of (1.1) is the same as the stability of

$$H_1 = |p| - \frac{2}{\pi} \beta/|x|, \tag{1.2}$$

where

$$\beta = \pi\alpha z/2. \tag{1.3}$$

Note that (1.2) is homogeneous under length scaling and therefore $E_1 \equiv \inf \operatorname{spec} H_1$ is either 0 or $-\infty$ by the scaling $\psi(x) \to \lambda^{3/2}\psi(\lambda x)$.

A first important fact about (1.2) is the existence of a critical $\beta_c = 1$, similar to that of the Klein-Gorden or Dirac theories. Kato [17] stated that $\beta_c \geqq 1$ and Herbst [16] showed that $\beta_c = 1$. The ground state energy for the Hamiltonian (1.2) is $E_1 = -\infty$ if $\beta > 1$ and $E_1 = 0$ if $\beta \leqq 1$. (In the Dirac theory $\beta_c = \pi/2$.)

Returning to the many-body case, suppose we have N electrons with coordinates $x_1, \ldots, x_N$ in $\mathbb{R}^3$ and K nuclei with coordinates $R_1, \ldots, R_K$ in $\mathbb{R}^3$ and with positive charges $z_1, \ldots, z_K$. We shall consider the following relativistic Schrödinger Hamiltonian, H_{NK}, for fermions with q spin states ($q = 2$ for real electrons). It is the analogue of (1.2):

$$H_{NK} \equiv \sum_{i=1}^{N} |p_i| + \alpha V_c(x_1, \ldots, x_N; R_1, \ldots, R_K), \tag{1.4}$$

$$V_c(x_1, \ldots, x_N; R_1, \ldots, R_K) \equiv \sum_{1 \leqq i < j \leqq N} |x_1 - x_j|^{-1} - \sum_{i=1}^{N} \sum_{j=1}^{K} z_j |x_i - R_j|^{-1} + \sum_{1 \leqq i < j \leqq K} z_i z_j |R_i - R_j|^{-1}. \tag{1.5}$$

Note that *charge neutrality is not assumed in* (1.4), *or anywhere else in this paper.*

Mathematically, the Hamiltonian H_{NK} is a quadratic form on the q-state physical subspace $\mathscr{H}^q$ of $L^2(\mathbb{R}^{3N})$. More precisely, $\psi \in \mathscr{H}^q$ if and only if there exists a partition $P = \{\pi_1, \ldots, \pi_q\}$ of $\{1, \ldots, N\}$ such that $\psi(x_1, \ldots, x_N)$ is an antisymmetric function of the variables in each π_j, for all $1 \leqq j \leqq q$. When $q = N$, there is no restriction and the ground state energy for H_{NK} is just the ground state energy for bosons.

Physically, the nuclear kinetic energies should be included in (1.4) since the Born-Oppenheimer approximation (i.e. the neglect of the nuclear kinetic energies) is inadequate in the extreme relativistic regime. For simplicity, we shall confine ourselves to the Born-Oppenheimer approximation.

In reality, our goal is to discuss stability of the second kind for $H_{NK}(m)$, which is given by (1.4) but with $|p|$ replaced by $(p^2 + m^2)^{1/2} - m$ there. For this purpose, however, it suffices to study only stability of the first kind for H_{NK} in (1.4). The reason is the following. Let $E_{NK}(R_1, \ldots, R_K)$ denote the ground state energy ($=$inf spec) of H_{NK} and let E_{NK} be the infimum of $E_{NK}(R_1, \ldots, R_K)$ over all choices of the R's. By simple scaling ($\psi(x_1, \ldots, x_N) \to \lambda^{3N/2}\psi(\lambda x_1, \ldots, \lambda x_N)$ and $R_j \to R_j/\lambda$), we see that E_{NK} is either zero or $-\infty$. On the other hand, if $E_{NK}(m)$ is defined analogously, then, since $|p| - m < (p^2 + m^2)^{1/2} - m < |p|$, we have that $E_{NK} \geqq E_{NK}(m) \geqq E_{NK} - mN$. Thus *stability of the first kind for* H_{NK} (in the sense that E_{NK} is bounded below independent of the R_j) *is equivalent to stability of the second kind for* $H_{NK}(m)$. Our goal then – and that is the purpose of this paper – is to find necessary conditions and sufficient conditions on z and α so that $E_{NK}(R_1, \ldots, R_K) \geqq 0$ for all N and all K and all $R_1, \ldots, R_K$.

If everything is held fixed except for q, then $E_{NK}(R_1, \ldots, R_K)$ is a monotone decreasing function of q. The reason is that specifying q is the same thing as requiring that the admissable wave functions $\psi(x_1, \ldots, x_N)$ are antisymmetric in each of q sets of variables. The number of variables in each set is unimportant, zero being an allowed number. Thus, a valid function for q is trivially a valid function for $q+1$.

A further remark about (1.4) can be made. Using a convexity argument, Daubechies and Lieb [8] proved that the stability of H_{NK} for $z_1 = z_2 = \ldots = z_K = z$ implies the stability of H_{NK} when all the nuclear charges are no greater than z, i.e. $0 \leqq z_j \leqq z$ for all j. With this remark, we shall assume from now on $z_1 = \ldots = z_k = z$.

Let $E_{NK}(\alpha, z)$ denote the dependence of E_{NK} on α and z. We shall use the following terminology: *$H(\alpha, z)$ is stable means that $E_{NK}(\alpha, z) = 0$ for all N and K. Otherwise we say that $H(\alpha, z)$ is unstable.*

The coupling constant of the electrons to the nuclei is $z\alpha = 2\beta/\pi$ and, from the hydrogen atom result, it is clearly necessary to have $\beta \leqq 1$ for stability. It is frequently convenient, therefore, to adopt α and β as the independent variables instead of α and z. When doing so we shall refer to the stability or instability of $H(\alpha, \beta)$ – hopefully without confusion. Indeed α and β are the natural variables from the following point of view. The electron-nuclear coupling is $2\beta/\pi$ while the nuclear-nuclear repulsion constant is $z^2\alpha = (2/\pi)^2\beta^2/\alpha$. Suppose that $K > 1$ and $\beta < 1$, but $K\beta > 1$. Then, if the nuclear-nuclear repulsion is ignored, the K nuclei can come to one common point and the system will collapse – even with only one electron. What discourages this from happening is the repulsion which is proportional to β^2/α. With β fixed, we see that α is required to be small in order that this repulsion prevents collapse. It is a striking fact, and it is the main theme of this paper, that *for every fixed $\beta \leqq 1$ and q there is a critical α (call it $\alpha_c(\beta)$) so that $H(\alpha, \beta)$ is stable when $\alpha < \alpha_c(\beta)$. There is another critical α (call it $\bar{\alpha}_c(\beta)$) so that $H(\alpha, \beta)$ is unstable when $\alpha > \bar{\alpha}_c(\beta)$.* These facts are the reason behind the contention above that α and β are natural. *We do not know whether or not* $\alpha_c(\beta) = \bar{\alpha}_c(\beta)$. Note that by the above monotonicity in z remark, stability for some (α, β_1) implies stability for all (α, β) with $\beta < \beta_1$.

There is an additional piece of information. Suppose that stability occurs for a pair α_1, z. Then stability occurs for a pair α, z if $\alpha \leqq \alpha_1$. The reason for the monotonicity in α is that $\inf\operatorname{spec}(\sum |p_i| + \alpha V_C) \geqq (1 - \alpha/\alpha_1)\ \inf\operatorname{spec}(\sum |p_i|) + (\alpha/\alpha_1)$ $\inf\operatorname{spec}(\sum |p_1| + \alpha_1 V_c) \geqq 0$.

Before stating our main results in detail, let us review some recent progress with this and related problems that also have the feature of critical coupling constants.

(1) The Chandrasekhar critical mass was established up to a factor of 4 in the framework of the relativistic Schrödinger equation by Lieb-Thirring [26]. Later, Lieb-Yau [27] proved that not only is the Chandrasekhar critical mass exactly correct, but the Chandrasekhar semiclassical equation can be derived rigorously from the relativistic Schrödinger equation in the limit that the gravitational constant $G \to 0$. In particular, in the physically interesting case, the discrepancy between the Chandrasekhar semiclassical critical mass and the quantum mechanical critical mass was shown in [27] to be less than 0.01%.

(2) For the non-relativistic Schrödinger equation, but with magnetic fields present that couple to both the electronic orbital motion and electronic spin, the existence of a critical nuclear charge for the stability of the hydrogen atom was proved by Fröhlich, Lieb, Loss, and Yau [15, 28]. The results were extended to the one-electron molecule and many-electron atom by Lieb and Loss [23]. The stability criteria are very similar to that of the relativistic stability considered in this paper. For stability, one should keep *both* $\alpha^2 z$ and α small. The general case for this model (many electrons and nuclei) remains an interesting open problem.

(3) The relativistic stability of matter itself. For $N=1$ and K arbitrary, Daubechies and Lieb [8] were the first to note the existence of a critical α and β fixed. They proved that H_{1K} is stable in the critical case $\beta = \pi\alpha z/2 = 1$ if $\alpha \leqq 1/3\pi$. The first person to solve a general case for all N and K was Conlon [3], who proved that the Hamiltonian $H(\alpha, z)$ is stable when $z=1$ provided $\alpha \leqq 10^{-200}$ and $q=1$. Using a different method, Fefferman and de la Llave [14] improved Conlon's result for $z=1$ to $\alpha \leqq 1/2.06\pi$, and again $q=1$. The Fefferman-de la Llave proof used computer assisted proofs extensively. Without using a computer, their bound would be worse by a factor 2.5, thereby reducing α to $1/5\pi$. Recently, Fefferman [13] announced a result for the critical case $\beta=1$ provided some numerical computer calculations can be made rigorous. The stability criterion announced in [13] is that stability occurs in the critical case $\beta=1$ if $\alpha \leqq 1/20$ and $q=1$. A complete proof, however, was not available when the present paper was written. Since $H(\alpha, \beta)$ collapses for $\beta > 1$ no matter how small the difference $\beta - 1$ may be, the application of computer assisted proofs to the $\beta = 1$ case is delicate and difficult. Fefferman [13] states that "arbitrarily small roundoff errors are apparently fatal."

All the results mentioned above address the situation $q=1$. The methods employed are not, in our opinion, easily generalized to treat arbitrary q, as is done here. The ability to treat arbitrary q without increasing the complexity of the proof as q increases is, in our opinion, one of the main advantages of our method. Another is that we have no intrinsic need to invoke the computer. *The essence of our method is that for all q the many-body problem is reduced to a tractable one-body problem (see e.g. Theorems 6 and 11). This method also makes it possible to prove, for the first time, that stability occurs up to and including the critical value* $\beta = 1$.

We should point out that the main tool in proving the nonrelativistic stability of matter, the Thomas-Fermi theory, fails to predict stability in the relativistic case. The semiclassical kinetic energy decreases in the high momentum region from (const) $\int \varrho^{5/3}$ in the nonrelativistic case to (const) $\int \varrho^{4/3}$ in the relativistic case. This semiclassical kinetic energy, $\int \varrho^{4/3}$, cannot control the Coulomb singularity $z\alpha/r$ for *any* $\alpha>0$. The fact that stability occurs only for some finite $\alpha>0$ and $z>0$ is not a trivial matter (see Conlon [3]). A good estimate for α, especially when β is set equal to its critical value 1, is very difficult to achieve and should resolve the following subtle points:

(i) The delicate balance of charge neutrality. If, for example, the attractive term in V_c is changed from $z\alpha\sum\sum|x_i-R_j|^{-1}$ to $z\alpha(1+\varepsilon)\sum\sum|x_i-R_j|^{-1}$ for some $\varepsilon>0$, then stability will not occur *for any positive* α *and* z. Physically, an attractive gravitational interaction is present and it does alter the Hamiltonian in precisely this manner – collapse does indeed occur. But the gravitational constant is small, and this collapse happens only when N and K are extremely large – the order of a solar mass [26, 27]. Indeed, the problem of determining the critical mass when Coulomb and gravitational interactions are both taken into account is a difficult open problem.

(ii) An improved version of the basic inequality $|p|-\frac{2}{\pi}|x|^{-1}\geqq 0$ is needed. This is apparently crucial since each electron in general feels attractions from more than one nucleus. One may argue that, by virtue of screening, each electron feels only one attraction from its nearest nucleus, but it is difficult to find a simple, precise mathematical statement about screening. Indeed, some corrections (e.g. van der Waals force) are obviously unavoidable and can only be controlled by the kinetic energy.

(iii) The nonlocality of the operator $|p|$. The technical problems caused by this non-locality are serious, especially since the Coulomb potential is long-ranged.

Our main results are the following four theorems about stability and instability.

Theorem 1 (Simple Stability Criterion). *For any* $z>0$ *and* q, *the Hamiltonian* $H(\alpha, z)$ *is stable if*

$$\alpha\leqq\sup_{z'\geqq z}A_q(z'), \tag{1.6}$$

where

$$A_q(z)=(2/\pi)z^{-1}[1+q^{1/3}z^{-1/3}C(z)^{-1/3}]^{-1}, \tag{1.7}$$

$$C(z)=3.0844\{[1.6617+1.7258z^{-1}+0.9533z^{-1/2}]^4+(4/\pi)^3[1+(2z)^{-1/2}]^8\}^{-1}. \tag{1.8}$$

Corollary. *Fix* $\beta\equiv z\alpha\pi/2<1$. *Then stability occurs if*

$$q\alpha\leqq\begin{cases}0.062980(1-\beta)^3\beta^{-2} & \text{if } \beta\geqq 0.49910\\ 0.031774 & \text{if } \beta\leqq 0.49910.\end{cases} \tag{1.9}$$

Remark. There is a number z_1, which is roughly 0.6, such that if $z\geqq z_1$ then the supremum in (1.6) occurs for $z'=z$, while if $z\leqq z_1$ the supremum occurs for $z'=z_1$.

Theorem 2 (Stability criterion for $\beta\leqq 1$). *Fix* $\beta\leqq 1$. *Then the Hamiltonian* $H(\alpha,\beta)$ *is stable if*

$$q\alpha\leqq 1/47.$$

Theorem 3 (Instability for all z and q). *There is a critical value* α_1 *such that if* $\alpha>\alpha_1$ *then* $H(\alpha, z)$ *is unstable for every* $q\geqq 1$ *and every nuclear charge* $z>0$ *(not necessarily* *integral), no matter how small z may be. This means that if* $\alpha > \alpha_1$, *one can always choose N and K so that* $E_{NK}(\alpha, z) = -\infty$. *In order to achieve this collapse, it is only necessary to use one electron, i.e.* $N=1$. *One can take* $\alpha_1 = 128/15\pi$.

Theorem 4 (Instability dependence on q). *Let* $\beta = \pi\alpha z/2$ *as in* (1.3). *There is a critical value* α_2 *such that if*

$$\alpha > \alpha_2 q^{-1} \beta^{-2}, \tag{1.10}$$

then $H(\alpha, \beta)$ *is always unstable. To achieve this collapse, only* $N=q$ *electrons are needed. One can take* $\alpha_2 = 115, 120$. *Alternatively,* $\alpha > 36 q^{-1/3} z^{2/3}$.

Corollary. *If the electrons are bosons then* $H(\alpha, z)$ *is unstable for all* $\alpha > 0$ *and all fixed* $z > 0$. *The number of electrons necessary to achieve this collapse satisfies* $N \leqq 4\pi^{-2} \alpha_2 z^{-2} \alpha^{-3}$.

Remarks. In view of Theorem 3, the number 115, 120 should not be taken seriously. Its large value merely demonstrates how difficult it is to find simple, rigorous bounds – even variational upper bounds – for the relativistic Coulomb problem.

These theorems, taken together, give a clear picture about the stability of relativistic matter. The relevant parameters for stability are αq (if β is fixed) and $\alpha q^{1/3}$ (if z is fixed). An upper bound for α which is independent of z and q is given in Theorem 3. β is never larger than 1. Theorem 1 clearly fails to predict stability for the critical case $\alpha z = 2/\pi$, but its proof is considerably simpler than that of Theorem 2. It also gives the correct q dependence (when z is fixed), and its bound on α for small z is better than that of Theorem 2.

To gain perspective on how good these bounds are, we specialize our results to the following two cases. First, in the critical case, our upper bound (Theorem 2) and lower bound (Theorem 3) differ by a factor of 128 for $q=1$. Second, for $z=1$ and $q=1$, Theorem 1 predicts stability for $\alpha \leqq 1/3.23\pi$, which is not appreciably worse than the computer assisted proof bound $1/2.06\pi$ in [14]. Our bounds in Theorem 1 and Theorem 2 can certainly be improved, as will become clear in the proofs given below. We refrain from the temptation to optimize our results by complicating the technicalities. Our goal is to give a simple conceptual proof which has the correct q dependence and reasonable estimates.

Our proofs for Theorem 3 and 4 follow the same idea used in [23, 20]. Theorems 1 and 2 are much more difficult. Our basic strategy is first to reduce the Coulomb potential to a one-body potential, W. Then, by localizing the kinetic energy $|p|$, we can control the short distance Coulomb singularity of W, leaving a bounded potential W^* as remainder. The last task is to bound the sum of the negative eigenvalues of $|p| + W^*$, but this is standard and can be done by using semiclassical bounds ([6]).

The following Theorem 5 is a consequence of our localization for $|p|$ and combinatorial ideas in [26]. Theorem 5 was announced in [27, Appendix B], where it was proved for the special case $q=N$. Earlier, Fefferman and de la Llave [14] proved it for $q=1$. This theorem is not needed in the present work, but it is independently interesting. (Note that the definition of δ_i below is the reciprocal of that in [27].)

Theorem 5 (Domination of the nearest neighbor attraction by kinetic energy). *Let $\delta_i = \delta_i(x_1, \ldots, x_N)$ be the nearest neighbor distance for particle i relative to $N-1$ other particles, i.e.*

$$\delta_i \equiv \min\{|x_i - x_j| \,|\, j \neq i\}. \tag{1.11}$$

Let $\psi \in L^2(\mathbb{R}^{3N})$ be an N particle fermionic function of space-spin with q spin states. Then

$$\sum_{i=1}^{N} (\psi, |p_i|\psi) \geqq C_1 q^{-1/3} \sum_{i=1}^{N} (\psi, \delta_i^{-1}\psi), \tag{1.12}$$

$$\sum_{i=1}^{N} (\psi, p_i^2\psi) \geqq C_2 q^{-2/3} \sum_{i=1}^{N} (\psi, \delta_i^{-2}\psi), \tag{1.13}$$

where

$$C_1 = 0.129, \quad C_2 = 0.0209. \tag{1.14}$$

The organization of the rest of this paper is as follows:

In Sects. II and III, we prove Theorems 1 and 2 assuming an electrostatic inequality for the Coulomb potential and localization estimates for $|p|$. The theorems used in Sects. II and III are then proved in Sects. IV–VII. The presentation has been broken up this way in order to stress the conceptual underpinnings of Theorems 1 and 2.

Theorem 5 is proved in Sect. V. Some details of our numerical calculations are explained in Sect. VIII. In the final Sect. IX we prove Theorems 3 and 4.

II. Proof of Theorem 1 ($z\alpha < 2/\pi$)

The proofs of Theorems 1 and 2 are conceptually much simpler than the following detailed calculations and technicalities would suggest. There are three main steps for Theorem 1 and five steps for Theorem 2. Step A is the same for both theorems.

Step A. Reduction of the many-body Coulomb potential to a sum of one-body potentials plus a positive constant, namely $-\sum_1^N W(x_i) + C$. This reduces the problem to that of showing that q times the sum of the negative eigenvalues of the operator $|p| - W$ is not less than $-C$.

In the next step we decompose $\mathbb{R}^3$ into regions $B_0, B_1, \ldots, B_K$ where the B_i are disjoint balls centered at the R_i and B_0 is everything else.

Step B. We write $|p| = \beta|p| + (1-\beta)|p|$ with $\beta = z\alpha\pi/2 < 1$. In the balls B_i, $i = 1, \ldots, K$ we use $\beta|p|$ to control the Coulomb singularity of W and prove the operator inequality

$$\beta|p| - \alpha W(x) \geqq -U(x), \tag{2.1}$$

where $U = W$ in B_0 and U is a continuous function inside each ball.Thus $|p| - \alpha W \geqq (1-\beta)|p| - U$.

Step C. The sum of the negative eigenvalues of $(1-\beta)|p| - U$ is bounded by using the semiclassical bound due to Daubechies [6].

Steps B, C, D, and E for Theorem 2 will be explained in Sect. III.

In this section we shall state the basic theorems for steps A and B. These will be proved later in Sects. IV and V. These theorems will be combined here in step C, thus completing the proof of Theorem 1.

Step A. Reduction of the Coulomb Potential to a One-Body Potential

This step has nothing to do with quantum mechanics or the nature of the kinetic energy operator. It has to do with screening in classical potential theory. The total Coulomb potential, V_c, is given in (1.5). There are K nuclei located at distinct points $R_1, \ldots, R_K$ in $\mathbb{R}^3$ and having the same charge, z. There are N electrons.

Introduce the nearest neighbor, or Voronoi, cells $\{\Gamma_j\}_{j=1}^K$ defined by

$$\Gamma_j = \{x \mid |x - R_j| \leqq |x - R_k| \text{ for all } k \neq j\}. \tag{2.2}$$

The boundary of Γ_j, $\partial\Gamma_j$, consists of a finite number of planes. Another important quantity is the distance

$$D_j = \operatorname{dist}(R_j, \partial\Gamma_j) = \tfrac{1}{2}\min\{|R_k - R_j| \mid j \neq k\}. \tag{2.3}$$

The following theorem will be proved in Sect. IV. Recall (1.5).

Theorem 6 (Reduction of the Coulomb potential). *For any* $0 < \lambda < 1$

$$V_c(x_1, \ldots, x_N; R_1, \ldots, R_K) \geqq -\sum_{i=1}^{N} W^\lambda(x_i) + \frac{1}{8} z^2 \sum_{j=1}^{K} D_j^{-1} \tag{2.4}$$

and, for x *in the cell* Γ_j, $W^\lambda(x) = W_j^\lambda(x) \equiv G_j(x) + F_j^\lambda(x)$ *with*

$$G_j(x) = z|x - R_j|^{-1} \tag{2.5}$$

$$F_j^\lambda(x) = \begin{cases} \tfrac{1}{2} D_j^{-1}(1 - D_j^{-2}|x - R_j|^2)^{-1} & \textit{for} \quad |x - R_j| \leqq \lambda D_i \\ (\sqrt{2z} + \tfrac{1}{2})|x - R_j|^{-1} & \textit{for} \quad |x - R_j| > \lambda D_i. \end{cases} \tag{2.6}$$

Theorem 6 says that when the electron-electron and nucleus-nucleus Coulomb repulsion is taken into account, V_c is bounded below by a *positive term* [the last term in (2.4)] consisting of a residue of the nucleus-nucleus repulsion (in fact one quarter of the nearest neighbor repulsion) and an attractive single particle part W^λ. In each cell Γ_j, W_j^λ is essentially the attraction to the nearest nucleus (this is the G_j part of W_j^λ); there is also a small attractive error F_j^λ.

There are two essential points in (2.4). One is that the charge z appearing in G_j is the same as in the original potential V_c. The other is the existence of the positive term. The error term F_j^λ can certainly be improved, especially the long-range part $|x - R_i| > \lambda D_j$; we have not tried to optimize F_j^λ.

It is interesting to compare our Theorem 6 with Baxter's Proposition 1 [1] which says that

$$V_c \geqq -(1 + 2z) \sum_{j=1}^{N} \delta(x_j)^{-1} \tag{2.7}$$

with

$$\delta(x) = \min\{|x - R_j| \mid j = 1, \ldots, K\} = |x - R_j| \quad \text{when} \quad x \in \Gamma_j. \tag{2.8}$$

Fefferman and de la Llave [14] later improved this when $z = 1$ from $1 + 2z = 3$ to 8/3. Our proof is completely different from both proofs of (2.7), as is Theorem 6 itself. To reiterate the essential points, our bound has the *correct* singularity near the nucleus (namely z and not $1+2z$) and it also has a *positive* repulsive term.

Step B. Control of the Coulomb Singularity in Balls

The following formula is well known. For $f\in L^2$ with Fourier transform $\hat{f}$,

$$(f,|p|f)=(2\pi)^{-3}\int|\hat{f}(p)|^2|p|dp=(2\pi^2)^{-1}\int\int|f(x)-f(y)|^2|x-y|^{-4}dxdy\,. \quad (2.9)$$

One way to derive this formula is to write

$$(f,|p|f)=\lim_{t\downarrow 0}t^{-1}\{(f,f)-(f,e^{-t|p|}f)\}\,. \quad (2.10)$$

The convergence is a simple consequence of dominated convergence in Fourier space. The kernel of $\exp(-t|p|)$ can easily be calculated to be

$$e^{-t|p|}(x,y)=\pi^{-2}t[|x-y|^2+t^2]^{-2}\,. \quad (2.11)$$

Inserting (2.11) in (2.10) yields (2.9).

A formula similar to (2.9) can be derived this way for $(p^2+m^2)^{1/2}$ in place of $|p|$.

$$(f,(p^2+m^2)^{1/2}f)=\tfrac{1}{4}\pi^{-2}m^2\int\int|f(x)-f(y)|^2|x-y|^{-2}K_2(m|x-y|)dxdy\,, \quad (2.12)$$

where K_2 is a Bessel function. This follows from [11]

$$\exp[-t(p^2+m^2)^{1/2}](x,y)=\tfrac{1}{2}\pi^{-2}m^2t(|x-y|^2+t^2)^{-1}K_2(m(|x-y|^2+t^2)^{1/2})\,. \quad (2.13)$$

Starting with formula (2.9) we have

Theorem 7 (Kinetic energy in balls). *Let B be a ball of radius D centered at $z\in\mathbb{R}^3$ and let $f\in L^2(B)$. Define*

$$(f,|p|f)_B\equiv\frac{1}{2\pi^2}\int_B\int_B|f(x)-f(y)|^2|x-y|^{-4}dxdy \quad (2.14)$$

and assume this is finite. Then

$$(f,|p|f)_B\geqq D^{-1}\int_B Q(|x-z|/D)|f(x)|^2dx\,, \quad (2.15)$$

where $Q(r)$ is defined for $0<r\leqq 1$ by

$$Q(r)=2/(\pi r)-Y_1(r)\,,$$

$$Y_1(r)=\frac{2}{\pi(1+r)}+\frac{1+3r^2}{\pi(1+r^2)r}\ln(1+r)-\frac{1-r^2}{\pi(1+r^2)r}\ln(1-r)-\frac{4r}{\pi(1+r^2)}\ln r$$
$$\leqq 1.56712\,. \quad (2.16)$$

The maximum of $Y_1(r)$ occurs at $r\approx 0.225975$ and was computed by S. Knabe. Note that $Y_1(|x|)$ is continuous for all $|x|\leqq 1$.

Using (2.9) we have

Corollary. *If $B_1,\ldots,B_K$ are disjoint balls in $\mathbb{R}^3$ centered at $R_1,\ldots,R_K$ and with radii $D_1,\ldots,D_K$,*

$$|p|\geqq\frac{2}{\pi}\sum_{j=1}^{K}|x-R_j|^{-1}B_j(x)-\sum_{j=1}^{K}D_j^{-1}Y_1(|x-R_j|/D_j)B_j(x)\,, \quad (2.17)$$

where $B_j(x)$ is the characteristic function of B_j.

Theorem 7 is proved in Sect. V. Theorem 12, which is the analogue of Theorem 7 with p^2 in place of $|p|$, is stated and proved in Sect. V.

Step C. Semiclassical Bounds and the Conclusion of the Proof of Theorem 1

The problem of showing that $H=\sum|p_i|+\alpha V_c\geqq 0$ has been reduced to the following. In step A we showed that $H\geqq\sum_1^N \tilde{h}_i+C$, where

$$\tilde{h}_i=|p_i|-\alpha W^\lambda(x_i), \tag{2.18}$$

$$C=\frac{1}{8}z^2\alpha\sum_{j=1}^K D_j^{-1}. \tag{2.19}$$

If we write $|p|=\beta|p|+(1-\beta)|p|$, with $\beta=z\alpha\pi/2$, then step B shows that it suffices to replace $\tilde{h}_i$ in H by h_i where

$$h_i=(1-\beta)|p_i|-U(x_i), \tag{2.20}$$

$$U(x)=\alpha F_j^\lambda(x)+\beta D_j^{-1}Y_1(|x-R_j|/D_j)B_j(x)+z\alpha|x|^{-1}(1-B_j(x))\quad\text{when}\quad x\in\Gamma_j. \tag{2.21}$$

Proving that $\sum_1^N h_i+C\geqq 0$ for all numbers, N, of q-state fermions amounts to the following inequality in terms of density matrices satisfying $0\leqq\gamma\leqq q$. [A density matrix is a positive definite trace class operator on $L^2(\mathbb{R}^3)$.]

$$\mathrm{Tr}\gamma h\geqq -C\quad\text{for all }\gamma, \tag{2.22}$$

with $h=(1-\beta)|p|-U(x)$. ($\mathrm{Tr}\gamma h$ is shorthand for $\sum_k(f_k,hf_k)\gamma_k$, where (f_k,γ_k) are the eigenfunctions and eigenvalues of γ.) For more details see [21].

The tool we shall use to prove (2.22) is Daubechies' extension of the Lieb-Thirring semiclassical bound from p^2 to $|p|$.

Theorem 8 (Daubechies). *Let γ be a density matrix satisfying $0\leqq\gamma\leqq q$. (q need not be an integer.) Let $U(x)$ be any positive function in $L^4(\mathbb{R}^3)$. Then for $\mu>0$,*

$$\mathrm{Tr}\gamma(\mu|p|-U)\geqq -0.0258q\mu^{-3}\int U(x)^4dx. \tag{2.23}$$

To complete the proof we merely insert (2.21) into (2.23). A simple bound is obtained by extending the integral over each Γ_j to an integral over all of $\mathbb{R}^3$. This will give K terms on the right side of (2.23) (each of which scales like D_j^{-1}) to be compared with the K terms in C (2.19). Our condition is then (recalling that $\beta=z\alpha\pi/2$)

$$0.0258q(1-\beta)^{-3}\left\{\int_{|x|<1}[\alpha F^\lambda(|x|)+\beta Y_1(|x|)]^4dx\right.$$
$$\left.+\int_{|x|>1}[\alpha F^\lambda(|x|)+z\alpha|x|^{-1}]^4dx\right\}\leqq\tfrac{1}{8}z^2\alpha \tag{2.24}$$

for some choice of $0<\lambda<1$ and where

$$F^\lambda(r)=\begin{cases}\frac{1}{2}(1-r^2)^{-1} & \text{for}\quad 0\leqq r\leqq\lambda\\ (\sqrt{2z}+\frac{1}{2})r^{-1} & \text{for}\quad \lambda\leqq r.\end{cases} \tag{2.25}$$

The second integral ($|x|>1$) in (2.24) (call it I_+) is easy to evaluate. It is independent of λ,

$$I_+ = (4/\pi)^3 \beta^4 [1+(2z)^{-1/2}]^8 . \tag{2.26}$$

Next, the integral of Y_1^4 over $|x|<1$ has been done numerically by S. Knabe. The following is actually an upper bound.

$$\int_{|x|<1} Y_1(x)^4 dx = 7.6245 \equiv I_1 . \tag{2.27}$$

We shall take $\lambda = 10/11$. Then

$$\int_{\lambda<|x|<1} F^\lambda(x)^4 dx = (4\pi/10)\left[\frac{1}{2}+(2z)^{1/2}\right]^4 \equiv I_2 , \tag{2.28}$$

$$\int_{|x|<\lambda} F^\lambda(x)^4 dx \leqq (\pi/4)\lambda \int_0^\lambda (1-r^2)^{-4} r dr \equiv I_3$$
$$= (\pi\lambda/24)[(1-\lambda^2)^{-3}-1] = 22.645 . \tag{2.29}$$

To bound the first integral ($|x|<1$) in (2.24) one can use the triangle inequality $\int (f+g+h)^4 \leqq [(\int f^4)^{1/4}+(\int g^4)^{1/4}+(\int h^4)^{1/4}]^4$. Thus our condition for stability is satisfied if

$$0.0258q(1-\beta)^{-3}\{[1.6617\beta+1.0588\alpha(\tfrac{1}{2}+(2z)^{1/2})+2.1815\alpha]^4$$
$$+(4/\pi)^3\beta^4[1+(2z)^{-1/2}]^8\} \leqq (2/\pi)^2\beta^2/8\alpha . \tag{2.30}$$

Let us rewrite the stability condition (2.30) as

$$q^{-1} z C(z) \geqq \beta^3(1-\beta)^{-3} \tag{2.31}$$

with $C(z)$ given by (1.8), namely

$$1/C(z) \equiv (0.0258)4\pi\{[1.6617+1.7258z^{-1}+0.9533z^{-1/2}]^4+(4/\pi)^3[1+(2z)^{-1/2}]^8\} . \tag{2.32}$$

By taking the cube root in (2.31) we have that (2.31) is equivalent to the assertion that stability occurs if

$$\alpha \leqq A_q(z) \equiv (2/\pi)z^{-1}\{1+q^{1/3}z^{-1/3}C(z)^{-1/3}\}^{-1} . \tag{2.33}$$

Using the monotonicity in z for fixed α [8] mentioned in Sect. I, (2.33) can be improved to the statement that stability occurs if

$$\alpha \leqq \sup\{A_q(z')|z' \geqq z\} , \tag{2.34}$$

and this is precisely Theorem 1. □

Next, we address the question of finding a bound on α that depends only on β and not on z. For this purpose return to (2.31) and solve the equation $q^{-1}zC(z) = \beta^3(1-\beta)^{-3}$. Since $z \to C(z)$ is monotone increasing, this equation has a unique solution. Call it $Z_q(\beta)$. Then stability occurs for any given β if

$$\alpha \leqq \alpha_q^*(\beta) \equiv (2/\pi)\sup\{\beta'/Z_q(\beta')|\beta' \geqq \beta\} . \tag{2.35}$$

Again we have used the aforementioned fact that stability for (α, β') implies stability for (α, β) if $\beta \leqq \beta'$.

Formula (2.35) is correct but lacks transparency. We shall now present a way to find a function $\alpha_q^{**}(\beta)$ which is less than or equal to $\alpha_q^*(\beta)$ but which has the same general features as $\alpha_q^*(\beta)$. It is this function, $\alpha_q^{**}(\beta)$ that is given in the corollary.

Choose an arbitrary z_0. Let $\alpha_0 = A_q(z_0)$ and let $\beta_0 = (2/\pi)\alpha_0 z_0$. Define

$$\alpha_q^{**}(\beta) = \begin{cases} (2/\pi q) C(z_0)(1-\beta)^3 \beta^{-2} & \text{if} \quad \beta \geqq \beta_0 \\ (2/\pi q) C(z_0)(1-\beta_0)^3 \beta_0^{-2} & \text{if} \quad \beta \leqq \beta_0 \,. \end{cases} \tag{2.36}$$

We claim that $\alpha \leqq \alpha_q^{**}(\beta)$ implies stability. First, suppose that $\beta \geqq \beta_0$. Then we have

$$z \equiv (2/\pi)\alpha^{-1}\beta \geqq (2/\pi)[\alpha_q^{**}(\beta)]^{-1}\beta_0 \geqq (2/\pi)[\alpha_q^{**}(\beta_0)]^{-1}\beta_0 \text{ (since } \beta \geqq \beta_0) = z_0 \,.$$

By the monotonicity of C, we have $C(z) \geqq C(z_0)$. Therefore

$$z = (2/\pi)\alpha^{-1}\beta \geqq (2/\pi)[\alpha_q^{**}(\beta)]^{-1}\beta \geqq qC(z)^{-1}\beta^3(1-\beta)^{-3} \text{ (since } C(z) \geqq C(z_0)) \,.$$

This is (2.31).

Second, suppose that $\beta \leqq \beta_0$. To prove the stability, we only have to verify (2.35). For this purpose, it suffices to show that $\alpha \leqq \frac{2}{\pi}\beta_0 / Z_q(\beta_0)$ with $Z_q(\beta_0)$ solving $q^{-1}zC(z) = \beta_0^3(1-\beta_0)^{-3}$. Since by definition $q^{-1}z_0C(z_0) = \beta_0^3(1-\beta_0)^{-3}$, we have from the uniqueness of the solution of the above equations that $Z_q(\beta_0) = z_0$ and $\alpha_q^{**}(\beta) = (2/\pi q)C(z_0)(1-\beta_0)^3\beta_0^{-2} = \frac{2}{\pi}\beta_0/Z_q(\beta_0)$. Hence $\alpha \leqq \alpha_q^{**}(\beta)$ is the same as $\alpha \leqq \frac{2}{\pi}\beta_0/Z_q(\beta_0)$ and thus stability occurs for (α, β) with $\alpha \leqq \alpha_q^{**}(\beta)$ and $\beta \leqq \beta_0$.

Let us choose $z_0 = 10$. Then $(2/\pi)C(10) = 0.062980$ and $\beta_0 = 0.49910$. This together with (2.36) proves the Corollary of Theorem 1. □

III. Proof of Theorem 2 ($z\alpha \leqq 2/\pi$)

In the proof of Theorem 1 we first reduced the many-body Coulomb potential to a one-body potential in Step A. Then we split the kinetic energy $|p|$ into two pieces. One of them was used to control the Coulomb singularity and the other was used to control the long range part of the potential. If the method of Theorem 1 is used when $z\alpha = 2/\pi$, all of $|p|$ must be used for the singularities and nothing remains to control the long-range potential. In this section both parts of the potential will be controlled without splitting $|p|$, but this requires inventing a suitable localization formula for $|p|$. We shall henceforth take $z\alpha = 2/\pi$; by the monotonicity in z, this case will cover all the cases $z\alpha \leqq 2/\pi$.

There are five steps.

Step A is the same as before. The Coulomb potential V_c is replaced by a one-body potential W^λ plus a positive constant. Henceforth we shall take $\lambda = 0.97$ and omit the superscript on W.

Step B. Here we show that if $\chi_1(x)$ is a C^1 function which is approximately the characteristic function of a ball, and if γ is a density matrix with $0 \leqq \gamma \leqq q$ and if $\chi_2(x)$

is defined by $\chi_1(x)^2+\chi_2(x)^2=1$, then

$$\begin{aligned}\operatorname{Tr}\gamma(|p|-W) &\geqq \operatorname{Tr}\chi_1\gamma\chi_1(|p|-\text{potential energy correction } -W)\\ &\quad+\operatorname{Tr}\chi_2\gamma\chi_2(|p|-\text{potential energy correction } -W)-q\cdot\text{const}. \end{aligned}\tag{3.1}$$

The important aspect of this inequality is this: It might have been thought that since $|p|$ is not a local operator, the potential energy corrections would have to be very long range. In fact they have support only inside a ball which is only slightly larger than the original ball. The long range nature of $|p|$ manifests itself in the term q-constant which depends on $\|\gamma\|$ but not on $N=\operatorname{Tr}\gamma$.

Step C. The ball referred to in step B is taken to be B_1 centered at R_1 (see Sect. II). To control the first term on the right side of (3.1) we have to bound q times the sum of the negative eigenvalues of $|p|$ – potential energy correction – W in a ball, where W is the one-body potential defined in step A.

Step D. For the second term on the right side of (3.1), the localization process in steps B and C are repeated $K-1$ times for nuclei, $2, \ldots, K$. This finally leaves us with a term $\operatorname{Tr}\chi_0\gamma\chi_0(|p|-$potential energy corrections) where χ_0 is essentially the characteristic function of the complement of the K balls. To estimate this term, Daubechies' semiclassical bound, Theorem 8, is used.

Step E. The above process leads to a lower bound on inf spec(H) in terms of certain integrals which depend on certain parameters that remain to be specified. These numerical facts are presented in this step. The details of the computation are given in Sect. VIII.

Step B. Localization of the Kinetic Energy

By way of comparison we begin by reminding the reader of the IMS localization formula (see [5, Theorem 3.2]) for $p^2=-\Delta$ instead of $|p|$. Let $\chi_0, \chi_1, \ldots, \chi_K$ be real valued functions on $\mathbb{R}^3$ satisfying

$$\sum_{j=0}^{K} \chi_j(x)^2=1 \quad \text{for all } x. \tag{3.2}$$

Then an elementary calculation yields the following operator identity.

$$-\Delta=\sum_{j=0}^{K} \chi_j(x)(-\Delta)\chi_j(x)-\sum_{j=0}^{K}|\nabla\chi_j(x)|^2. \tag{3.3}$$

This is a *localization of* $-\Delta$. If we assume additionally that χ_j has support in some set A_j (which are not pairwise disjoint, of course) then for any $f\in L^2(\mathbb{R}^3)$ and any arbitrary potential V,

$$(f,[-\Delta+V(x)]f)=\sum_{j=0}^{K}(\chi_j f,[-\Delta+V(x)-U(x)]\chi_j f) \tag{3.4}$$

with

$$U(x)=\sum_{j=0}^{K}|\nabla\chi_j(x)|^2. \tag{3.5}$$

The advantage of (3.4) is that in the j^{th} term of (3.4) only $[V(x)-U(x)]1_{A_j}(x)$ appears [where $1_A(x)=1$ if $x\in A$ and $1_A(x)=0$ if $x\notin A$] and one can utilize different bounds on $V-U$ according to the region A_j under consideration. Furthermore, since $\chi_j f$ has support in A_j one can replace $-\Delta$ by the larger operator $-\Delta$ with Dirichlet boundary conditions on ∂A_j. The price one has to pay for all this is the negative potential operator $-U(x)$.

For the operator $|p|$ the following analogue of (3.3) is much more complicated because $|p|$ is not a local operator. We also state its generalization to $(p^2+m^2)^{1/2}$. The proof is immediate starting with (2.9) and (2.12).

Theorem 9 (Localization of kinetic energy-general form). *Let $\chi_0, \ldots, \chi_K$ be Lipschitz continuous functions satisfying* (3.2). *Then for any $f\in L^2(\mathbb{R}^3)$,*

$$(f,|p|f)=\sum_{j=0}^{K}(\chi_j f,|p|\chi_j f)-(f,Lf), \tag{3.6}$$

where L is a bounded operator with the kernel

$$L(x,y)=\frac{1}{2\pi^2}|x-y|^{-4}\sum_{j=0}^{K}[\chi_j(x)-\chi_j(y)]^2. \tag{3.7}$$

More generally,

$$(f,(p^2+m^2)^{1/2}f)=\sum_{j=0}^{K}(\chi_j f,(p^2+m^2)\chi_j f)-(f,L^{(m)}f), \tag{3.8}$$

where $L^{(m)}$ is a bounded operator with the kernel

$$L^{(m)}(x,y)=(2\pi)^{-2}m^2|x-y|^{-2}K_2(m|x-y|)\sum_{j=0}^{K}[\chi_j(x)-\chi_j(y)]^2 \tag{3.9}$$

and K_2 is a Bessel function.

Formula (3.6) was proposed to us by M. Loss, to whom we are grateful.

A simple, but important corollary of Theorem 9 concerns q-state, density matrices. As defined in Sect. II, this is any bounded operator on $L^2(\mathbb{R}^3)$ which satisfies the operator inequality $0\leqq\gamma\leqq q$ and for which $\mathrm{Tr}\gamma<\infty$.

Corollary. *For any density matrix, γ,*

$$\mathrm{Tr}\gamma|p|=\sum_{j=0}^{K}\mathrm{Tr}\gamma_j|p|-\mathrm{Tr}\gamma L, \tag{3.10}$$

where $\gamma_j\equiv\chi_j\gamma\chi_j$, with χ_j being thought of as a multiplication operator.

To exploit (3.10) we now impose a condition on $\chi_0, \ldots, \chi_K$. Let $R_1, \ldots, R_K$ be distinct points in $\mathbb{R}^3$ (namely the nuclear coordinates) and let D_j be given by (2.3). The K disjoint balls $B_j=\{x|x-R_j|<D_j\}$ were defined in Sect. II. Choose some $0<\sigma<1$ and consider the smaller balls

$$B_j^{(\sigma)}=\{x||x-R_j|\leqq(1-\sigma)D_j\}. \tag{3.11}$$

Let $\chi_0, \ldots, \chi_K$ satisfy (3.2) with χ_j supported in $B_j^{(\sigma)}$ for $j=1, \ldots, K$. The explicit choice for χ_j will be made in step D.

First, consider the case $K=1$. We decompose the L of (3.7) into a long-range part, L^0, and a short-range part, L_1^*, with $L=L^0+L_1^*$. Furthermore, $L_1^*(x,y)$ vanishes if x or y is not in B_1 or if $|x-y|>\sigma$, namely

$$L_1^*(x,y)=\begin{cases}\pi^{-2}|x-y|^{-4}[1-\chi_0(x)\chi_0(y)-\chi_1(x)\chi_1(y)]B_1(x)B_1(y) & \text{if } |x-y|\leqq\sigma\\ 0 & \text{if } |x-y|>\sigma,\end{cases} \tag{3.12}$$

where $B_1(x)=1$ if $x\in B_1$ and $B_1(x)=0$ otherwise. Recall that $\chi_0(x)^2+\chi_1(x)^2=1$ in the $K=1$ case. With these conventions, we have the following theorem which will be proved in Sect. VI.

Theorem 10 (Localization of kinetic energy-explicit bound in the one-center case). *For $K=1$, let L_1^* be given by (3.12) and $L^0=L-L_1^*$, with L given by (3.7). For any positive function, h_1, defined on the ball B_1, let*

$$\theta_1(x)=h_1(x)^{-1}\int_{B_1} L_1^*(x,y)h_1(y)dy. \tag{3.13}$$

Let $\Omega_1=\frac{1}{2}D_1^2\operatorname{Tr}(L^0)^2$, i.e.

$$\Omega_1\equiv\tfrac{1}{2}D_1^2\int[L(x,y)-L_1^*(x,y)]^2dxdy\equiv I^{(1)}+I^{(2)}, \tag{3.14}$$

$$I^{(1)}=\frac{1}{2}\pi^{-4}D_1^2\iint_{\substack{x,y\in B_1^{(\sigma)}\\ ||x|-|y||\geqq\sigma D_1}}|x-y|^{-8}[1-\chi_0(x)\chi_0(y)-\chi_1(x)\chi_1(y)]^2dxdy, \tag{3.15}$$

$$I^{(2)}=\pi^{-4}D_1^2\iint_{\substack{x\in B_1^{(\sigma)}\\ y\notin B_1^{(\sigma)}\\ |y|-|x|\geqq\sigma D_1}}|x-y|^{-8}[1-\chi_0(x)]^2dxdy. \tag{3.16}$$

Then, for any density matrix γ with $\|\gamma\|\leqq q$, and any $\varepsilon>0$,

$$\operatorname{Tr}\gamma|p|\geqq\operatorname{Tr}\chi_1\gamma\chi_1(|p|-U_1^*(x))+\operatorname{Tr}\chi_0\gamma\chi_0(|p|-U_1^*(x))-q(\varepsilon D_1)^{-1}\Omega_1, \tag{3.17}$$

where $U_1^*(x)=0$ for $x\notin B_1$ and, for $x\in B_1$,

$$U_1^*(x)\equiv(\varepsilon/D_1)B_1^{(\sigma)}(x)+\theta_1(x). \tag{3.18}$$

Inequality (3.17) looks complicated, but it is not vastly different from (3.3). The first two terms in (3.17) are the localized kinetic energies (inside and outside the ball B_1). The U_1^* term is a potential energy correction like the U in (3.4), but this potential has support only in the ball B_1. The last term is novel; it involves only the norm of γ and not a trace over γ. One might expect that the non-local nature of $|p|$ would give rise to a long range contribution to U, but these long range effects can be bounded by the norm of γ – as is done in the last term of (3.17).

Step C. Bound on Negative Eigenvalues in a Ball

Our goal is to give a lower bound to $\operatorname{Tr}\chi_1\gamma\chi_1(|p|-W(x)-U_1^*(x))$. The following is our main tool. It will be proved in Sect. VII.

Theorem 11 (Lower bound to the short-range energy in a ball). *Let $C>0$ and $R>0$ and let*

$$H_{CR}=|p|-\frac{2}{\pi}|x|^{-1}-C/R \tag{3.19}$$

be defined on $L^2(\mathbb{R}^3)$ as a quadratic form. Let $0 \leqq \gamma \leqq q$ be a density matrix as before and let χ be any function with support in $B_R = \{x \mid |x| \leqq R\}$. Then

$$\operatorname{Tr} \bar{\chi}\gamma\chi H_{CR} \geqq -4.4827 C^4 R^{-1} q \{(3/4\pi R^3) \int |\chi(x)|^2 dx\}. \tag{3.20}$$

Remark. When $\chi \equiv 1$ in B_R then the factor in braces $\{\ \}$ in (3.20) is 1.

To apply Theorem 11 to our case we take R in Theorem 11 to be $(1-\sigma)D_1$ and we take C to be an upper bound for $(1-\sigma)D_1\{\alpha W(x) + U_1^*(x) - (2/\pi)|x|^{-1}\} = (1-\sigma)D_1\{\alpha F_1(x) + U_1^*(x)\}$ in the ball $|x| \leqq (1-\sigma)D_1$. This computation will be done in Step E.

Step D. The Negative Eigenvalues for the Long Range Potential

Associated with each ball B_j of radius D_j centered at R_j will be a cutoff function χ_j defined by

$$\chi_j(x) = \chi(|x - R_j|/D_j), \tag{3.21}$$

where the universal χ is given by

$$\chi(r) = \begin{cases} 1 & \text{for} \quad r \leqq 1 - 3\sigma \\ \cos[\pi(r - 1 + 3\sigma)/4\sigma] & \text{for} \quad 1 - 3\sigma \leqq r \leqq 1 - \sigma \\ 0 & \text{for} \quad 1 - \sigma \leqq r. \end{cases} \tag{3.22}$$

Here, it is important that $\sigma < 1/3$. We also choose a function $h_j(x)$ for $x \in B_j$,

$$h_j(x) = h(|x - R_j|/D_j), \tag{3.23}$$

$$rh(r) = \begin{cases} 1 & \text{for} \quad r \leqq 1 - 3\sigma \ \text{and}\ 1 - \sigma \leqq r \leqq 1 \\ 2 - \sigma^{-1}|r - 1 + 2\sigma| & \text{for} \quad 1 - 3\sigma \leqq r \leqq 1 - \sigma. \end{cases} \tag{3.24}$$

Starting with Theorem 10, Eq. (3.17), we choose some ε and compute Ω_1, $\theta_1(x)$, $U_1^*(x)$ using (3.13)–(3.16). We also compute some bound

$$C \geqq (1-\sigma)D_1\{\alpha F_1(x) + U_1^*(x)\} \tag{3.25}$$

in $B_1^{(\sigma)}$. By scaling, C does not depend on D_1. Then, using Theorem 11, Eq. (3.20), we have that

$$E = \inf_\gamma \operatorname{Tr}\gamma(|p| - \alpha W) \geqq -qA/D_1 + \inf_\gamma \operatorname{Tr}(1-\chi_1^2)^{1/2}\gamma(1-\chi_1^2)^{1/2}(|p| - \alpha W - U_1^*). \tag{3.26}$$

The first term, qA/D_1, is a sum of two pieces. One is the $q(\varepsilon D_1)^{-1}\Omega_1$ in (3.17); the other is the right side of (3.20) (call it qA_2). The sum is written as qA/D_1 because the various quantities that have been introduced scale in just the right way – so that A really is independent of D_1 and q.

For the second term on the right side of (3.26) we note the identity

$$(1-\chi_1(x)^2)[\alpha W(x) + U_1^*(x)] = (1-\chi_1(x)^2)[\alpha W(x)\beta_1(x) + U_1^*(x)\beta_1(x)], \tag{3.27}$$

where $\beta_1(x) = 1$ if $|x - R_1| \geqq 1 - 3\sigma D_1$ and $\beta_1(x) = 0$ otherwise. Since $(1-\chi_1^2)^{1/2}\gamma(1-\chi_1^2)^{1/2}$ is a q-state density matrix whenever γ is, the last term in (3.26) can be bounded below by

$$\inf_{\gamma} \operatorname{Tr}\gamma(|p| - \alpha W(x)\beta_1(x) - U_1^*(x)\beta_1(x)). \tag{3.28}$$

Now we can apply Theorems 10 and 11 to (3.28), using the ball B_2 in place of B_1. Since $U_1^*(x)=0$ for $x \notin B_1$ we see that $(\alpha W(x) + U_1^*(x))\beta_1(x) = \alpha W(x)$ for $x \notin B_1$. This process can be repeated until all the balls $B_1, \ldots, B_K$ have been used. Our final result (with U_j^* defined as in (3.18) with R_1, D_1 replaced by R_j, D_j) is

$$E \geqq -A \sum_{j=1}^{K} D_j^{-1} + \inf_{\gamma} \operatorname{Tr}\gamma \left[|p| - \left(\alpha W + \sum_{j=1}^{K} U_j^*(x) \right) \prod_{j=1}^{K} \beta_j(x) \right]. \tag{3.29}$$

To bound the last term in (3.29) we use Theorem 8. This will result in a sum of K integrals, one for each cell Γ_j. As in the proof of Theorem 1, a further bound is obtained by pretending that each Γ_j extends to all of $\mathbb{R}^3$. Thus

$$E \geqq -q(A+J) \sum_{j=1}^{K} D_j^{-1}, \tag{3.30}$$

where

$$J = 0.0258 \int_{|x|>1-3\sigma} [(2/\pi)|x|^{-1} + \alpha F(|x|) + U^*(|x|)]^4 dx, \tag{3.31}$$

and where $F(r)$ is given in (2.25) with $\lambda = 0.97$, and $U^*(x)$ is given by (3.18) with $D_1 = 1$ there.

From (3.30) and (2.4), stability holds if

$$q(A+J) \leqq \tfrac{1}{8} z^2 \alpha = (2\pi^2)^{-1} \alpha^{-1}. \tag{3.32}$$

Step E. Numerical Results

We take $\sigma = 0.3$ and $\varepsilon = 0.2077$ (recall that λ was previously chosen to be 0.97). Since all quantities have the correct length scaling, we shall refer everything to a standard ball of unit radius $D_1 = 1$. The following are the results of the computations given in Sect. VIII.

Starting with $\chi(r)$ in (3.22) we compute $\Omega_1 \equiv \Omega$ in (3.13)–(3.16),

$$I^{(1)} = 0.05529, \qquad I^{(2)} = 0.06042,$$
$$\Omega = I^{(1)} + I^{(2)} = 0.1157, \qquad \varepsilon^{-1}\Omega = 0.5571. \tag{3.33}$$

From the definition (3.13) and (3.24) we find that $\theta_1(x) \equiv \theta(|x|)$ satisfies $\theta(r) \leqq \theta^*(r)$ and

$$\theta^*(r) = \begin{cases} (3\pi/32)(2-\sqrt{2})\sigma^{-1} = 0.5751 & \text{for} \quad r \leqq 1-\sigma \\ (\pi/64)\sigma^{-5}(1+2\sigma-r)(1-r)^3 & \text{for} \quad 1-\sigma < r \leqq 1 . \end{cases} \tag{3.34}$$

Using this we have, from (3.18), that

$$U^*(r) \leqq \varepsilon B^{(\sigma)}(r) + \theta^*(r) \tag{3.35}$$

with $B^{(\sigma)}(r) = 1$ for $r < 1 - \sigma = 0.7$ and $B^{(\sigma)}(r) = 0$ otherwise.

Next, we want to find some C satisfying (3.25). Since $\lambda = 0.97 > 1 - \sigma = 0.7$, we need only concern ourselves with the first line of (2.25). Note that α appears in (3.25) in the form $\alpha F_1(x)$ and, since $F_1(x)$ does not depend on z in the region $r<\lambda$, the quantity $\alpha F_1(x)$ is proportional to α when $z\alpha$ is fixed. Our goal is to prove stability when $\alpha<1/47q\leqq 1/47$, and therefore we can replace $\alpha F_1(x)$ by $F_1(x)/47$ in (3.25). Then

$$C=0.7\{0.02086+0.2077+0.5751\}=0.5629 \tag{3.36}$$

satisfies (3.25) for $r<1-\sigma=0.7$.

The right side of (3.20) (with $R=1-\sigma=0.7$) can now be easily calculated. It is

$$qA_2=0.1661q\,. \tag{3.37}$$

Adding $\varepsilon^{-1}\Omega$ and A_2 we have

$$A=0.7232\,. \tag{3.38}$$

Finally, the integral in (3.31) must be computed. To bound $\alpha F(r)$ we can use $(1/47)F(r)$ for $r<\lambda$, while for $r>\lambda$ we write $z=2/\pi\alpha$ in (2.25). When $r>\lambda$ this results in two terms in αF, one of which is proportional to $\alpha^{1/2}$ and the other to α. In both terms we can take $\alpha=1/47$. Thus, we bound $\alpha F(r)$ by $0.1753/r$ for $r>\lambda$ and by $(1/94)(1-r^2)^{-1}$ for $r<\lambda$. We then find that

$$\begin{aligned}(0.0258)^{-1}(4\pi)^{-1}J\leqq &\int_{0.1}^{0.7}[2/\pi r+(1/94)(1-r^2)^{-1}+0.2077+0.5751]^4r^2dr\\ &+\int_{0.7}^{0.97}[(2/\pi r+(1/94)(1-r^2)^{-1}+20.20(1.6-r)(1-r)^3]^4r^2dr\\ &+\int_{0.97}^{1}[2/\pi r+0.1753/r+20.20(1.6-r)(1-r)^3]^4r^2dr\\ &+\int_{1}^{\infty}[2/\pi r+0.1753r^{-1}]^4r^2dr\,.\end{aligned} \tag{3.39}$$

The first integral, J_1, can be bounded by replacing $(1-r^2)^{-1}$ by $(1-(0.7)^2)^{-1}$ and then doing the integral analytically. The second integral, J_2, was done on a computer. In the third integral, J_3, $1.6-r$ was replaced by $1.6-0.97$ and $(1-r^3)$ was replaced by $(1-0.97)^3$; it was then done analytically. The fourth integral, J_4, can be done analytically. We find $J_1\leqq 4.435$, $J_2\leqq 0.17$, $J_3\leqq 0.0135$, and $J_4\leqq 0.435$. Thus

$$J\leqq 1.64 \tag{3.40}$$

and, from (3.32), stability occurs if $\alpha q<1/47$. This completes the proof of Theorem 2. □

IV. An Electrostatic Inequality

Our goal here is to prove Theorem 6 about the Coulomb potential V_c given in (1.5). A similar theorem can be derived for the Yukawa potential $|x|^{-1}\exp(-\mu|x|)$, but we shall not do so here. We recall the definition (2.2) of the K Voronoi cells $\Gamma_1, \ldots, \Gamma_K$ for K nuclei located at $R_1, \ldots, R_K\in\mathbb{R}^3$, and also the radii D_j in (2.3) which is the distance of R_j to $\partial\Gamma_j$. Since Theorem 6 is trivial when $K=1$, we shall assume henceforth that $K>1$. We set

$$V(x)=\sum_{j=1}^{K}|x-R_j|^{-1}\,, \tag{4.1}$$

which is the potential of K nuclei of unit charge located at the R_j, and

$$\delta(x)=\min\{|x-R_j|\,|\,1\leqq j\leqq K\}, \tag{4.2}$$

which is the distance of a particle at x to the set of K nuclei. We set

$$\Phi(x)=V(x)-\delta(x)^{-1}, \tag{4.3}$$

which is the potential of all the nuclei except for the nucleus in the cell Γ_j in which x is located. Φ is continuous but not differentiable.

Let ν be any Borel measure (possibly signed) on $\mathbb{R}^3$. We say that ν is a bounded measure if $|\nu|(\mathbb{R}^3)<\infty$. In this case $\int\Phi(x)d\nu(x)$ is well defined since Φ is continuous and bounded. We define

$$\mathscr{E}_{\Phi,z}(\nu)=\frac{1}{2}\iint|x-y|^{-1}d\nu(x)d\nu(y)-z\int\Phi(x)d\nu(x)+z^2\sum_{1\leqq i<j\leqq K}|R_i-R_j|^{-1}. \tag{4.4}$$

The first term on the right side of (4.4) is well defined (in the sense that it is either finite or $+\infty$) since $|x-y|^{-1}$ is a positive definite kernel. The following is basic to our analysis.

Lemma 1. *Let ν be any bounded measure, let $z>0$ and let Φ be given by* (4.3). *Then*

$$\mathscr{E}_{\Phi,z}(\nu)\geqq\frac{1}{8}z^2\sum_{j=1}^{K}D_j^{-1}. \tag{4.5}$$

Proof. There is a (positive) measure μ that satisfies the equation

$$|x|^{-1}*\mu=z\Phi \tag{4.6}$$

and μ has support on $\partial\Gamma\equiv\bigcup_{j=1}^{K}\partial\Gamma_j$. In fact, μ can be computed explicitly as

$$\mu=-(z/4\pi)\Delta\Phi. \tag{4.7}$$

More precisely, $\partial\Gamma$ consists of pieces of 2 dimensional planes separating some Γ_i from some Γ_j; on $\partial\Gamma_j$

$$d\mu(x)=-(z/2\pi)\mathbf{n}\cdot\nabla|x-R_j|^{-1}d^2x, \tag{4.8}$$

where d^2x is two-dimensional Lebesgue measure on $\partial\Gamma_j$, and $\mathbf{n}$ is the unit normal pointing *out* of Γ_j. Let

$$A=-\tfrac{1}{2}z\int\delta(x)^{-1}d\mu(x). \tag{4.9}$$

Then

$$\begin{aligned}\frac{1}{2}\iint|x-y|^{-1}d\mu(x)d\mu(y)&=\frac{1}{2}\int\Phi(x)d\mu(x)=\frac{z}{2}\sum_{j=1}^{K}\int|x-R_j|^{-1}d\mu(x)+A\\&=\frac{z^2}{2}\sum_{j=1}^{K}\Phi(R_j)+A=z^2\sum_{1\leqq i<j\leqq K}|R_i-R_j|^{-1}+A.\end{aligned} \tag{4.10}$$

On the other hand, if each part of $\partial\Gamma$ is counted twice we obtain

$$A=(z^2/8\pi)\sum_{j=1}^{K}\int_{\partial\Gamma_j}|x-R_j|^{-1}\mathbf{n}\cdot\nabla|x-R_j|^{-1}d^2x. \tag{4.11}$$

Let I_j denote the integral in (4.11). The integrand is $\frac{1}{2}\mathbf{n}\cdot\nabla|x-R_j|^{-2}$. With Λ_j denoting the complement of Γ_j in $\mathbb{R}^3$ (so that $\partial\Lambda_j=\partial\Gamma_j$) we have

$$I_j=\frac{1}{2}\int_{\partial\Gamma_j}\mathbf{n}\cdot\nabla|x-R_j|^{-2}d^2x=-\frac{1}{2}\int_{\Lambda_j}\Delta|x-R_j|^{-2}dx=-\int_{\Lambda_j}|x-R_j|^{-4}dx. \tag{4.12}$$

For convenience in evaluating (4.12) we can take $R_j=0$ and assume that Λ_j contains the half-space $\{(x,y,z)|x\geqq D_j\}$; the reason for this is that (assuming $D_j \neq \infty$) there is another nucleus at some R_i such that the midplane between R_j and R_i is given (after rotation of coordinates) by $\{(x,y,z)|x=D_j\}$. Thus

$$I_j\leqq-\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dydz\int_{D_j}^{\infty}dx(x^2+y^2+z^2)^{-2}=-\pi/D_j, \tag{4.13}$$

and therefore

$$A\leqq-\frac{1}{8}z^2\sum_{j=1}^{K}D_j^{-1}. \tag{4.14}$$

Using (4.6) and (4.10) we have that

$$\mathscr{E}_{\Phi,z}(v)=\tfrac{1}{2}\iint|x-y|^{-1}d(v-\mu)(x)d(v-\mu)(y)-A. \tag{4.15}$$

The integral in (4.15) is nonnegative (since $|x-y|^{-1}$ is positive definite), and the lemma follows from (4.14). □

Proof of Theorem 6. There are N points $x_1,\ldots,x_N$. If x_i is in some cell Γ_j we shall replace the unit point charge at x_i by a unit charge distributed on a sphere S_i but, in general, the center of S_i will not be x^i and the charge distribution on S_i will not be uniform. Also, S_i is not always contained entirely in Γ_j. (If x_i is in more than one Γ_j then an arbitrary choice can be made.) The definition of S_i and the charge distribution v_i on S_i is the following:

(i) If $|x_i-R_j|\leqq\lambda D_j$, then S_i is the sphere $\partial B_j=\{x||x-R_j|=D_j\}$. The charge v_i is determined so that its (continuous) potential $V_i\equiv|x|^{-1}*v_i$ satisfies

$$V_i(x)=\begin{cases}|x-x_i|^{-1} & \text{for}\quad |x-R_j|\geqq D_j\\ |x-x_i^*|^{-1}|x_i-R_j|^{-1}D_j & \text{for}\quad |x-R_j|\leqq D_j,\end{cases} \tag{4.16}$$

where x_i^* is the image of x_i with respect to S_j, namely

$$x_i^*-R_j=D_j^2|x_i-R_j|^{-2}(x_i-R_j). \tag{4.17}$$

The potential $V_i(x)$ is harmonic inside and outside B_j, and v_i can be computed from the formula $-\Delta V_i=4\pi v_i$, but we shall not need this. It is important to note that v_i is nonnegative.

(ii) If $|x_i-R_j|>\lambda D_j$ and $x_i\in\Gamma_j$, then S_i is a sphere centered at x_i and of radius t_i given by

$$t_i=|x_i-R_j|(1+\sqrt{2z})^{-1}. \tag{4.18}$$

The charge distribution v_i on S_i is the uniform one with unit total charge.

Now we apply Lemma 1 with

$$v=\sum_{i=1}^{N}v_i. \tag{4.19}$$

In order to utilize inequality (4.5) it is necessary to relate $\mathscr{E}_{\Phi,z}(v)$ to V_c. The last term in (4.4) is, of course, exactly the nuclear repulsion. The first term on the right side of (4.4) (call it I) satisfies

$$I = \sum_{1 \leq i<k \leq N} \iint |x-y|^{-1} dv_i(x) dv_k(y) + \frac{1}{2} \sum_{i=1}^{N} \iint |x-y|^{-1} dv_i(x) dv_i(y). \quad (4.20)$$

Each $v_i v_k$ integral in (4.20) is less than or equal to $|x_i - x_k|^{-1}$. This is so because, by construction

$$(|x|^{-1} * v_i)(x) \leqq |x-x_i|^{-1}, \quad \text{all } x, \quad (4.21)$$

and hence

$$\int (|x|^{-1} * v_i)(x) dv_k(x) \leqq (|x|^{-1} * v_k)(x_i) \leqq |x_k - x_i|^{-1}. \quad (4.22)$$

The $v_i v_i$ integral in (4.20) is just the self energy of v_i. Call it e_i. There are two cases.

(i) $|x_i - R_j| \leqq \lambda D_j$. Then, from (4.16)

$$\begin{aligned} e_i &= \iint |x-y|^{-1} dv_i(x) dv_i(y) = \int |x-x_i|^{-1} dv_i(x) = V_i(x_i) \\ &= |x_i - x_i^*|^{-1} |x_i - R_j|^{-1} D_j = D_j^{-1}(1 - D_j^{-2}|x_i - R_j|^2)^{-1}. \end{aligned} \quad (4.23)$$

(ii) $|x_i - R_j| > \lambda D_j$ and $x_i \in \Gamma_j$. Here $e_i = 1/t_i$ since v_i is uniformly distributed on a sphere of radius t_i.

To summarize,

$$I \leqq \sum_{1 \leq i<k \leq N} |x_i - x_k|^{-1} + \frac{1}{2} \sum_{i=1}^{N} \begin{Bmatrix} \text{Eq. (4.23)} & \text{in case (i)} \\ 1/t_i & \text{in case (ii)} \end{Bmatrix}. \quad (4.24)$$

The second term on the right side of (4.4) is a sum of $z \int \Phi dv_i$. Again, there are two cases.

(i) $|x_i - R_j| \leqq \lambda D_j$. From the definition of W and the fact that $(|x|^{-1} * v_i)(x) = |x - x_i|^{-1}$ when $x \notin \Gamma_j$, we have

$$\int \Phi(x) dv_i(x) = \sum_{k=1}^{K} |x_i - R_k|^{-1} - |x_i - R_j|^{-1}. \quad (4.25)$$

(ii) $|x_i - R_j| > \lambda D_j$ and $x_i \in \Gamma_j$. By the definition of Φ

$$\int \Phi(x) dv_i(x) = \sum_{k=1}^{K} \int |x - R_k|^{-1} dv_i(x) - \int \delta(x)^{-1} dv_i(x), \quad (4.26)$$

where $\delta(x)$ is the distance to the nearest nucleus. Since every R_k (including R_j) is outside S_i, the first term in (4.26) is merely $\sum_{k=1}^{K} |x_i - R_k|^{-1}$. The difficulty in estimating the second term in (4.4) stems from the fact that v_i can have support in several cells – not just Γ_j. We have, however, that for $|x - x_i| = t_i$ and any k,

$$|x - R_k| + t_i = |x - R_k| + |x - x_i| \geqq |R_k - x_i| \geqq |R_j - x_i|. \quad (4.27)$$

Hence $\delta(x) \geqq |R_j - x_i| - t_i$, and therefore in case (ii),

$$\int \Phi(x) dv_i(x) \geqq \sum_{k=1}^{K} |x_i - R_k|^{-1} - (|R_j - x_i| - t_i)^{-1}. \quad (4.28)$$

Using these inequalities and the definition (4.18) we find that

$$\mathscr{E}_{\Phi,z}(v) \leqq V_c + \sum_{i=1}^{N} W^\lambda(x_i), \tag{4.29}$$

with $W^\lambda(x)$ given in (2.5), (2.6). This, together with Lemma 1, proves Theorem 6. □

V. Simple Localization of the Kinetic Energy

Here we shall prove Theorem 7, but before doing so let us motivate Theorem 7 by stating the analogous Theorem 12 below for p^2 instead of $|p|$. This latter theorem is simple to prove, but we have not seen it in the literature.

Theorem 12 (The energy of p^2 in balls). *Let B be a ball of radius R centered at $z \in \mathbb{R}^3$ and let $f \in L^2(B)$ and $\nabla f \in L^2(B)$. Define*

$$(f, p^2 f)_B = \int_B |\nabla f(x)|^2 dx. \tag{5.1}$$

Then

$$(f, p^2 f)_B \geqq R^{-2} \int_B H((x-z)/R)|f(x)|^2 dx, \tag{5.2}$$

where $H(x)$, for $|x|<1$, is any function of the form $H(x) = -h^{-1}(x)\Delta h(x)$ and where h is a smooth, strictly positive function with vanishing normal derivative on the boundary $|x|=1$. In particular, by taking $h(x) = (|x|^2+t)^{-1/4} \exp[\frac{1}{4}|x|^2/(1+t)]$, and then letting $t \to 0$ (using Fatou's lemma) we have that (5.2) *holds with*

$$H(x) = \tfrac{1}{4}|x|^{-2} - Y_2(|x|), \qquad Y_2(r) = 1 + \tfrac{1}{4}r^2. \tag{5.3}$$

Remark. It is important to note that $\frac{1}{4}$, the coefficient of the $|x|^{-2}$ singularity, is precisely the sharp constant for the uncertainty principle in all of $\mathbb{R}^3$, $(f, p^2 f) \geqq \frac{1}{4}\int |f|^2 |x|^{-2} dx$.

Proof. Write $f(x) = g(x)h(x)$ so that $\nabla f = h\nabla g + g\nabla h$. Then

$$\int_B |\nabla f|^2 = \int_B h^2|\nabla g|^2 + \int_B |g|^2(\nabla h)^2 + \int_B (\nabla g^2)h\nabla h. \tag{5.4}$$

Integrating the last integral by parts

$$\int_B |\nabla f|^2 \geqq -\int_B g^2 h\Delta h = \int_B f^2 H. \tag{5.5}$$

Equation (5.3) is merely a calculation. □

We turn now to the problem of proving Theorem 7 which is the analogue of Theorem 12 for

$$(f, |p| f)_B = (2\pi^2)^{-1} \int_B \int_B |f(x) - f(y)|^2 |x-y|^{-4} dx dy. \tag{5.6}$$

If B is $\mathbb{R}^3$ then this is just $(f, |p| f)$; see (2.9).

Proof of Theorem 7. Without loss of generality we can take $z=0$ and $R=1$. First, we regularize $|x-y|^{-4}$ to $L_t(x,y) = (|x-y|^2+t)^{-2}$. The theorem will follow by letting $t \to 0$ and using dominated convergence and Fatou's lemma.

With L_t in place of $|x-y|^{-4}$ we have

$$(f,|p|f)_{B,t}=\pi^{-2}\int_B |f(x)|^2 K_t(x)dx-\pi^{-2}\int_B\int_B f(x)\bar{f}(y)L_t(x,y)dxdy\,, \tag{5.7}$$

$$K_t(x)=\int_B L_t(x,y)dy\,. \tag{5.8}$$

The second integral in (5.7) can be bounded above using the Schwarz inequality as follows. Choose a real valued function h with $h(x)>0$ for all $|x|\leqq 1$. Then

$$\begin{aligned}\int f\bar{f}L_t&=\int_B\int_B [f(x)h(y)^{1/2}/h(x)^{1/2}][\bar{f}(y)h(x)^{1/2}/h(y)^{1/2}]L_t(x,y)dxdy\\&\leqq \int_B |f(x)|^2\eta_t(x)dx\end{aligned} \tag{5.9}$$

with

$$\eta_t(x)=h(x)^{-1}\int_B L_t(x,y)h(y)dy\,. \tag{5.10}$$

We make the choice that h is radial, i.e. $h(x)=h(r)$ with $r=|x|$. To compute K_t and η_t we can do the angular y integration. With $|y|=s$ we have

$$l_t(r,s)\equiv\int L_t(x,y)d\omega_y=[\pi/rs]\{[(r-s)^2+t]^{-1}-[(r+s)^2+t]^{-1}\}\,. \tag{5.11}$$

Combining (5.7)–(5.11) we have that

$$(f,|p|f)_{B,t}\geqq\int_B |f(x)|^2 Q_t(|x|)dx\,, \tag{5.12}$$

with

$$Q_t(r)=\pi^{-2}\int_0^1 l_t(r,s)[1-h(s)/h(r)]s^2ds\,. \tag{5.13}$$

Finally, we choose

$$h(r)=(1+r^2)/r\,. \tag{5.14}$$

(Note that $dh/dr=0$ at $r=1$.) The integrand in (5.13) is then

$$\pi r^{-1}(1+r^2)^{-1}(s-r)(1-rs)\{[(r-s)^2+t]^{-1}-[(r+s)^2+t]^{-1}\}\,. \tag{5.15}$$

At this point we can let $t\to 0$ by recognizing that the integral in (5.13) becomes a principal value integral in the limit, i.e. $Q_t\to Q$ with

$$Q(r)=4\pi^{-1}(1+r^2)^{-1}⨍(s-r)^{-1}(r+s)^{-2}(s-rs^2)ds\,. \tag{5.16}$$

To do this integral (call it I) we set

$$I_1=⨍_0^1(s-r)^{-1}(r+s)^{-2}sds=[2r(1+r)]^{-1}-(4r)^{-1}\ln[(1+r)/(1-r)]\,. \tag{5.17}$$

The remainder of I (namely the rs^2 term) is

$$-\int_0^1 rs(r+s)^{-2}ds-r^2I_1=-r\ln[(1+r)/r]+r(r+1)^{-1}-r^2I_1\,. \tag{5.18}$$

By combining (5.17), (5.18), Eq. (2.16) is derived. The maximum of $Y_1(r)$ was computed numerically by S. Knabe. □

With the help of Theorems 7 and 12, the proof of Theorem 5, which was stated in Sect. 1, can now be given.

Proof of Theorem 5. Fix $0<L<N$ and $M=N-L$ and consider any partition $P=(\pi_1,\pi_2)$ of $\{1,\dots,N\}$ into two disjoint sets with L integers in π_1 and M integers in π_2. There are $\binom{N}{L}$ such partitions. For each P we define

$$\delta_i(\pi_2)=\min\{|x_i-x_j|\,|\,j\in\pi_2 \quad\text{and}\quad j\neq i \quad\text{if}\quad i\in\pi_2\}. \tag{5.19}$$

First the operator $|p|$ will be considered. Define the N-particle operator

$$h_P=\sum_{i\in\pi_1}|p_i|-\lambda\sum_{i\in\pi_1}\delta_i(\pi_2)^{-1}+\alpha\sum_{i\in\pi_2}\delta_i(\pi_2)^{-1} \tag{5.20}$$

for some λ, $\alpha>0$ to be determined later. Let the N-particle operators H and $\hat{H}$ be given by

$$H=\binom{N}{L}^{-1}\frac{N}{L}\sum_P h_p, \tag{5.21}$$

$$\hat{H}=\sum_{i=1}^{N}|p_i|-C_1q^{-1/3}\sum_{i=1}^{N}\delta_i^{-1}. \tag{5.22}$$

If H and $\hat{H}$ are compared we observe that the $|p_i|$ terms are identical. The potential energy terms are more complicated, but we wish to choose λ and α so that $\hat{H}\geqq H$. To this end, fix $x_1,\dots,x_N$ and let $x_{j(i)}$ be a nearest neighbor of x_i, that is $|x_{j(i)}-x_i|=\min\{|x_k-x_i|\,|k\neq i\}$. It is obvious that $\delta_i(\pi_2)^{-1}\leqq\delta_i^{-1}$, so that the last term in (5.20), when summed on P, is at most $\alpha\tau\sum_1^N\delta_i^{-1}$, where

$$\tau=\binom{N}{L}^{-1}\frac{N}{L}\binom{N-1}{L}=\frac{N-L}{L}. \tag{5.23}$$

To bound the middle, or λ, term in h_P we note that for each $i\in\{1,\dots,N\}$ there will be $\binom{N-2}{L-1}$ partitions in which $i\in\pi_1$ and $j(i)\in\pi_2$. Therefore this middle sum in h_P, when summed on all partitions, is at least $\lambda\nu\sum_1^N\delta_i^{-1}$, where

$$\nu=\binom{N}{L}^{-1}\frac{N}{L}\binom{N-2}{L-1}=\frac{N-L}{N-1}. \tag{5.24}$$

Consequently, $\hat{H}\geqq H$ if

$$C_1q^{-1/3}\leqq(N-L)[\lambda(N-1)^{-1}-\alpha L^{-1}]. \tag{5.25}$$

Assuming (5.25), Theorem 5 will be proved if we show that $(\psi, h_P\psi)\geqq 0$ for every P. Since permutation of the labels in π_1 and π_2 is irrelevant, it suffices to prove this for any one P. To this end we henceforth change notation so that $x_1,\dots,x_L\in\mathbb{R}^3$ are the variables in the π_1 block and $R_1,\dots,R_M\in\mathbb{R}^3$ are the variables in the π_2 block. Obviously we can assume that the R_i are fixed and distinct and that ψ is then a function of $x_1,\dots,x_L$ with q-state Fermi statistics. We shall also drop the subscript P on h_P. Thus, we want to show that $h \geqq 0$ for all choices of the R_i. Since h is a sum of one-body operators, we have to show that for any density matrix γ with $0 \leqq \gamma \leqq q$,

$$\mathrm{Tr}\gamma(|p|-V) \geqq -\alpha \sum_{j=1}^{M} (2D_j)^{-1}, \tag{5.26}$$

where $V(x)$ and D_j are defined by

$$V(x) = -\lambda \delta(x)^{-1}, \tag{5.27}$$

$$2D_j = \min\{|R_j - R_k| \,|\, k=1, \ldots, M \text{ but } k \neq j\}, \tag{5.28}$$

$$\delta(x) = \min\{|x-R_j| \,|\, j=1, \ldots, M\}. \tag{5.29}$$

Under the assumption that $\lambda < 2/\pi$, we write $|p|$ as the sum of two pieces $|p| = (\lambda\pi/2)|p| + (1-\lambda\pi/2)|p|$. We also introduce the Voronoi cells $\Gamma_j = \{x \,|\, |x-R_j| \leqq |x-R_k| \text{ for all } k \neq y\}$ and the balls $B_j \subset \Gamma_j$ defined by $B_j = \{x \in \Gamma_j \,|\, |x-R_j| \leqq D_j\}$. Obviously

$$(f, |p| f) \geqq \sum_{j=1}^{M} (f, |p| f)_{B_j}, \tag{5.30}$$

where the right side is the sum of the kinetic energies in the balls B_j defined in Theorem 7, (2.14). Using Theorem 7, we have that

$$(\lambda\pi/2)(f, |p| f) \geqq (\lambda\pi/2) \sum_{j=1}^{M} D_j^{-1} \int_{B_j} |f(x)|^2 Q(|x-R_j|/D_j) dx, \tag{5.31}$$

with Q given by (2.16). Hence

$$\mathrm{Tr}\gamma(|p|-V) \geqq \mathrm{Tr}\gamma[(1-\lambda\pi/2)|\mathrm{p}| - \lambda W], \tag{5.32}$$

where W is given in each Γ_j by

$$W_j(x) = \begin{cases} |x-R_j|^{-1} & \text{if } |x-R_j| > D_j \\ (\pi/2) D_j^{-1} Y_1(|x-R_j|/D_j) & \text{if } |x-R_j| \leqq D_j \end{cases} \tag{5.33}$$

with Y_1 given in (2.16).

Next, we use the Daubechies bound, Theorem 8,

$$\mathrm{Tr}\gamma[(1-\lambda\pi/2)|p| - \lambda W] \geqq -0.0258 q [1-\lambda\pi/2]^{-3} \lambda^4 \int W(x)^4 dx. \tag{5.34}$$

The integral in (5.34) is a sum of integrals over each Γ_j. To obtain a bound we shall merely integrate each $|x-R_j|$ term in W [see (5.33)] over all $|x-R_j| > D_j$ and omit the restriction that $x \in \Gamma_j$. The integral outside each ball B_j is thus

$$\int_{\sim B_j} W_j^4 = 4\pi/D_j. \tag{5.35}$$

The integral inside B_j is (see (2.27))

$$\int_{B_j} W_j^4 = (\pi/2)^4 D_j^{-1} \int_{|x|<1} Y_1(x)^4 dx = 46.418/D_j. \tag{5.36}$$

Combining (5.34)–(5.36) we find that (5.26) is satisfied provided

$$qA\lambda^4(1-\lambda\pi/2)^{-3} \leqq \tfrac{1}{2}\alpha \tag{5.37}$$

with

$$A=0.0258[4\pi+46.418]=1.522 \tag{5.38}$$

and provided $\lambda<2/\pi$. We shall choose α so that (5.37) is an equality. We shall also write $\lambda=Xq^{-1/3}$. Then (5.25) is satisfied if C_1 satisfies the following for some $0\leqq X\leqq 2/\pi$ and some $0<L<N$:

$$C_1\leqq(N-L)[X(N-1)^{-1}-AX^4(1-X\pi/2)^{-3}L^{-1}]. \tag{5.39}$$

(Here we have used the bound that $\lambda\pi/2<X\pi/2$, which holds since $q\geqq 1$.)

Consider the case $N\geqq 3$. To utilize (5.39) we make the following choices

$$X=1/5 \quad \text{and} \quad L=\{(B/X)^{1/2}N\}, \tag{5.40}$$

where $B\equiv AX^4(1-X\pi/2)^{-3}=0.0075486$ and where $\{a\}$ denotes the smallest integer $\geqq a$. Write $L=l+\varepsilon$ with $l=N(B/X)^{1/2}$ and $0\leqq\varepsilon<1$. We claim that when $N\geqq 3$,

$$(L-1)X/(N-1)+BN/L\leqq lX/N+BN/l. \tag{5.41}$$

Assuming this for the moment, we would then have that (5.39) is satisfied with

$$C_1=(X^{1/2}-B^{1/2})^2\geqq 0.129, \tag{5.42}$$

which proves Theorem 5 when $N\geqq 3$. If $N=1$ there is nothing to prove. If $N=2$, Theorem 3 is trivial because it asserts that

$$|p_1|+|p_2|\geqq 0.129q^{-1/3}|x_1-x_2|^{-1}, \tag{5.43}$$

but we already have the simple bound $|p_1|\geqq(2/\pi)|x_1-x_2|^{-1}$ for all x_2.

To prove (5.41), insert $L=l+\varepsilon$ in the left side and multiply by $N(N-1)Ll$ (recalling that $l\equiv N(B/X)^{1/2}$). Then (5.41) is equivalent to

$$Nl-l(l+2\varepsilon)+N\varepsilon(1-\varepsilon)\geqq 0. \tag{5.44}$$

Since $l<N/5$, (5.44) holds for $N\geqq 3$.

The proof for p^2 in place of $|p|$ follows the same route, but using Theorem 12 in place of Theorem 7 and using the Lieb-Thirring [25] bound in place of the Daubechies bound. This is

$$\mathrm{Tr}\gamma(\mu p^2-\lambda W)\geqq -q\sigma\mu^{-3/2}\lambda^{5/2}\int W(x)^{5/2}dx.$$

The best bound for σ is obtained in [22] and is $\sigma=0.040305$. We split the operator p^2 into $4\lambda p^2+(1-4\lambda)p^2$, and take the μ above to be $(1-4\lambda)$. Using Theorem 12, W is given in each cell Γ_j by

$$W(x)=\begin{cases}|x-R_j|^{-2} & \text{if } |x-R_j|>D_j\\ 4D_j^{-2}Y_2(|x-R_j|/D_j) & \text{if } |x-R_j|<D_j.\end{cases} \tag{5.45}$$

The analogue of (5.35), (5.36) using $Y_2(r)=1+r^2/4$, is

$$w\equiv D_j^2\int_{\mathbb{R}^3}W_j(x)^{5/2}dx=2\pi+128\pi\int_0^1(1+r^2/4)^{5/2}r^2dr.$$

Using $(1+r^2/4)^{1/2}\leqq 1+r^2/8$ in the above integral we find $w<198.2$.

Setting $\lambda = Xq^{-2/3}$, the analogue of (5.39) is

$$C_2 \leqq (N-L)[X(N-1)^{-1} - AX^{5/2}(1-4X)^{-3/2}L^{-1}] \tag{5.46}$$

with $A = \sigma w = 7.988$. For $N \geqq 3$ we make the following choices:

$$X = 1/20 \quad \text{and} \quad L = \{(B/X)^{1/2} N\}, \tag{5.47}$$

with $B = AX^{5/2}(1-4X)^{-3/2} = 0.006241$. Again, setting $L = l + \varepsilon$ with $l = (B/X)^{1/2} N$, we have to verify (5.41), which is equivalent to (5.44). This inequality is true for $N \geqq 4$ since $l = 0.3533N$. With (5.41) satisfied we have that

$$C_2 \geqq (X^{1/2} - B^{1/2})^2 \geqq 0.0209. \tag{5.48}$$

This proves Theorem 3 for $N \geqq 4$. When $N = 1$ there is nothing to prove, while for $N = 2$ we require

$$p_1^2 + p_2^2 \geqq 0.0209 q^{-2/3} |x_1 - x_2|^{-2}. \tag{5.49}$$

Since $p_1^2 \geqq \frac{1}{4}|x_1 - x_2|^{-2}$ for all x_2, inequality (5.49) is satisfied. For $N = 3$ it suffices to have

$$p_1^2 \geqq 0.0209 q^{-2/3} \{|x_1 - x_2|^{-2} + |x_1 - x_3|^{-2}\}, \tag{5.50}$$

and this is clearly true by the inequality just mentioned. □

Remarks. In the above proof, the inequality for p^2 was proved in a fashion analogous to that for $|p|$ by substituting Theorem 12 for Theorem 7. However, another proof for p^2 can be given by using the IMS localization [see (3.3)] instead of Theorem 12.

VI. Refined Localization of the Kinetic Energy

Proof of Theorem 10 (Sect. III). Starting from the Corollary of Theorem 9, we see from (3.10) that our task is to find an upper bound to $\mathrm{Tr}\gamma L$ with $L = L^0 + L_1^*$ and with

$$L(x, y) = \pi^{-2} |x - y|^4 [1 - \chi_0(x)\chi_0(y) - \chi_1(x)\chi_1(y)] \tag{6.1}$$

and

$$L_1^*(x, y) = \begin{cases} L(x, y) B_1(x) B_1(y) & \text{if} \quad |x - y| \leqq \sigma \\ 0 & \text{if} \quad |x - y| > \sigma. \end{cases} \tag{6.2}$$

Recall that B_1 is a ball of radius D_1 centered at the origin. By simple scaling we can, and shall take $D_1 = 1$; we shall also write $B_1 = B$. We have $\chi_1(x) = 0$ unless $|x| \leqq (1 - \sigma)$, i.e. unless $x \in B^{(\sigma)}$.

We first bound $\mathrm{Tr}\gamma L^0$. Notice that when $|x| < |y|$, $L^0(x, y) = 0$ unless $|x| \leqq (1 - \sigma)$. Using the symmetry of L_0 we can write

$$\mathrm{Tr}\gamma L^0 = 2\mathrm{Re} \iiint_{|x| < |y|} \gamma^{1/2}(x, z)\gamma^{1/2}(z, y) L^0(x, y) B^{(\sigma)}(x)\, dx\, dy\, dz, \tag{6.3}$$

where $\gamma^{1/2}$ is the operator square root of γ. We do the y integration first and then apply Minkowski's inequality to the x integration. For any $\varepsilon > 0$,

$$\begin{aligned}\operatorname{Tr}\gamma L^0 \leqq \varepsilon \iint |\gamma^{1/2}(x,z)|^2 B^{(\sigma)}(x)\,dx\,dz \\ + \varepsilon^{-1} \iint \left| \int_{|y|>|x|} \gamma^{1/2}(z,y) L^0(x,y)\,dy \right|^2 B^{(\sigma)}(x)\,dx\,dz\,.\end{aligned} \tag{6.4}$$

The first integral is just

$$\int \gamma(x,x) B^{(\sigma)}(x)\,dx\,. \tag{6.5}$$

In the second integral we do the z integration before the x integration and obtain

$$\iint \gamma(y,y') \left(\int_A L^0(x,y) L^0(x,y')\,dx \right) dy\,dy'\,, \tag{6.6}$$

where A is the region $|x| \leqq \min((1-\sigma), |y|, |y'|)$. The factor in parentheses in (6.6) is the kernel of a positive definite operator, so we can bound (6.6) by

$$\|\gamma\| \iint_A L^0(x,y)^2\,dx\,dy\,, \tag{6.7}$$

where A is the region $|x| \leqq (1-\sigma)$ and $|y| \geqq |x|$. In view of the fact that $L^0(x,y)$ is symmetric and $L^0(x,y) = 0$ unless at least one of $|x|$ or $|y|$ is less than $(1-\sigma)$, and given that $\|\gamma\| = q$ by assumption, (6.7) is just $\frac{1}{2} q \operatorname{Tr}(L^0)^2$. Thus,

$$\operatorname{Tr}\gamma L^0 \leqq \varepsilon \int \gamma(x,x) B^{(\sigma)}(x)\,dx + q\varepsilon^{-1}\Omega_1 \tag{6.8}$$

with $\Omega_1 = \frac{1}{2}\operatorname{Tr}(L^0)^2$. The verification of the two integrals for Ω_1 in (3.15), (3.16) is evident if one recognizes that $\chi_0(x) = 1$ and $\chi_1(x) = 0$ for $|x| \geqq (1-\sigma)$.

Now we turn to $\operatorname{Tr}\gamma L_1^*$. Since γ is a positive operator, its kernel satisfies $|\gamma(x,y)|^2 \leqq \gamma(x,x)\gamma(y,y)$. Hence, since $L_1^*(x,y) > 0$ and $h_1(x) > 0$,

$$\begin{aligned}\operatorname{Tr}\gamma L_1^* &= \iint \gamma(x,y) L_1^*(x,y)\,dx\,dy \\ &\leqq \iint [\gamma(x,x) h_1(y)/h_1(x)]^{1/2} [\gamma(y,y) h_1(x)/h_1(y)]^{1/2} L_1^*(x,y)\,dx\,dy \\ &\leqq \iint [\gamma(x,x) h_1(y)/h_1(x)] L_1^*(x,y)\,dx\,dy \\ &= \int \gamma(x,x)\theta_1(x)\,dx\,.\end{aligned} \tag{6.9}$$

The second inequality in (6.9) is the Schwarz inequality, together with the symmetry in x and y. The idea of using the Schwarz inequality in this fashion goes back to Hardy and Littlewood; see [18] for another application.

When inequalities (6.8) and (6.9) are inserted into (3.10), the Corollary of Theorem 9, the result is Theorem 10. □

VII. Estimates of Negative Eigenvalues

Proof of Theorem 11 (Sect. III). It obviously suffices to consider the case $q = 1$. Let the kernel of γ be

$$\gamma(x,y) = \sum_\alpha \tau_\alpha f_\alpha(x) \overline{f_\alpha(y)} \tag{7.1}$$

with $0 \leqq \tau_\alpha \leqq 1$ and $\sum \tau_\alpha < \infty$ and with the f_α being orthonormal. Let $g_\alpha(x) \equiv \chi(x) f_\alpha(x)$. We want to prove that, with $V(x) = 2/(\pi|x|) + C/R$,

$$E \equiv \sum_\alpha (g_\alpha, (|p| - V) g_\alpha) \geqq -4.4827 (3/4\pi R^3) C^4 R^{-1} \|\chi\|_2^2\,. \tag{7.2}$$

By scaling it clearly suffices to prove the theorem for $R=1$, which we assume henceforth.

It is convenient to use Fourier transforms. Let

$$\varrho(p,q)=\int\int \bar{\chi}(x)\chi(y)\gamma(x,y)\exp(ip\cdot x-iq\cdot y)dxdy. \tag{7.3}$$

Since $\bar{\chi}\gamma\chi$ is positive semidefinite, so is ϱ, and hence

$$|\varrho(p,q)|\leqq\varrho(p,p)^{1/2}\varrho(q,q)^{1/2}\equiv\mu(p)\mu(q) \tag{7.4}$$

with $\mu(p)=\varrho(p,p)^{1/2}$. From (7.3) and the fact that $0\leqq\gamma\leqq 1$ as an operator,

$$\mu(p)^2=(n_p,\gamma n_p)\leqq(n_p,n_p)=\int|\chi(x)|^2dx\equiv M^2, \tag{7.5}$$

where $n_p(x)=\chi(x)\exp(-ip\cdot x)$ and $M=\|\chi\|_2$. Using the Fourier transform of $|x|^{-1}$, namely

$$4\pi|p|^{-2}=\int|x|^{-1}\exp(ip\cdot x)dx, \tag{7.6}$$

E can be written as

$$E=(2\pi)^{-3}\{\int\varrho(p,p)(|p|-C)dp-\pi^{-3}\int\int\varrho(p,q)|p-q|^{-2}dpdq\}. \tag{7.7}$$

Using (7.5) we have that

$$E\geqq(2\pi)^{-3}\inf\{\tilde{E}(\mu)|0\leqq\mu(p)\leqq M \quad \text{for all } p\}, \tag{7.8}$$

where $\tilde{E}(\mu)$ is defined by

$$\tilde{E}(\mu)=\int\mu(p)^2(|p|-C)dp-\pi^{-3}\int\int\mu(p)\mu(q)|p-q|^{-2}dpdq. \tag{7.9}$$

To bound the second integral in (7.9), let

$$h(p)=\begin{cases}A^{-2} & \text{if} \quad |p|\leqq A\\ |p|^{-2} & \text{if} \quad |p|>A,\end{cases} \tag{7.10}$$

where A is some constant to be determined later. Employing the same strategy as in (6.9) we have

$$\begin{aligned}&\int\int\mu(p)\mu(q)|p-q|^{-2}dpdq\\ &=\int\mu(p)(h(q)/h(p))^{1/2}\mu(q)(h(p)/h(q))^{1/2}|p-q|^{-2}dpdq\leqq\int\mu(p)^2t(p)dp,\end{aligned} \tag{7.11}$$

with

$$\begin{aligned}t(p)&=h(p)^{-1}\int|p-q|^{-2}h(q)dq\\ &=h(p)^{-1}\{\int|p-q|^{-2}q^{-2}dq-s(p)\}=h(p)^{-1}\{\pi^3|p|^{-1}-s(p)\},\end{aligned} \tag{7.12}$$

and with

$$s(p)=\int_{|q|<A}|p-q|^{-2}(q^{-2}-A^{-2})dq. \tag{7.13}$$

To calculate $s(p)$ we use bipolar coordinates, i.e. for any functions f and g

$$\int f(|p-q|)g(|q|)d^3q=(2\pi/|p|)\int_0^\infty\beta f(\beta)\left\{\int_{||p|-\beta|}^{|p|+\beta}\alpha g(\alpha)d\alpha\right\}d\beta. \tag{7.14}$$

Thus,

$$s(p)=(2\pi/|p|)\int_0^A(\beta^{-1}-\beta A^{-2})\left\{\int_{||p|-\beta|}^{|p|+\beta}\alpha^{-1}d\alpha\right\}d\beta$$
$$=(2\pi/|p|)\int_0^{1/\xi}(u^{-1}-u\xi^2)\ln\left(\frac{1+u}{|1-u|}\right)du \tag{7.15}$$

with $\xi=|p|/A$.

We claim that

$$s(p)\geqq\tilde{s}(p)\equiv\begin{cases}(8\pi/3)A & \text{for} \quad |p|\geqq A\\ 4\pi|p|^{-1}[\frac{10}{9}+\frac{\pi^2}{8}-2\xi+\frac{1}{6}\xi^2+\frac{5}{36}\xi^3] & \text{for} \quad |p|\leqq A.\end{cases} \tag{7.16}$$

We shall prove (7.16) later. For now, let us insert (7.16) into (7.12), and then into (7.11) and (7.9),

$$\tilde{E}(\mu)\geqq\int_{|p|>A}\mu(p)^2[8A(3\pi^2)^{-1}-C]dp+\int_{|p|<A}\mu(p)^2[|p|-A^2|p|^{-1}$$
$$+\pi^{-3}A^2\tilde{s}(p)-C]dp. \tag{7.17}$$

We choose

$$A=3\pi^2C/8 \tag{7.18}$$

so that the first integral in (7.17) vanishes. Then, using (7.18) and performing the angular integration,

$$\tilde{E}(\mu)\geqq 4\pi A^4\int_0^1\mu(Aw)^2\left\{w+2w^2/3\pi^2+5w^3/9\pi^2\right.$$
$$\left.-\left[\frac{1}{2}-40/(9\pi^2)\right]w^{-1}-32/(3\pi^2)\right\}w^2dw. \tag{7.19}$$

As is easily seen, the factor $\{\ \}$ in (7.19) has its maximum at $w=1$ and it is negative there. Therefore the infimum of the right side of (7.19) over the set $\mu(Aw)\leqq M$ occurs for $\mu(Aw)=M$ for all $0\leqq w\leqq 1$. The right side of (7.19) with $\mu=M$ is

$$-(598/135\pi)A^4M^2. \tag{7.20}$$

Returning to (7.8) and using (7.18) and (7.20) (with 598 replaced by 600) we have that

$$E\geqq-\frac{5}{9}\left(\frac{3\pi}{8}\right)^4C^4M^2. \tag{7.21}$$

Since $M=\|\chi\|_2$, (7.21) is the same as (7.2).

To complete the proof we must bound (7.15) by (7.16). When $u\leqq 1/\xi$, the factor $u^{-1}-u\xi^2\geqq 0$. When $\xi\geqq 1$ (i.e. $|p|\geqq A$), $u\leqq 1$ and we have the bound

$$\ln[(1+u)/(1-u)]\geqq 2u. \tag{7.22}$$

Inserting (7.22) into (7.15) yields the first part of (7.16).

If $|p|\leqq A$, then $\xi<1$. The integral in (7.15) from 0 to 1 can be done explicitly,

$$\int_0^1(u^{-1}-u\xi^2)\ln[(1+u)/(1-u)]du=\pi^2/4-\xi^2. \tag{7.23}$$

To bound the integral from 1 to $1/\xi$, use the fact that for $u>1$,

$$\ln[(1+u)/(u-1)] \geqq 2u^{-1}+\tfrac{2}{3}u^{-3}. \tag{7.24}$$

Then

$$\int_1^{1/\xi}(u^{-1}-u\xi^2)\ln[(1+u)/(u-1)]\,du$$
$$\geqq \int_1^{1/\xi}(u^{-1}-u\xi^2)\left(2u^{-1}+\frac{2}{3}u^{-3}\right)du = 20/9-4\xi+4\xi^2/3+4\xi^3/9. \tag{7.25}$$

When (7.25) is combined with (7.23) (and the $4\xi^3/9$ term is replaced by the smaller quantity $5\xi^3/18$) the result is the second part of (7.16). □

VIII. Some Numerical Calculations

Our goal here is to derive the bounds (3.33) for Ω and (3.34) for $\theta(r)$.

(A) Evaluation of Ω. Ω is defined as the sum of the two integrals in (3.15), (3.16). Recall that $\sigma=0.3$ and $\chi_1(x)=\chi(|x|)$ is given in (3.22) while $\chi_0(x)^2=1-\chi_1(x)^2$. We already set $D_1=1$.

To evaluate $I^{(1)}$ we use the spherical symmetry of χ and first do the angular integration on x and y. This integral is

$$\int |x-y|^{-8}d\omega_y = 2\pi\int_0^{\pi}(x^2+y^2-2xy\cos\theta)^{-4}\sin\theta d\theta$$
$$=(\pi/3)(|x|\,|y|)^{-1}\{(|x|-|y|)^{-6}-(|x|+|y|^{-6})\}. \tag{8.1}$$

Thus,

$$I^{(1)}=4(3\pi^2)^{-1}\int_0^{1-2\sigma}sds\int_{s+\sigma}^{1-\sigma}tdt[(t-s)^{-6}$$
$$-(t+s)^{-6}][1-(1-\chi(s)^2)^{1/2}(1-\chi(t)^2)^{1/2}-\chi(s)\chi(t)]^2. \tag{8.2}$$

(Note that we integrate over $t>s+\sigma$ and $s,t<1-\sigma$, and then multiply by 2. Since $s<t-\sigma$ and $t<1-\sigma$, we have that $s<1-2\sigma$.) This integral is not elementary, but because it is an integral of a continuous, bounded function over a bounded domain in $\mathbb{R}^2$ it can be confidently evaluated on a computer. The result is (3.33).

To evaluate $I^{(2)}$, the angular integration over y is done first as before, with the result (8.1). Then $I^{(2)}$ is the sum of three integrals according as $|x|<1-3\sigma$, $1-3\sigma \leqq |x|<1-2\sigma$, $1-2\sigma \leqq |x| \leqq 1-\sigma$. Thus,

$$I^{(2)}=(4/3\pi^2)\int_0^{1-3\sigma}sds\int_{1-\sigma}^{\infty}tdt[(t-s)^{-6}-(t+s)^{-6}]$$
$$+(16/3\pi^2)\int_{1-3\sigma}^{1-2\sigma}sds\int_{1-\sigma}^{\infty}tdt[(t-s)^{-6}-(t+s)^{-6}]\sin^4\left[\frac{\pi}{8\sigma}(1-\sigma-s)\right]$$
$$+(16/3\pi^2)\int_{1-2\sigma}^{1-\sigma}sds\int_{s+\sigma}^{\infty}tdt[(t-s)^{-6}-(t+s)^{-6}]\sin^4\left[\frac{\pi}{8\sigma}(1-\sigma-s)\right]. \tag{8.3}$$

In each case the t integration can easily be done analytically. This transforms (8.3) into three integrals over the bounded intervals $0 \leqq s < 1-3\sigma$, $1-3\sigma \leqq s < 1-2\sigma$ and $1-2\sigma \leqq s \leqq 1-\sigma$. The integrands are again bounded and continuous so numerical integration can be used. The result is (3.33).

(B) Bound on $\theta(r)$, Eq. (3.34). The function $\theta \equiv \theta_1$ is defined in (3.13) with h defined in (3.24). Again we take $D_1 = 1$. The kernel L_1^* is given in (3.12) with $\chi_1 \equiv \chi$ given in (3.22) and $\chi_0^2 \equiv 1 - \chi^2$.

We want to compute

$$I(r) = \int L_1^*(x, y) h(|y|) dy \tag{8.4}$$

with $r = |x|$. Since the angular integral of $|x-y|^{-4}$ is less than $\pi(rs)^{-1}(r-s)^{-2}$, with $s = |y|$, we have that

$$I(r) \leqq (1/\pi r) \int_0^1 (r-s)^{-2} h(s) m(r,s) s ds, \tag{8.5}$$

where $m(r,s) = m(s,r)$ and, for $r \leqq s$, $m(r,s)$ is given by

$$m(r,s) = \begin{cases} 1 - \cos[\pi(s-\tau)/4\sigma] & \text{for} \quad 0 \leqq r \leqq \tau \leqq s \leqq r + \sigma \\ 1 - \cos[\pi(s-r)/4\sigma] & \text{for} \quad \tau \leqq r \leqq s \leqq \min(\tau + 2\sigma, r + \sigma) \\ 1 - \cos[\pi(2\sigma + \tau - r)/4\sigma] & \text{for} \quad s - \sigma \leqq r \leqq \tau + 2\sigma \leqq s \leqq 1 \\ 0 & \text{otherwise}. \end{cases} \tag{8.6}$$

In (8.6), $\tau = 1 - 3\sigma$.

The arguments of the cosines in (8.6) are all at most $\pi/4$ and one can use the inequality $\cos b \geqq 1 - b^2/2$ for $|b| \leqq \pi/4$. If we use this inequality in (8.6) and then insert the result in (8.5), the integral (8.5) is seen to be elementary but tedious [recall (3.24)]. Finally, $\theta(r) = I(r)/h(r)$.

Let us verify (3.34) when $r \geqq 1 - \sigma$. Then $rh(r) = 1$ and thus

$$\theta(r) = (\pi/32\sigma^2) \int_{r-\sigma}^{1-\sigma} sh(s)(r-s)^{-2}(1-\sigma-s)^2 ds. \tag{8.7}$$

The second line of (3.24) is appropriate for this region. In the region $r - \sigma \leqq s \leqq 1 - \sigma$ the function $(r-s)^{-2}(1-\sigma-s)^2$ is monotone decreasing in s and so has its maximum at $s = r - \sigma$. Thus,

$$\theta(r) \leqq (\pi/32\sigma^2)\sigma^{-2}(1-r)^2 \int_{r-\sigma}^{1-\sigma} \{2 - \sigma(s - 1 + 2\sigma)\} ds, \tag{8.8}$$

and this agrees with (3.34) for $r \geqq 1 - \sigma$.

The verification of the $r \leqq 1 - \sigma$ case of (3.34) is elementary and we omit the details.

IX. The Occurrence of Collapse for Large α

In the previous sections it was shown that the Hamiltonian H_{NK} (1.4) under consideration is stable if α is small enough. There are two parameters in the problem, $z\alpha$ *and* α. For stability of one electron and one nucleus it is necessary and sufficient that $z\alpha \leqq 2/\pi$, but, assuming this condition, there is stability in the many-body case if $\alpha < \alpha_0/q$ with $\alpha_0 > 1/47$. In this section we shall prove that this stability bound is not just an artifact of our proof but that instability definitely occurs if α is too large. Theorems 3 and 4 will be proved here.

Proof of Theorem 3. The method of proof here is the same as the method employed in [23] to prove the instability of one-electron molecules in a magnetic field. Let $\phi \in L^2(\mathbb{R}^3)$ be real with $\|\phi\|_2 = 1$ and let $\tau = (\phi, |p|\phi)$ which is assumed to be finite. Then

$$E = (\phi, H_{NK}\phi) = \tau - z\alpha \int \phi^2(x) \sum_{j=1}^{K} |x - R_j|^{-1} dx + z^2\alpha \sum_{1 \leqq i < j \leqq K} |R_i - R_j|^{-1} . \quad (9.1)$$

With ϕ fixed let us try to position the R_i so as to minimize the right side of (9.1). This minimum (call it e) is less than any average of E over positions of the R_i. In particular, we use $\psi = \prod_{j=1}^{K} \phi(R_j)^2$ as a probability density for such an average. Then

$$Av(E) = \tau - \sigma[z\alpha K - z^2\alpha K(K-1)/2] = \tau + \tfrac{1}{2}\sigma\{z^2\alpha[K - \tfrac{1}{2} - z^{-1}]^2 - \tfrac{1}{4}z^2\alpha - \alpha - z\alpha\}, \quad (9.2)$$

where

$$\sigma = \int \phi(x)^2 \phi(y)^2 |x - y|^{-1} dx dy . \quad (9.3)$$

Now K can be chosen so that $|K - \frac{1}{2} - z^{-1}| \leqq \frac{1}{2}$. Using this K, we have

$$e \leqq Av(E) \leqq \tau - \tfrac{1}{2}\sigma\alpha . \quad (9.4)$$

If we set $\alpha_1 = 2\tau/\sigma$, then when $\alpha > \alpha_1$, $e < 0$, and we can drive e to $-\infty$ simply by dilation, i.e. $\phi(x) \to \lambda^{3/2}\phi(\lambda x)$ and $R_j \to \lambda R_j/\lambda$ with $\lambda \to \infty$.

To obtain a numerical value for α_1, choose $\phi(x) = \pi^{-1/2}\exp(-r)$ with $r = |x|$. The Fourier transforms of ϕ and ϕ^2 are

$$\hat{\phi}(p) = 8\pi^{1/2}(1 + p^2)^{-2} , \qquad \widehat{\phi^2}(p) = 16(4 + p^2)^{-2} . \quad (9.5)$$

Then

$$\tau = (2\pi)^{-3} \int \hat{\phi}(p)^2 |p| dp = 8/3\pi , \qquad \sigma = (2\pi)^{-3} \int \widehat{\phi^2}(p)(4\pi/|p|^2) dp = 5/8 , \quad (9.6)$$

and $2\tau/\sigma = 128/15\pi$. □

Proof of Theorem 4. The method of proof here is similar to that used in [20] to prove that the energy of N nonrelativistic bosons interacting with fixed nuclei via Coulomb forces diverges as $-N^{5/3}$. Again, let $\phi \in L^2(\mathbb{R}^3)$ be real with $\|\phi\|_2 = 1$ and $\tau = (\phi, |p|\phi)$. Since there are q spin states, we can put $N = q$ electrons into the state ϕ. The energy is then

$$E = q\tau - z\alpha q \int \phi^2(x) \sum_{j=1}^{K} |x - R_j|^{-1} dx + z^2\alpha \sum_{1 \leqq i < j \leqq K} |R_i - R_j|^{-1} + \frac{1}{2}q(q-1)\sigma \quad (9.7)$$

with σ given in (9.3). Let us first prove the theorem under the condition $q/z \geqq 1$; at the end of the proof we shall show how to handle the case $q/z < 1$.

To construct ϕ we first define $g \in L^2(\mathbb{R}^3)$ *by*

$$g(x,y,z)=f(x)f(y)f(z), \tag{9.8}$$

where $f \in L^2(\mathbb{R}^1)$ is given by $f(x)=\sqrt{3/2}(1-|x|)$ for $|x| \leqq 1$ and $f(x)=0$ for $|x| \geqq 1$. This f has $\|f\|_2=1$, and thus $\|g\|_2=1$. Let $h \in L^2(\mathbb{R}^3)$ be some other function with compact support and with $(h,|p|h)<\infty$ and $\|h\|_2=1$. Define the integers n and K and the positive number λ by

$$\begin{aligned} n=[(q/z)^{1/3}] \geqq 1, \quad & K=n^3, \\ \lambda=n^3 z/q=Kz/q, & \end{aligned} \tag{9.9}$$

where $[b]$ means integral part of b. Clearly, $1 \geqq \lambda \geqq 1/8$. Finally, we construct a sequence of functions $\phi^{(s)}(x)$, $x \in \mathbb{R}^3$, by

$$\phi^{(s)}(x)^2=\lambda g(x)+(1-\lambda)s^{-3}h(x/s+(0,0,s^2))^2. \tag{9.10}$$

Now choose some fixed locations $R_1, \ldots, R_K$ of K nuclei. Because of the scaling of h by s^{-1} and translation by $(0,0,s^2)$, we have that E converges to the following E' as $s \to \infty$:

$$E'=q\lambda\tau - z\alpha\lambda q \int g^2(x) \sum_{j=1}^{K} |x-R_j|^{-1}dx + z^2\alpha \sum_{1 \leqq i<j \leqq K} |R_i-R_j|^{-1} + \frac{1}{2}\lambda^2 q(q-1)\sigma\alpha, \tag{9.11}$$

where τ now means $(g,|p|g)$ and σ is given in (9.3) with g in place of ϕ.

We claim that it is possible to choose the locations $R_1, \ldots, R_K$ so that

$$\sum_{1 \leqq i<j \leqq K} |R_i-R_j|^{-1} - K\int g^2(x) \sum_{j=1}^{K} |x-R_j|^{-1}dx + \frac{1}{2}K^2\sigma \leqq -K^{4/3}/6. \tag{9.12}$$

If (9.12) holds then, recalling (9.9),

$$E' \leqq q\lambda\tau - \tfrac{1}{6}z^2\alpha(\lambda q/z)^{4/3}. \tag{9.13}$$

Recalling that $\lambda > 1/8$ we have that $E'<0$ whenever

$$\beta^2\alpha q \geqq 8(6\tau)^3(\pi/2)^2. \tag{9.14}$$

We also have that $\tau=(g,|p|g) \leqq (g,p^2 g)^{1/2}=3$ (by the Schwarz inequality). Thus, collapse occurs if $\alpha \geqq \alpha_2 q^{-1}\beta^{-2}$ with $\alpha_2=(\pi/2)^2 8(18)^3=115,120$, provided $q/z \geqq 1$.

If, on the other hand, $q/z<1$ and if $\alpha>\alpha_2 q^{-1}\beta^{-2}=\alpha_2 q^{-1}z^{-2}\alpha^{-2}(2/\pi)^2$, we have that $(\pi/2)^2(z\alpha)^3>\alpha_2 z/q>\alpha_2$. Since $\alpha_2 \gg (2/\pi)^5$, we are in the situation that $z\alpha>2/\pi$, which certainly entails collapse. Therefore, the theorem is proved for all ratios q/z with the α, given above.

There remains to prove (9.12). Choose $n-1$ numbers $\beta_1, \ldots, \beta_{n-1}$ satisfying $-1 \equiv \beta_0<\beta_1<\ldots<\beta_{n-1}<\beta_n \equiv 1$ such that

$$\int_{\beta_j}^{\beta_{j+1}} f(x)^2 dx = 1/n \quad \text{for all } j.$$

Let L_j be the interval $[\beta_{j-1}, \beta_j]$ in $\mathbb{R}^1$ and, with m denoting a triplet (i,j,k), let $\Gamma(m) \subset \mathbb{R}^3$ be the rectangular parallelepiped $L_i \times L_j \times L_k$. Then, for each m,

$$\int_{\Gamma(m)} g^2(x)dx = 1/n^3 = 1/K. \tag{9.15}$$

There are n^3 of these parallelepipeds. To prove (9.12) we shall place one of the R_i's in each $\Gamma(m)$ and average its location with respect to the density $g^2(x)$ restricted to $\Gamma(m)$. If the average satisfies (9.12) then there is surely some choice of the R_i's that satisfies (9.12). Apart from a self energy contribution from each parallelepiped, the average of the left side of (9.12) is zero. Thus the average of the left side is given by the self energy terms

$$W = -\frac{1}{2} n^6 \sum_m \int_{\Gamma(m)} \int_{\times \Gamma(m)} g(x)^2 g(y)^2 |x-y|^{-1} dx dy . \tag{9.16}$$

Each integral is the self energy of a charge density g^2 in $\Gamma(m)$. However $\Gamma(m)$ lies inside a ball $B(m)$ of radius $r(m) = (s^2+t^2+u^2)^{1/2}$, where $2s$, $2t$, and $2u$ are the lengths of $\Gamma(m)$, namely $(\beta_i - \beta_{i-1})$, $(\beta_j - \beta_{j-1})$, $(\beta_k - \beta_{k-1})$. The self energy is greater than the *minimum* self energy of a charge $1/K$ distributed in $B(m)$; the minimum occurs for a uniform charge distribution on the boundary of $B(m)$ and is $r(m)^{-1}/K^2$. Thus,

$$W \leqq -\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} (s^2+t^2+u^2)^{-1/2} . \tag{9.17}$$

Now $(s^2+t^2+u^2)^{-1/2} > (s+t+u)^{-1}$. Substituting this latter expression in (9.17) and then using the convexity of the function $(s,t,u) \to (s+t+u)^{-1}$ and recalling that $K = n^3$, we have that

$$W \geqq -\tfrac{1}{2} K (a+b+c)^{-1} , \tag{9.18}$$

where a, b, and c are the averages of s, t, and u. But $a=b=c=1/n$, and thus (9.12) is proved. □

Acknowledgements. The authors thank Michael Loss for helpful discussions and comments and they thank Stefan Knabe for performing numerical calculations.

References

1. Baxter, J.R.: Inequalities for potentials of particle systems. Ill. J. Math. **24**, 645–652 (1980)
2. Chandrasekhar, S.: Phil. Mag. **11**, 592 (1931); Astro. J. **74**, 81 (1931); Monthly Notices Roy. Astron. Soc. **91**, 456 (1931); Rev. Mod. Phys. **56**, 137 (1984)
3. Conlon, J.G.: The ground state energy of a classical gas. Commun. Math. Phys. **94**, 439–458 (1984)
4. Conlon, J.G., Lieb, E.H., Yau, H.-T.: The $N^{7/5}$ law for charged bosons. Commun. Math. Phys. **116**, 417–448 (1988)
5. Cycon, H.L., Froese, R.G., Kirsch, W., Simon, B.: Schrödinger operators. Berlin, Heidelberg, New York: Springer 1987
6. Daubechies, I.: An uncertainty principle for fermions with generalized kinetic energy. Commun. Math. Phys. **90**, 511–520 (1983)
7. Daubechies, I.: One electron molecules with relativistic kinetic energy: properties of the discrete spectrum. Commun. Math. Phys. **94**, 523–535 (1984)
8. Daubechies, I., Lieb, E.H.: One-electron relativistic molecules with Coulomb interaction. Commun. Math. Phys. **90**, 497–510 (1983)
9. Dyson, F.J.: Ground state energy of a finite system of charged particles. J. Math. Phys. **8**, 1538–1545 (1967)

10. Dyson, F.J., Lenard, A.: Stability of matter I and II. J. Math. Phys. **8**, 423–434 (1967); ibid **9**, 698–711 (1968). See also Lenard's Battelle lecture. In: Lecture Notes in Physics, vol. 23. Berlin, Heidelberg, New York: Springer 1973
11. Erdelyi, A., Magnus, W., Oberhettinger, F., Tricomi, F.G.: Tables of integral transforms, Vol. 1. New York, Toronto, London: McGraw-Hill 1954, p. 75, 2.4 (35)
12. Federbush, P.: A new approach to the stability of matter problem. II. J. Math. Phys. **16**, 706–709 (1975)
13. Fefferman, C.: The N-body problem in quantum mechanics. Commun. Pure Appl. Math. Suppl. **39**, S67–S109 (1986)
14. Fefferman, C., de la Llave, R.: Relativistic stability of matter. I. Rev. Math. Iberoamericana **2**, 119–215 (1986)
15. Fröhlich, J., Lieb, E.H., Loss, M.: Stability of Coulomb systems with magnetic fields. I. The one-electron atom. Commun. Math. Phys. **104**, 251–270 (1986)
16. Herbst, I.: Spectral theory of the operator $(p^2+m^2)^{1/2}-ze^2/r$. Commun. Math. Phys. **53**, 285–294 (1977); Errata ibid **55**, 316 (1977)
17. Kato, T.: Perturbation theory for linear operators. Berlin, Heidelberg, New York: Springer 1966. See remark 5.12, p. 307
18. Kovalenko, V., Perelmuter, M., Semenov, Ya.: Schrödinger operators with $L_w^{l/2}(\mathbb{R}^l)$ potentials. J. Math. Phys. **22**, 1033–1044 (1981)
19. Lieb, E.H.: Stability of matter. Rev. Mod. Phys. **48**, 553–569 (1976)
20. Lieb, E.H.: The $N^{5/3}$ law for bosons. Phys. Lett. **70**A, 71–73 (1979)
21. Lieb, E.H.: Density functionals for Coulomb systems. Int. J. Quant. Chem. **24**, 243–277 (1983)
22. Lieb, E.H.: On characteristic exponents in turbulence. Commun. Math. Phys. **92**, 473–480 (1984)
23. Lieb, E.H., Loss, M.: Stability of Coulomb systems with magnetic fields. II. The many electron atom and the one electron molecule. Commun. Math. Phys. **104**, 271–282 (1986)
24. Lieb, E., Simon, B.: Thomas Fermi theory of atoms, molecules and solids. Adv. Math. **23**, 22–116 (1977)
25. Lieb, E.H., Thirring, W.: Bound for the kinetic energy of fermions which proves the stability of matter. Phys. Rev. Lett. **35**, 687–689 (1975). Errata, ibid **35**, 1116 (1975); see also their article: Inequalities for the moments of the eigenvalues of the Schrödinger Hamiltonian and their relation to Sobolev inequalities. In: Studies in Mathematical Physics, Essays in honor of Valentine Bargmann. Lieb, E.H., Simon, B., Wightman, A.S. (eds.). Princeton, NJ: Princeton University Press 1976
26. Lieb, E.H., Thirring, W.: Gravitational collapse in quantum mechanics with relativistic kinetic energy. Ann. Phys. (NY) **155**, 494–512 (1984)
27. Lieb, E.H., Yau, H.-T.: The Chandrasekhar theory of stellar collapse as the limit of quantum mechanics. Commun. Math. Phys. **112**, 147–174 (1987). See also Lieb, E.H. and Yau, H.-T.: A rigorous examination of the Chandrasekhar theory of stellar collapse. Astro. J. **323**, 140–144 (1987)
28. Loss, M., Yau, H.-T.: Stability of Coulomb systems with magnetic fields. III. Zero energy bound states of the Pauli operator. Commun. Math. Phys. **104**, 283–290 (1986)
29. Weder, R.: Spectral analysis of pseudodifferential operators. J. Funct. Anal. **20**, 319–337 (1975)

Communicated by A. Jaffe

Received May 12, 1988