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BOUNDS ON SCHRÖDINGER OPERATORS AND GENERALIZED SOBOLEV TYPE INEQUALITIES

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Start with the usual Sobolev inequality on $\mathbb{R}^n$, $n \geqslant 3$:

(1) $$\int_{\mathbb{R}^n} |\nabla f|^2 \geqslant S_n \{ \int_{\mathbb{R}^n} |f|^{\frac{2n}{n-2}} \}^{\frac{n-2}{n}} .$$

Apply Hölder's inequality to the right side to obtain

(2) $$\int_{\mathbb{R}^n} |\nabla f|^2 \geqslant K_n^1 \int_{\mathbb{R}^n} \rho^{\frac{n+2}{n}} / \{\int\rho\}^{2/n}$$

with $\rho(x) \equiv |f(x)|^2$. The superscript 1 indicates that in (2) we are considering only 1 function, f . In general $K_n^1 \geqslant S_n$; in fact $K_n^1 < \infty$ for all $n \geqslant 1$ while $S_n = 0$ for $n < 3$. Eq. (2), unlike (1) has the following important property : The non-linear term $\int\rho^{\frac{n+2}{n}}$ enters with the power 1 (and not n-2/n) and is therefore "extensive". The price we have to say for this is $\| f \|_2^{4/n}$ in the denominator, but since we shall apply (2) to cases in which $\| f \|_2 = 1$ (L^2 normalization condition) this is not serious.

Inequality (2) is equivalent to the following : Consider the Schrödinger operator on $\mathbb{R}^n$

(3) $$H = -\Delta - V(x)$$

and let $e_1 = \inf \operatorname{spec}(H)$. (We assume H is self-adjoint.)

Then

(4) $$e_1 \geqslant - L_{1,n}^1 \int V_+(x)^{\frac{n+2}{2}} dx$$

with

(5) $$L_{1,n}^1 = (\frac{n}{2K_n^1})^{n/2} (1 + \frac{n}{2})^{-1-\frac{n}{2}}$$

Here is the proof of the equivalence in one direction (the other direction is even easier.) We have

$$e_1 \geqslant \inf_f \{\int|\nabla f|^2 - \int\rho V_+ \quad | \quad \| f \|_2 = 1 \text{ and } \rho = f^2\} .$$

Use (2) and Hölder to obtain (with $X = \|\rho\|_{\frac{n+2}{n}}$)

$$(6) \qquad e_1 \geq \inf_X \{K_n^1 \; X^{\frac{n+2}{n}} - \|V_+\|_{\frac{n+2}{2}} X\}$$

Minimizing (6) with respect to X yields (4) .

So far this is trivial, but now we turn to a more interesting question. Let $e_1 \leq e_2 \leq \ldots \leq 0$ be the negative spectrum of H (which may be empty).

Is there abound of the form

$$(7) \qquad \Sigma\, e_i \geq - L_{1,n} \int V_+(x)^{\frac{n+2}{2}}\, dx$$

for some universal V and N independent constant $L_n > 0$ (which, of course, is $\leq L_n^1$) ? The point is that the right side of (7) has the same form as the right side of (4). More generally, given $\gamma \geq 0$, does

$$(8) \qquad \Sigma\, |e_i|^\gamma \leq L_{\gamma,n} \int V_+(x)^{\gamma + \frac{n}{2}}\, dx$$

hold for suitable $L_{\gamma,n}$? When $\gamma = 0$, $\Sigma|e_i|^o$ is interpreted as the number of $e_i \leq 0$.

The answer to these questions is yes in the following cases :

<u>n = 1</u> : All $\gamma > \frac{1}{2}$. The case $\gamma = \frac{1}{2}$ is unsettled. For $\gamma < \frac{1}{2}$ there is no bound of the form (8).

<u>n = 2</u> : All $\gamma > 0$. There is no bound when $\gamma = 0$.

<u>n ⩾ 3</u> : All $\gamma \geq 0$.

The cases $\gamma > 0$ were first done in [8] , [9] . The $\gamma = 0$ case for $n \geq 3$ was done in [2], [4] , [11] , with [4] giving the best estimate for $L_{o,n}$. For a review of what is currently known about these constants and conjectures about the sharp values of $L_{\gamma,n}$, see [6].

There is a natural "guess" for $L_{\gamma,n}$ in terms of a semiclassical approximation (and which is not unrelated to the theory of pseudodifferential operators):

$$(9) \qquad \Sigma\, |e_i|^\gamma \approx (2\pi)^{-n} \int_{\mathbb{R}^n} dp \int_{\mathbb{R}^n} dx\, [V(x)-p^2]^\gamma$$

$$p^2 \leq V(x)$$

$$(10) \qquad \equiv L^c_{\gamma,n} \int V_+(x)^{\gamma+n/2}$$

From (9),

$$(11) \qquad L^c_{\gamma,n} = (4\pi)^{-n/2} \; \Gamma(\gamma+1)/\Gamma(1+\gamma+n/2) \; .$$

It is easy to prove that

$$(12) \qquad L_{\gamma,n} \geqslant L^c_{\gamma,n} \quad .$$

The evaluation of the sharp $L_{\gamma,n}$ is an interesting open problem - especially $L_{1,n}$. In particular, for which γ, n is $L_{\gamma,n} = L^c_{\gamma,n}$? It is known [1] that for each fixed n , $L_{\gamma,n}/L^c_{\gamma,n}$ is decreasing in γ . Thus, if $L_{\gamma_o,n} = L^c_{\gamma_o,n}$ for some γ_o , then $L_{\gamma,n} = L^c_{\gamma,n}$ for all $\gamma > \gamma_o$. In particular, $L_{\frac{3}{2},1} = L^c_{\frac{3}{2},1}$ [9] so $L_{\gamma,1} = L^c_{\gamma,1}$, for $\gamma \geqslant 3/2$. No other sharp values of $L_{\gamma,n}$ are known .

Just as (4) is related to (2), eq. (7) is related to a generalization of (2). Let $\varphi_1,\ldots,\varphi_N$ be any set of L^2 orthonormal functions on $\mathbb{R}^n$ and define

$$(13) \qquad \rho(x) \equiv \sum_{i=1}^{N} |\varphi_i(x)|^2 \quad .$$

$$(14) \qquad T \equiv \sum_{i=1}^{N} \int |\nabla\varphi_i|^2$$

Then

$$(15) \qquad T \geqslant K_n \int \rho(x)^{1+2/n}$$

with K_n related to $L_{1,n}$ as in (5), i.e.

$$(16) \qquad L_{1,n} = \left(\frac{n}{2K_n}\right)^{n/2} \left(1+\frac{n}{2}\right)^{-1-\frac{n}{2}} \quad .$$

We might call (15) <u>a Sobolev type inequality for orthonormal functions</u>. The point is that if the φ_i are nerely normalized, but not orthogonal, then the best one could say is

$$(17) \qquad T \geqslant N^{-\frac{2}{n}} K^1_n \int \rho(x)^{1+2/n}$$

The orthogonality eliminates the factor $N^{-2/n}$.

(17) can be easily extended to the following : Let $\psi(x_1,\dots,x_N) \in L^2((\mathbb{R}^n)^N)$ $x_i \in \mathbb{R}^n$. Suppose $\|\psi\|_2 = 1$ and ψ is antisymmetric. Define

(18) $$\rho(x) \equiv N \int |\psi(x,x_2,\dots,x_N)|^2 \, dx_2 \dots dx_N$$

(19) $$T \equiv N \int |\nabla_1 \psi|^2 \, dx_1 \dots dx_N \ .$$

Then (15) holds (with the same K_n). This is a generalization of (13)-(15) since we can take

(20) $$\psi(x_1,\dots,x_N) = (N!)^{-1/2} \det \{\varphi_i(x_j)\}_{i,j=1}^{N} \ .$$

One application of (8) is to the Riesz and Bessel potentials of orthonormal functions [5] . Again, $\varphi_1,\dots,\varphi_N$ are L^2 orthonormal and let

(21) $$u_i \equiv (-\Delta+m^2)^{-1/2}\varphi_i$$

(22) $$\rho(x) \equiv \sum_{i=1}^{N} |u_i(x)|^2$$

Then there are constants L, B_p, A_n such that

(23) $\underline{n = 1}$: $\|\rho\|_\infty \leqslant L/m \qquad m > 0$

(24) $\underline{n = 2}$: $\|\rho\|_p \leqslant B_p \, m^{-2/p} N^{1/p} \ , \ 1 \leqslant p < \infty \ , \ m > 0$

(25) $\underline{n \geqslant 3}$: $\|\rho\|_p \leqslant A_n N^{1/p} \qquad p = n/(n-2), \ m \geqslant 0$.

If the orthogonality condition is dropped then the right sides of (23)-(25) have to be multiplied by N , $N^{1-1/p}$, $N^{1-1/p}$ respectively. Similar results can be derived [5] for $(-\Delta+m^2)^{-\alpha/2}$ in place of $(-\Delta+m^2)^{-1/2}$, with $\alpha < n$ when $m = 0$.

Inequality (15) also has applications in mathematical physics.

Application 1. Suppose $\Omega \subset \mathbb{R}^n$ is bounded with volume $|\Omega|$ and consider

$$H = -\Delta - V(x)$$

on Ω with Dirichlet boundary conditions. Let $\lambda_1 \leqslant \lambda_2 \leqslant \dots$ be the eigenvalues of H . Let $\overline{N}$ be the smallest integer, N , such that

(26) $$E_N \equiv \sum_{i=1}^{N} \lambda_i \geqslant 0 .$$

We want to find an upper bound for $\bar{N}$.

If φ_1 , $\varphi_2, \dots$ are the normalized eigenfunctions then, from (13)-(15) with $\varphi_1, \dots, \varphi_N$,

(27) $$E_N = T - \int \rho V \geqslant K_n \int \rho^{1+n/2} - \int V_+ \rho \geqslant G(\rho)$$

with $(p = 1+n/2)$

(28) $$G(\rho) \equiv K_n \quad \|\rho\|_p^p - \|V_+\|_{p'} \|\rho\|_p \quad .$$

Thus, for all N ,

(29) $$E_N \geqslant \inf \quad \{G(\rho) \mid \ \|\rho\|_1 = N , \quad \rho(x) \geqslant 0\}$$

But $\|\rho\|_p \quad |\Omega|^{1/p'} \geqslant \|\rho\|_1 = N$ so , with $X \equiv \|\rho\|_p$,

(30) $$E_N \geqslant \inf \{J(X) \mid X \geqslant N \ |\Omega|^{-1/p'}\}$$

where

(31) $$J(X) \equiv K_n X^p - \|V_+\|_{p'} X \quad .$$

$J(X) \geqslant 0$ for $X \geqslant X_o = \{\|V\|_{p'}/K_n\}^{1/(p-1)}$, whence

(32) $$N \geqslant |\Omega|^{1/p'} \{\|V_+\|_{p'}/K_n\}^{1/(p-1)} \Rightarrow E_N \geqslant 0 .$$

Therefore

(33) $$\bar{N} \leqslant |\Omega|^{1/p'} \{\|V_+\|_{p'} \ /K_n\}^{1/(p-1)}$$

The bound (33) can be applied [6] (following an idea of Ruelle) to the Navier-Stokes equation . There, $\bar{N}$ is interpreted as the Hausdorff dimension of an attracting set for the N-S equation while $V(x) \equiv \frac{1}{\nu^{3/2}} \varepsilon(x)$, where $\varepsilon(x) = \nu \left| \frac{\partial v}{\partial x} \right|^2$ is the average energy dissipation per unit mass in a flow v . ν is the viscosity.

<u>Application 2</u>. This is the original one [8] . In the quantum mechanics of

Coulomb systems (electrons and nuclei) one wants a lower bound for :

$$H = -\sum_{i=1}^{N} \Delta_i - \sum_{i=1}^{N} \sum_{j=1}^{K} z_j |x_i - R_j|^{-1} + \sum_{1 \leq i < j \leq N} |x_i - x_j|^{-1}$$

(34)

$$+ \sum_{1 \leq i < j \leq K} z_i z_j \, |R_i - R_j|$$

on the L^2 space of antisymmetric functions $\psi(x_1, \ldots, x_2), x_i \in \mathbb{R}^3$. Here, N is the number of elections (with coordinates x_i) and $R_1, \ldots, R_K \in \mathbb{R}^3$ are fixed vectors representing the locations of fixed nuclei of charges $z_1, \ldots, z_K > 0$. The desired bound is linear :

(35) $$H \geq - A(N+K)$$

for some A independent of N , K, $R_1, \ldots, R_K$ (assuming all $z_i <$ some $\bar{z}$).

The main point is that antisymmetry of ψ is crucial for (35) and this is reflected in the fact that (15) holds with antisymmetry but only (17) holds without it. By using (15) one can eliminate the differential operators Δ_i . The functional $\psi \to (\psi, H\psi)$, with $(\psi,\psi) = 1$ can be bounded below using (15) by a functional involving only $\rho(x)$ (called the Thomas-Fermi functional). The minimization of this latter functional with respect to ρ is tractable and leads to (35).

Application 3. Going from atoms to stars, we now consider N neutrons which attract each other gravitationally with a constant $\kappa = Gm^2$. (34) is replaced by

(36) $$H_N = \sum_{i=1}^{N} (-\Delta_i)^{1/2} - \kappa \sum_{1 \leq i < j \leq N} |x_i - x_j|^{-1}$$

(again on antisymmetric functions).One finds that

(37)
$$\begin{aligned} \inf \operatorname{spec}(H_N) &= 0 \quad \text{if} \quad \kappa \leq C\, N^{-2/3} \\ &= -\infty \quad \text{if} \quad \kappa > C\, N^{-2/3} \end{aligned}$$

for some constant, C . Without antisymmetry, $N^{-2/3}$ must be replaced by N^{-1} . (37) is proved in [10] . An important role is played by Daubechies's generalization of (15) to the operator $(-\Delta)^{1/2}$, namely (for antisymmetric ψ with $\|\psi\|_2 = 1$)

(38) $$(\psi, \sum_{i=1}^{N} (-\Delta_i)^{1/2} \psi) \geq B_n \int \rho(x)^{1+1/n}$$

with ρ given by (18). In general, one has

(39) $$(\psi, \sum_{i=1}^{N} (-\Delta)^p \psi) \geq C_{p,n} \int \rho(x)^{1+p/2n} .$$

Application 4. The latest application is in [7] and concerns the stability of atoms in magnetic fields. $\psi(x_1,\dots,x_N)$ becomes a spinor valued function, i.e. ψ is an antisymmetric function in $\bigwedge_1^N L^2(\mathbb{R}^3; \mathbb{C}^2)$. The operator H of interest is as in (34) but with the replacement

(40) $$\Delta \to \{\sigma.(i\nabla - A(x))\}^2$$

where $\sigma_1, \sigma_2, \sigma_3$ are the 2×2 Pauli matrices and $A(x)$ is a given vector field (called the magnetic vector potential). Let

(41) $$E_0(A) = \inf \operatorname{spec}(H)$$

after the replacement of (40) in (34). As $A \to \infty$ (in a suitable sense), $E_0(A)$ can go to $-\infty$. The problem is this : Is

(42) $$\tilde{E}(A) \equiv E_0(A) + \frac{1}{8\pi} \int (\mathrm{curl}\ A)^2$$

bounded below for all A ? In [7] the problem is resolved for $K = 1$, all N and $N = 1$, all K. It turns out that $\tilde{E}(A)$ is bounded below in these cases if and only if all the z_i satisfy $z_i < z^c$ where z^c is some fixed constant independent of N and K.

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