PHYSICAL REVIEW LETTERS

VOLUME 35 15 SEPTEMBER 1975 NUMBER 11

Bound for the Kinetic Energy of Fermions Which Proves the Stability of Matter

Elliott H. Lieb*
Departments of Mathematics and Physics, Princeton University, Princeton, New Jersey 08540

and

Walter E. Thirring
Institut für Theoretische Physik der Universität Wien, A-1090 Wien, Austria

(Received 8 July 1975)

We first prove that $\sum|e(V)|$, the sum of the negative energies of a single particle in a potential V, is bounded above by $(4/15\pi)\int|V|^{5/2}$. This, in turn, implies a lower bound for the kinetic energy of N fermions of the form $\frac{3}{5}(3\pi/4)^{2/3}\int\rho^{5/3}$, where $\rho(x)$ is the one-particle density. From this, using the no-binding theorem of Thomas-Fermi theory, we present a short proof of the stability of matter with a reasonable constant for the bound.

The basis of all theories of bulk matter is the stability theorem of the N-electron Hamiltonian,[1]

$$H_N=\sum_{i=1}^{N}p_i^2-\sum_{i=1}^{N}\sum_{k=1}^{M}Z_k|x_i-R_k|^{-1}+\sum_{i>j}|x_i-x_j|^{-1}+\sum_{k>m}\frac{Z_kZ_m}{|R_k-R_m|}\geq AN. \tag{1}$$

Equation (1) has been proved by Dyson and Lenard.[2] Unfortunately, their analysis is complicated and their constant A gigantic, about 10^{14}. Despite subsequent improvements,[3-5] a simple proof yielding a reasonable constant A has not yet been found. In this note we propose to fill this gap.

We start with the observation that if Thomas-Fermi (TF) theory were valid, then the no-binding theorem[6] would yield the desired result because the TF energy is proportional to the number of atoms. Our goal will be to show that the TF energy, with suitably modified constants, is a lower bound to H_N. To show this, we have to demonstrate two things: (i) The TF approximation for the N-fermion kinetic energy, $K\int\rho^{5/3}$, is a lower bound for some $K>0$; (ii) the TF approximation for the electron repulsion, $\iint\rho(x)\rho(y)|x-y|^{-1}d^3x\,d^3y$, can be converted into a bound by a further change of constants. The following is a sketch of our proof. Fine points of rigor, together with some variations of the inequalities given here, will be presented elsewhere.

(i) *Kinetic energy of N fermions.*—Consider the Schrödinger equation for one particle in a potential $V(x)$. Schwinger[7] has derived an upper bound for $N_E(V)$, the number of energy levels with energies $\geq E$. For $\alpha>0$, and with $|f(x)|_-\equiv -f(x)$ for $f<0$ and 0 otherwise,

$$N_{-\alpha}(V)\leq N_{-\alpha/2}(|V+\alpha/2|_-)\leq(4\pi)^{-2}\int d^3x\,d^3y\,|V(x)+\alpha/2|_-|x-y|^{-2}\exp[-(2\alpha)^{1/2}|x-y|]|V(y)+\alpha/2|_-$$
$$\leq(4\pi)^{-1}(2\alpha)^{-1/2}\int d^3x\,|V(x)+\alpha/2|_-^{\,2}. \tag{2}$$

The last inequality is Young's. Consequently, the sum of the negative energy eigenvalues of p^2+V is bounded by

$$\sum_j |e_j(V)| = \int_0^\infty N_{-\alpha}(V)\,d\alpha \leq (8\pi)^{-1}2^{1/2}\int d^3x \int_0^{2|V(x)|_-} d\alpha\,\alpha^{-1/2}[V(x)+\alpha/2]^2 = (4/15\pi)\int d^3x\,|V(x)|_-^{5/2} \tag{3}$$

By comparison, the classical value is

$$(2\pi)^{-3}\int d^3x \int d^3p\,|p^2+V(x)|_- = (15\pi^2)^{-1}\int d^3x\,|V(x)|_-^{5/2}. \tag{4}$$

We conjecture that (4) is actually a bound. In one dimension an analog of (3) holds with $\int |V|_-^{3/2}$, but we have a counterexample that shows that the classical value is not a bound.

Now let ψ be any N-particle normalized antisymmetric wave function of space-spin. Define

$$\rho_\pm(x) = N\int d^3x_2 \cdots d^3x_N \sum_{\sigma_2,\ldots,\sigma_N} |\psi(x,x_2,\ldots,x_N;\pm,\sigma_2,\ldots,\sigma_N)|^2, \tag{5}$$

$$T = \langle\psi| -\sum_{i=1}^N \Delta_i |\psi\rangle, \tag{6}$$

$$K = T\left(\int\rho_+^{5/3} + \int\rho_-^{5/3}\right)^{-1} > 0, \tag{7}$$

and $\pi_\pm$ are projections onto the single-particle spin states. Let $h_i = p_i^2 - (5K/3)[\rho_+^{2/3}(x_i)\pi_{i+} + \rho_-^{2/3}(x_i)\times\pi_{i-}]$ be a single-particle Hamiltonian and

$$H = \sum_{i=1}^N h_i.$$

If E_0 is the fermion ground-state energy of H then $E_0 \leq \langle\psi|H|\psi\rangle = T - (5K/3)(\int\rho_+^{5/3} + \int\rho_-^{5/3})$. On the other hand, E_0 is greater than or equal to the sum of all the negative eigenvalues of $p^2 - (5K/3)\rho_\pm^{2/3}$ together. By (3), $E_0 \geq -(4/15\pi)(5K/3)^{5/2}(\int\rho_+^{5/3} + \int\rho_-^{5/3})$. Combining these two inequalities[8,9] yields

$$K \geq \tfrac{3}{5}(3\pi/2)^{2/3}. \tag{8}$$

With

$$\rho(x) = \rho_+(x) + \rho_-(x), \tag{9}$$

and using the convexity of $\int\rho^{5/3}$, we obtain a weakened version of (8):

$$T \geq \tfrac{3}{5}(3\pi/4)^{2/3}\int\rho(x)^{5/3}d^3x. \tag{10}$$

If (4) were a bound, then the TF constant, $\frac{3}{5}(3\pi^2)^{2/3}$, could be used in (10).

(ii) *Electron repulsion.*—In this paper we shall use TF theory twice; the first use is to derive a theorem about electrostatics. The TF energy functional with $\gamma > 0$ and positive charges Z_k at locations R_k is

$$\mathcal{E}_\gamma(\rho) = (3/5\gamma)\int\rho^{5/3} - \sum_{k=1}^M \int d^3x\,\rho(x)|x-R_k|^{-1}Z_k + \tfrac{1}{2}\iint\rho(x)\rho(y)|x-y|^{-1}d^3x\,d^3y + \sum_{j<k} Z_jZ_k|R_j-R_k|^{-1}. \tag{11}$$

For any R_j, the minimum of $\mathcal{E}_\gamma(\rho)$ occurs when $\int\rho = \sum_j Z_j$ ($j=1$ to M), and this in turn has a minimum when the R_j are infinitely separated (no-binding theorem[6]). Thus

$$\mathcal{E}_\gamma(\rho) \geq -3.68\gamma\sum_{j=1}^M Z_j^{7/3}, \tag{12}$$

since a neutral atom of charge Z has an energy $-3.68\gamma Z^{7/3}$ in TF theory.

Consider (11) with R_j being the *electron* coordinates, x_j, $Z_j = 1$, $M = N$, and ρ given by (5) and (9). Multiply (11) by $|\psi|^2$ and integrate, and then use (12). Thus, for all $\gamma > 0$,

$$\langle\psi|\sum_{i<j}|x_i - x_j|^{-1}|\psi\rangle \geq \tfrac{1}{2}\iint\rho(x)\rho(y)|x-y|^{-1}d^3x\,d^3y - (3/5\gamma)\int d^3x\,\rho(x)^{5/3} - 3.68N. \tag{13}$$

Therefore we have an electrostatic theorem that the TF estimate for the electron repulsion [the first term on the right-hand side of (13)] is a lower bound provided one makes a kinetic energy correction and subtracts an energy proportional to the electron number.

(iii) *Stability of matter.*—Combining (10) and (13), with $\gamma > (4/3\pi)^{2/3}$ and R_k being the *nuclear* coordinates, yields

$$\langle\psi|H_N|\psi\rangle \geq \mathcal{E}_\delta(\rho) - 3.68\,N\gamma, \tag{14}$$

with $1/\delta = (3\pi/4)^{2/3} - 1/\gamma$ and ρ given by (5) and (9). A lower bound is obtained by minimizing $\mathcal{E}_\delta$ over all ρ such that $\int\rho = N$. For simplicity we shall only use the absolute minimum of $\mathcal{E}_\delta$. By (12)

$$\langle\psi|H_N|\psi\rangle \geq -3.68(N\gamma + \delta\sum_{j=1}^{M} Z_j^{7/3})^2. \qquad (15)$$

Optimizing (15) with respect to γ yields

$$\langle\psi|H_N|\psi\rangle \geq -2.08\, N\left[1+\left(\sum_{j=1}^{M}\frac{Z_j^{7/3}}{N}\right)^{1/2}\right]^2. \qquad (16)$$

Remarks.—(1) If the fermions are of q species (instead of 2 as in the electron case), then the right-hand side of (10) would acquire a factor $(2/q)^{2/3}$ and the right-hand side of (16) a factor $(q/2)^{2/3}$.

(2) If all $Z_j = Z$, our result (16) gives a $Z^{7/3}$ dependence instead of the known Z^2 bound.[3] If $MZ \leq N$ then $MZ^{7/3}/N \leq Z^{4/3}$, which is an improvement over Ref. 3. If $MZ > N$ then we have to use the $\int\rho = N$ condition in (14). The TF no-binding theorem also holds in the subneutral case. By convexity of the TF energy in $\int\rho$, the minimum occurs for M atoms with equal electron charge N/M. If $MZ \gg N$ the energy per atom is proportional to $(N/M)^{1/3}Z^2$. Then $\langle\psi|H_N|\psi\rangle$ is bounded below by $-aN - bZ^2M^{2/3}N^{1/3}$. While this has the correct Z dependence, it has the wrong M dependence[3]; $M^{2/3}$ should be replaced by $N^{2/3}$. This difficulty is inherent in TF theory. What one needs is a simple proof that if $MZ \gg N$, then one can remove most of the surplus nuclei without affecting the energy. Even for $N = 1$ this is not a simple problem. Nevertheless, our present bound is proportional to the *total* particle number, and this is sufficient for proving the existence of the thermodynamic limit.[10]

We thank J. F. Barnes and A. Martin for helpful correspondence and discussions. E. L. thanks the Institut für Theoretische Physik, Universität Wien, for its kind hospitality.

*Work supported by the U. S. National Science Foundation under Grant No. MPS 71-03375-A03 at the Massachusetts Institute of Technology.

[1]The notation is $\hbar = e = 2m = 1$; x_i and p_i are electron variables; R_k and $Z_k > 0$ are nuclear coordinates and charges ($\frac{1}{4} = 1$ Ry).

[2]F. J. Dyson and A. Lenard, J. Math. Phys. (N.Y.) 8, 423 (1967); A. Lenard and F. J. Dyson, J. Math. Phys. (N.Y.) 9, 698 (1968).

[3]A. Lenard, in *Statistical Mechanics and Mathematical Problems*, edited by A. Lenard (Springer, Berlin, 1973).

[4]P. Federbush, J. Math. Phys. (N.Y.) 16, 347, 706 (1975).

[5]J. P. Eckmann, "Sur la Stabilité de Matière" (to be published).

[6]E. Teller, Rev. Mod. Phys. 34, 627 (1962). A rigorous proof of this theorem is given by E. Lieb and B. Simon, "Thomas-Fermi Theory of Atoms, Molecules, and Solids" (to be published). See also E. Lieb and B. Simon, Phys. Rev. Lett. 31, 681 (1973).

[7]J. Schwinger, Proc. Nat. Acad. Sci. 47, 122 (1961).

[8]The connection between $N_E(V)$ and a bound on the kinetic energy was noted by A. Martin (private communication). One can show that the converse holds; i.e., an improvement in (8) implies an improvement in (3).

[9]By numerically solving the three-dimensional variational equation for K, Eq. (7), when $N = 1$, J. F. Barnes has shown that (8) holds with the TF constant $\frac{3}{5}(6\pi^2)^{2/3}$ when $N = 1$ (private communication).

[10]J. L. Lebowitz and E. H. Lieb, Phys. Rev. Lett. 22, 631 (1969); E. H. Lieb and J. Lebowitz, Adv. Math. 9, 316 (1972).

Simple Model for $1/f$ Noise*

Michael B. Weissman

Department of Physics, University of California, San Diego, La Jolla, California 92037

(Received 2 June 1975)

The noise produced by thermodynamic fluctuations (e.g., in carrier number) is shown to diverge for ideal contact (spreading) resistors. For diffusion-controlled fluctuations the frequency spectrum is shown to be proportional to ω^{-1} (i.e., $1/f$) for high frequencies. This behavior is shown to be approached by resistors whose surfaces have sharp corners. The relation to observed noise is briefly discussed.

Noise power proportional to the square of the applied voltage (V) with a frequency spectrum $S(\omega) \propto \omega^{-1}$ over a wide range of ω has been observed in a variety of electrical devices.[1,2] Several models for this noise, invoking either complicated processes (e.g., hydromagnetic turbulence[3]) or purely mathematical constructs (e.g., correlated pulses[4]), have not given successful