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A NEW PROOF OF THE CWIKEL-LIEB-ROSENBLJUM BOUND

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1. Introduction. Consider the operator $-\Delta + V$ acting on $L^2(\mathbf{R}^3)$, where $V(x)$ is a potential in $L^{3/2}(\mathbf{R}^3)$. Let $N(V)$ be the dimension of the spectral projection of $-\Delta + V$ on $(-\infty, 0]$. Then it is known **[1, 5, 8]** that

$$(1.1) \qquad N(V) \leqq C\int_{\mathbf{R}^3} |V_{-}(x)|^{3/3}\, dx,$$

which C is a constant and V_{-} denotes the negative part of V. The inequality (1.1) was derived in three quite different ways by Lieb **[5]**, Cwikel **[1]** and Rosenbljum **[8]**. The best value for the constant C was obtained by Lieb **[5]** and is $C = .116$. Attempts have been made to obtain the best constant C but the results are rather inconclusive **[3]**. However, it is known **[5]** that $C \geqq .0780$.

Here we obtain a new derivation of (1.1) with constant $C = .168$. Our approach is adapted from Lieb's method **[6, 7]** to show that Dirac's semi-classical formula for exchange energy **[2]** bounds the quantum exchange energy. In fact we merely paraphrase the arguments of **[7]** so that (1.1) may be regarded as a corollary of the exchange energy bound.

Another new proof of (1.1) has also recently been given by Li and Yau **[4]**. It is quite different from the one presented here as well as the three previous derivations. Despite the claim in **[4]** the constant obtained there is three times worse than Lieb's value of .116.

We turn to our proof of (1.1). As is standard in all approaches to this problem, we consider a different problem, which is equivalent by the Birman-Schwinger principle **[9]**. Thus we assume $V(x) \leqq 0$, for all $x \in \mathbf{R}^3$, and put $V(x) = -W(x)^2$, where $W(x) \geqq 0$ for $x \in \mathbf{R}^3$. We consider the operator A on $L^2(\mathbf{R}^3)$ with integral kernel

$$(1.2) \qquad a(x, y) = W(x)W(y)\,[4\pi|x - y|]^{-1}.$$

Since $W \in L^3(\mathbf{R}^3)$ with norm $\|W\|_3$ it follows that A is a positive Hilbert-Schmidt operator and thus has discrete spectrum $\mu_1 \geqq \mu_2 \geqq \cdots \geqq 0$. Then to prove (1.1) we need to show that for any $\lambda > 0$,

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$$\#\{\mu_i \geqq \lambda^{-1}: i = 1, 2, \cdots\} \leqq C\lambda^{3/2}\,\|W\|_3^3. \tag{1.3}$$

The inequality (1.3) is a consequence of the following theorem of Cwikel [1], which we intend to derive.

THEOREM.

$$\sum_{i=1}^{N} \mu_i \leqq C^{2/3}N^{1/3}\,\|W\|_3^2.$$

2. Proof of theorem. Let $\psi_i(x)$, $1 \leqq i \leqq N$, be an orthonormal set of functions in $L^2(\mathbf{R}^3)$ and $K(x, y)$ be the density matrix

$$K(x, y) = \sum_{i=1}^{N} \psi_i(x)\,\overline{\psi_i(y)}, \tag{2.1}$$

and $\rho(x)$ be the one body density

$$\rho(x) = K(x, x) \tag{2.2}$$

Let $g: \mathbf{R}^3 \to \mathbf{R}$ be a continuous nonnegative spherically symmetric function with support in the unit ball and L^1 norm equal to 1. We define a function $\mu: \mathbf{R}^3 \times \mathbf{R}^3 \to \mathbf{R}$ by

$$\mu(x, z) = h(z)g[h(z)^{1/3}(x - z)], \tag{2.3}$$

where $h: \mathbf{R}^3 \to \mathbf{R}$ is a positive function to be determined later.

Now, putting

$$f(x) = W(x)K(x, z) - W(z)\mu(x, z), \tag{2.4}$$

we expand out the inequality

$$\int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{f(x)\,\overline{f(y)}}{|x - y|}\,dx\,dy \geqq 0, \tag{2.5}$$

to obtain

$$\begin{aligned} &\iint \frac{W(x)W(y)K(x, z)K(z, y)}{|x - y|}\,dx\,dy \\ &- 2\,\mathrm{Re}\int W(x)K(x, z)W(z)\int \frac{\mu(y, z)}{|x - y|}\,dy\,dx \\ &+ \iint \frac{W(z)^2\mu(x, z)\mu(y, z)}{|x - y|}\,dx\,dy \geqq 0. \end{aligned} \tag{2.6}$$

Observe that the last integral on the left in (2.6) may be written as

$$\alpha W(z)^2 h(z)^{1/3}, \tag{2.7}$$

with

$$\alpha = \iint \frac{g(x)g(y)}{|x-y|}\,dx\,dy. \tag{2.8}$$

Next we integrate (2.6) with respect to z. Using the fact that

$$\int K(x,z)K(z,y)\,dz = K(x,y), \tag{2.9}$$

we obtain the inequality

$$\begin{aligned} &\iint \frac{W(x)W(y)K(x,y)}{|x-y|}\,dx\,dy \\ &\leqq \alpha \int W(z)^2 h(z)^{1/3}\,dz \\ &\quad + 2\,\mathrm{Re} \iint W(x)K(x,z)W(z)\left[\frac{1}{|x-z|} - \int \frac{\mu(y,z)}{|x-y|}\,dy\right] dx\,dz. \end{aligned} \tag{2.10}$$

We define a function $\xi\colon \mathbf{R}^3 \to \mathbf{R}$ by

$$\xi(v) = \frac{1}{|v|} - \int \frac{g(w)}{|v-w|}\,dw. \tag{2.11}$$

In view of the conditions on g it follows from Newton's theorem that ξ is spherically symmetric and decreases radially to zero with $\xi(v) = 0$ in $|v| \geqq 1$. It is easy to see that the function in square brackets in (2.10) may be written as

$$h(z)^{1/3}\xi[h(z)^{1/3}(x-z)]. \tag{2.12}$$

Thus from (1.2), (2.10) and (2.12) we obtain the basic inequality

$$\begin{aligned} 4\pi \sum_{i=1}^{N} \mu_i &\leqq \alpha \int W(z)^2 h(z)^{1/3}\,dz \\ &\quad + 2 \iint W(x)W(z)\rho(x)^{1/2}\rho(z)^{1/2}h(z)^{1/3}\xi[h(z)^{1/3}(x-z)]\,dx\,dz. \end{aligned} \tag{2.13}$$

Here we have chosen the functions $\psi_i(x)$ in (2.1) to be the first N eigenfunctions of the operator A defined by (1.2).

Next we make an appropriate choice for the function $h(z)$ by putting

$$h(z) = W(z)^{6/5}\rho(z)^{3/5}. \tag{2.14}$$

The first integral in (2.13) thus becomes

$$\int W(z)^{12/5}\rho(z)^{1/5}\,dz, \tag{2.15}$$

while the second integral may be written as

$$2\iint h(x)^{5/6}h(z)^{7/6}\xi[h(z)^{1/3}(x-z)]\,dx\,dz. \tag{2.16}$$

Using the fact that

$$\int \rho(z)dz = N, \tag{2.17}$$

and Holder's inequality, we conclude that the integral (2.15) is bounded by

$$N^{1/5}\,\|W\|_3^{12/5}. \tag{2.18}$$

We can bound (2.16) by making use of the Hardy-Littlewood maximal function [6, 10]. First note that $h(x)$ is integrable with

$$\|h\|_1 \leqq N^{3/5}\|W\|_3^{6/5}. \tag{2.19}$$

Let $M(x)$ be the maximal function corresponding to $h(x)^{5/6}$. Since $h(x)^{5/6}$ is in $L^{6/5}$, it follows [10] that $M(x) \in L^{6/5}$ and

$$\|M\|_{6/5} \leqq k\|h\|_1^{5/6}, \tag{2.20}$$

where k is a universal constant. Furthermore, for arbitrary $z \in \mathbf{R}^3$, we have [10]

$$\int h(x)^{5/6}h(z)\xi[h(z)^{1/3}(x-z)]\,dx \leqq \|\xi\|_1 M(z). \tag{2.21}$$

Thus (2.16) is bounded by

$$2\,\|\xi\|_1\int h(z)^{1/6}M(z)dz, \tag{2.22}$$

which by Holder's inequality and (2.20), is bounded by

$$2k\|\xi\|_1\|h\|_1 \leqq 2k\|\xi\|_1 N^{3/5}\|W\|_3^{6/5}. \tag{2.23}$$

Putting (2.18) and (2.23) together we conclude from (2.13) that

$$4\pi\sum_{i=1}^{N}\mu_i \leqq \alpha N^{1/5}\|W\|_3^{12/5} + 2k\|\xi\|_1 N^{3/5}\|W\|_3^{6/5}. \tag{2.24}$$

If we go through our argument again replacing $W(x)$ by $\gamma\,W(x)$ where $\gamma > 0$ is an arbitrary parameter, then we evidently obtain

$$4\pi\sum_{i=1}^{N}\mu_i \leqq \gamma^{2/5}\alpha N^{1/5}\|W\|_3^{12/5} + 2\,\gamma^{-4/5}\,k\,\|\xi\|_1 N^{3/5}\|W\|_3^{6/5}. \tag{2.25}$$

Optimizing the right side of (2.25), for $\gamma > 0$, yields the bound in the theorem, namely

$$4\pi\sum_{i=1}^{N}\mu_i \leqq 3.2^{-1/3}k^{1/3}\alpha^{2/3}\|\xi\|_1^{1/3}N^{1/3}\|W\|_3^2. \tag{2.26}$$

One can improve the bound in (2.26) by proceeding directly from (2.16) to the estimate (2.23) without recourse to the maximal function. Again we follow the argument of [7]. Thus let

$$\chi_a(x) = \int_a^\infty \delta(h(x) - u)du, \tag{2.27}$$

where δ denotes the Dirac δ function. Then

$$\begin{aligned} h(z)^{7/6}\xi[h(z)^{1/3}(x-z)] &= \int_0^\infty a^{7/6}\xi[a^{1/3}(x-z)]\delta(h(z)-a)da \\ &= \int_0^\infty \chi_a(z)\frac{\partial}{\partial a}[a^{7/6}\xi(a^{1/3}(x-z))]da. \end{aligned} \tag{2.28}$$

Hence the integral (2.16) may be written as

$$\int_0^\infty\int_0^\infty\int_{\mathbf{R}^3}\int_{\mathbf{R}^3}\frac{5}{3}b^{-1/6}\chi_b(x)\chi_a(z)\frac{\partial}{\partial a}[a^{7/6}\xi(a^{1/3}(x-z))]\,dxdz\,dadb. \tag{2.29}$$

Letting the subscript "+" denote the possitive part of a function we see that

$$\int_{\mathbf{R}^3}\left\{\frac{\partial}{\partial a}[a^{7/6}\xi(a^{1/3}w)]\right\}_+ dw = Ka^{-5/6}, \tag{2.30}$$

where the constant K is given by

$$K = \frac{4\pi}{3}\int_0^1\left\{\frac{\partial}{\partial r}[r^{7/2}\xi(r)]\right\}_+ r^{-1/2}\,dr. \tag{2.31}$$

Now we split the integral (2.29) into the sum of two integrals over the sets $\{a < b\}$ and $\{a \geqq b\}$. Thus we have

$$\int_{a<b} \leqq \int_{\mathbf{R}^3}\frac{5}{3}\int_0^\infty b^{-1/6}\,db\int_0^b Ka^{-5/6}\,da\chi_b(x)dx = 10K\|h\|_1. \tag{2.32}$$

In a similar fashion we have

$$\int_{b<a} \leqq \int_{\mathbf{R}^3}\frac{5}{3}\int_0^\infty Ka^{-5/6}\,da\int_0^a b^{-1/6}db\chi_a(z)dz = 2K\|h\|_1. \tag{2.33}$$

We conclude therefore that (2.16) is bounded by

$$12K\|h\|_1. \tag{2.34}$$

which leads to the bound

$$4\pi\sum_{i=1}^N \mu_i \leqq 3^{4/3}\alpha^{2/3}K^{1/3}N^{1/3}\,\|W\|_3^2. \tag{2.35}$$

This gives the constant C to be

$$C = 9(4\pi)^{-3/2}\alpha K^{1/2}. \tag{2.36}$$

If we take the function $g(x)$ to be constant in the unit ball $|x| \leqq 1$, then we get from (2.8) the value $\alpha = 6/5$. To evaluate the integral (2.31) for K, note that

$$\xi(r) = \frac{1}{r} - \frac{3}{2} + \frac{1}{2}r^2, \qquad 0 < r \leqq 1, \tag{2.37}$$

and hence

$$\frac{\partial}{\partial r}[r^{7/2}\xi(r)] = \frac{5}{2}r^{3/2} - \frac{21}{4}r^{5/2} + \frac{11}{4}r^{9/2}. \tag{2.38}$$

Thus K is given by

$$K = \frac{4\pi}{3}\int_0^R \left[\frac{5}{2}r - \frac{21}{4}r^2 + \frac{11}{4}r^4\right]dr. \tag{2.39}$$

with $R = .57661$. This yields the value $K = .482$. Hence we obtain from (2.36) the value $C = .168$.

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