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SCHRÖDINGER OPERATORS WHOSE POTENTIALS HAVE SEPARATED SINGULARITIES

JOHN D. MORGAN III

I. INTRODUCTION

This paper is mainly concerned with obtaining lower bounds to the bottom of the spectrum of a Schrödinger operator $-\nabla^2 + V$ on $\mathbf{R}^n$, where the real-valued potential V has separated singularities. The main result is that if there is a (possibly finite) sequence of smooth real-valued functions on $\mathbf{R}^n$ to $\mathbf{R}$ with

$$(1.1) \qquad \sum_i \varphi_i^2 \equiv 1 \text{ and } \sup\Big(\sum_i |\underset{\sim}{\nabla}\varphi_i|^2\Big) < +\infty,$$

such that for some real a and b

$$(1.2) \qquad \|\,|V|^{1/2}\,\varphi_i\psi\|^2 \leqslant a\,\|\underset{\sim}{\nabla}(\varphi_i\psi)\|^2 + b\,\|\varphi_i\psi\|^2$$

for all ψ in $D(-\mathrm{i}\underset{\sim}{\nabla})$, then there exists a constant c such that

$$(1.3) \qquad \|\,|V|^{1/2}\,\psi\|^2 \leqslant a\,\|\underset{\sim}{\nabla}\psi\|^2 + c\,\|\psi\|^2$$

for all ψ in $D(-\mathrm{i}\underset{\sim}{\nabla})$. That is, given a uniform local estimate of the form (1.2), we can derive an estimate of the form (1.3). We also present an operator version of this result given stronger differentiability assumptions on the φ_i's.

These estimates are useful in the following physical situation. Consider a Hamiltonian $H = -\nabla^2 + V$ on $\mathbf{R}^n$, where the potential $V = V_1 + V_2$. Suppose that V_1 and V_2 have separated singularities in the sense that there exists a real number K such that

$$(1.4) \qquad \overline{\{\underset{\sim}{x}\,|\,|V_1(\underset{\sim}{x})| > K\}} \quad \text{and} \quad \overline{\{\underset{\sim}{x}\,|\,|V_2(\underset{\sim}{x})| > K\}}$$

are separated by a minimum distance $R > 0$. Then it is natural to enquire whether the semiboundedness of both $H_1 = -\nabla^2 + V_1$ and $H_2 = -\nabla^2 + V_2$ implies that $H = -\nabla^2 + V_1 + V_2$ is semibounded. For example, in $\mathbf{R}^3$ the Hamiltonian $H(\alpha) = -\nabla^2 - \alpha/r^2$ is semibounded by 0 if $\alpha \leqslant 1/4$ and unbounded below if $\alpha > 1/4$; one might then ask whether for $\underset{\sim}{r}_0 \neq \underset{\sim}{0}$ the Hamiltonian $H(\alpha, \beta) = -\nabla^2 - \alpha/r^2 - \beta/|\underset{\sim}{r} - \underset{\sim}{r}_0|^2$ is semibounded if $\alpha, \beta \leqslant 1/4$ but $\alpha + \beta > 1/4$.

The basic technique is to partition the density distribution $|\varphi|^2$ of a function ψ in $Q(-\nabla^2)$ (the form-domain of $-\nabla^2$) as

$$|\varphi|^2 = |\psi_1|^2 + |\psi_2|^2, \tag{1.5}$$

where

$$\text{supp}\,(|\psi_1|) \cap \{\overline{\underset{\sim}{x} \,|\, |V_2(\underset{\sim}{x})| > K}\} = \tag{1.6}$$

$$= \text{supp}\,(|\psi_2|) \cap \{\overline{\underset{\sim}{x} \,|\, |V_1(\underset{\sim}{x})| > K}\} = \{\emptyset\},$$

and ψ_1 and ψ_2 are in $Q(-\nabla^2)$. Thus ψ_1 and ψ_2 will not 'see' the singularities of V_2 and V_1, respectively. Then *modulo* some terms which are easily seen to be bounded, the semiboundedness of H_1 and H_2 will imply the semiboundedness of H. The guiding philosophy, inspired by the fact that the semiboundedness of a quantum mechanical Hamiltonian is closely related to the absence of 'collapse' of the trajectories of the corresponding classical Hamiltonian [1], is that 'collapse' is a purely local phenomenon.

The technique of local partitioning goes back to Strichartz [2], who was considering the boundedness of a multiplier from a Sobolev space to itself. Shortly thereafter E. Nelson noticed that Strichartz' technique extended to the case of a multiplier from a Sobolev space to a different Sobolev space. Nelson's remark has been exploited by B. Simon *et al.* in some recent work on Hamiltonians whose potentials have multiple singularities [3, 4]. However, the method of local partitioning does not seem to be widely appreciated, and in 1977 it was independently rediscovered by T. Kato after some discussions with the author on the physical intuition behind the result. Unfortunately, Simon and Kato's technique used a less than optimal estimate which did not allow one to consider the case when V_1 and V_2 are form-bounded by $-\nabla^2$ with bound exactly 1. Very recently the author found a simple way of extending the method to this case. In fact, one can use the improved technique to derive rigorous lower bounds, which are asymptotically exact, to the potential energy curves of molecules in the Born-Oppenheimer approximation; this application will be discussed by Barry Simon and the author in a forthcoming paper [5]. For the above reasons the improved Strichartz technique is presented below.

II. THE RELATIVE BOUNDEDNESS OF A POTENTIAL WITH SEPARATED SINGULARITIES

A possibly infinite sequence $\{\varphi_i\}$ of real functions which satisfies

$$\sum_i \varphi_i^2 \equiv 1 \quad \text{and} \quad \sup\,(\sum_i |\underset{\sim}{\nabla}\varphi_i|^2) < +\infty \tag{2.1}$$

will be called a *local partition.* Notice that Hölder's inequality for sums implies that the series $\sum_i \varphi_i \nabla \varphi_i$ is absolutely convergent.

THEOREM 2.1. *Given a potential V, suppose there exist a local partition $\{\varphi_i\}$ and real constants a and b such that*

$$\| |V|^{1/2} \varphi_i \psi \|^2 \leqslant a \| \nabla (\varphi_i \psi) \|^2 + b \| \varphi_i \psi \|^2 \tag{2.2}$$

for all ψ in $D(-i\nabla)$. Then there exists a real constant c such that

$$\| |V|^{1/2} \psi \|^2 \leqslant a \| \nabla \psi \|^2 + c \| \psi \|^2 \tag{2.3}$$

for all ψ in $D(-i\nabla)$.

Proof.

$$\| \nabla (\varphi_i \psi) \|^2 = \| \varphi_i \nabla \psi + \psi \nabla \varphi_i \|^2 = \tag{2.4}$$

$$= \| \varphi_i \nabla \psi \|^2 + \| \psi \nabla \varphi_i \|^2 + \int \varphi_i \nabla \varphi_i \cdot (\psi^* \nabla \psi + \psi \nabla \psi^*).$$

Hence

$$\| |V|^{1/2} \psi \|^2 = \sum_i \| |V|^{1/2} \varphi_i \psi \|^2 \leqslant \tag{2.5}$$

$$\leqslant a \sum_i \left\{ \| \varphi_i \nabla \psi \|^2 + \| \psi \nabla \varphi_i \|^2 + \int \varphi_i \nabla \varphi_i \cdot (\psi^* \nabla \psi + \psi \nabla \psi^*) \right\} + b \sum_i \| \varphi_i \psi \|^2$$

Notice that from (2.1)

$$\sum_i \varphi_i \nabla \varphi_i = \frac{1}{2} \sum_i \nabla \varphi_i^2 = \frac{1}{2} \nabla \left(\sum_i \varphi_i^2 \right) = 0. \tag{2.6}$$

Hence the cross term in (2.6) vanishes, [1]) so

$$\| |V|^{1/2} \psi \|^2 \leqslant a \| \nabla \psi \|^2 + a \sum_i \| \psi \nabla \varphi_i \|^2 + b \| \psi \|^2. \tag{2.7}$$

Choosing

$$c = b + a \sup \left(\sum_i | \nabla \varphi_i |^2 \right) \tag{2.8}$$

yields (2.3) Q.E.D.

We would like to make some remarks:

(i) The analog of (1.2) is given by $\varphi_i = \varphi_i \psi$.

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[1]) We could handle the cross term even without (2.1) if the φ_i's are sufficiently smooth just by using the symmetric nature of $-i\nabla$:

$$\int \varphi_i \nabla \varphi_i \cdot (\psi^* \nabla \psi + \psi \nabla \psi^*) = -\frac{1}{2} \int \nabla^2 (\varphi_i^2) |\psi|^2.$$

(*ii*) Instead of (2.6), Simon and Kato used the estimate

$$\| \underset{\sim}{\nabla}(\varphi_i\psi)\|^2 = \|\varphi_i \underset{\sim}{\nabla}\psi + \psi \underset{\sim}{\nabla}\varphi_i\|^2 \leqslant \tag{2.9}$$

$$\leqslant (1+\varepsilon) \| \varphi_i \underset{\sim}{\nabla}\psi\|^2 + (1+\varepsilon^{-1}) \| \psi \underset{\sim}{\nabla} \varphi_i\|^2.$$

The nonzero ε does not allow one to prove semiboundedness of H if $a = 1$, and the ε^{-1} yields a bound of little quantitative interest at finite separations.

(*iii*) The result is independent of the dimension or the number of particles.

(*iv*) If V is the sum of N asymptotically vanishing potentials whose singularities are separated by a minimum distance R, the R-dependence of the φ_i's can be chosen such that as $R \to \infty$, $\sup (\sum_i |\underset{\sim}{\nabla}\varphi_i|^2) \to 0$ and $-b$ tends to the infimum over all cluster decompositions of the sum of the energies of each cluster. This fact plays a crucial role in [5].

(*v*) The theorem could be phrased in terms of general operators, where the φ_i's are replaced with bounded operators P_i.

This theorem is of value since the KLMN Theorem, one of the most useful ways of proving self-adjointness of $-\nabla^2 + V$ [6], requires an estimate of the form (2.3), and this method enables one to turn uniform local estimates into global estimates. For example, suppose there exists a positive constant l such that

$$\| \, |V|^{1/2} \chi_l(\cdot - \underset{\sim}{x}) \psi\|^2 \leqslant a \|\underset{\sim}{\nabla}\psi\|^2 + b \|\psi\|^2 \tag{2.10}$$

for all ψ in $D(-i\underset{\sim}{\nabla})$ and all $\underset{\sim}{x}$ in $\mathbf{R}^n$, where $\chi_l(\underset{\sim}{z})$ is the characteristic function of an n-dimensional hypercube of volume l^n centered at $\underset{\sim}{0}$. Then by choosing the φ_i's such that the support of each lies within a hypercube of volume l^n, we can show that V obeys (2.3).

A similar uniform localisation result holds for operators. Kato [7] has proved

THEOREM 2.2. *Suppose B is symmetric and A is essentially self-adjoint/self-adjoint on $D(A)$. If there exist a and b such that for all ψ in $D(A)$*

$$\|B\psi\|^2 \leqslant a \|A\psi\|^2 + b \|\psi\|^2, \tag{2.11}$$

then $A + B$ is essentially self-adjoint / self-adjoint on $D(A)$ depending on whether $a \leqslant 1$ or $a < 1$, respectively.

Notice that for $a = 1$, (2.11) is only apparently less general than

$$\|B\psi\|^2 \leqslant \|A\psi\|^2 + 2c(\psi, A\psi) + b\|\psi\|^2, \tag{2.12}$$

since the right side of (2.12) equals

$$\|A + cI\|^2 + (b - c^2) \|\psi\|^2, \tag{2.13}$$

and $A + cI$ is essentially self-adjoint iff A is.

THEOREM 2.3. *Given a local partition* $\{\varphi_i\}$ *such that*

(2.14) $$\sup\left(\sum_i |\varphi_i \nabla^4 \varphi_i|\right) < +\infty \text{ and } \sup\left|\sum_i \nabla^2(\varphi_i \nabla^2 \varphi_i)\right| < +\infty$$

suppose there exists a constant b such that for each i,

(2.15) $$\|V\varphi_i\psi\|^2 \leqslant \|\nabla^2(\varphi_i\psi\|^2 + b\,\|\varphi_i\psi\|^2$$

for all ψ *in* $D(-\nabla^2)$. *Then there exist constants a and c such that*

(2.16) $$\|V\psi\|^2 \leqslant \|\nabla^2\psi\|^2 + 2a\,(\psi, -\nabla^2\psi) + c\|\psi\|^2$$

for all ψ *in* $D(-\nabla^2)$.

Proof. Since

(2.17) $$\nabla^2(\varphi_i\psi) = \varphi_i\nabla^2\psi + \psi\nabla^2\varphi_i + 2\underset{\sim}{\nabla}\varphi_i\cdot\underset{\sim}{\nabla}\psi,$$

(2.18) $$\|\nabla^2(\varphi_i\psi)\|^2 = \|\varphi_i\nabla^2\psi\|^2 + 2\int\varphi_i\underset{\sim}{\nabla}\varphi_i\cdot(\nabla^2\psi^*\underset{\sim}{\nabla}\psi + \nabla^2\psi\underset{\sim}{\nabla}\psi^*) +$$
$$+ 4\int|\underset{\sim}{\nabla}\varphi_i\cdot\underset{\sim}{\nabla}\psi|^2 + \int\varphi_i\nabla^2\varphi_i(\psi\nabla^2\psi^* + \psi^*\nabla^2\psi) +$$
$$+ 2\int\nabla^2\varphi_i\underset{\sim}{\nabla}\varphi_i\cdot(\psi^*\underset{\sim}{\nabla}\psi + \psi\underset{\sim}{\nabla}\psi^*) + \|\nabla^2\varphi_i\psi\|^2.$$

Using the symmetry of $-i\underset{\sim}{\nabla}$, (2.6), and

(2.19) $$\sum_i \varphi_i\nabla^2\varphi_i = -\sum_i |\underset{\sim}{\nabla}\varphi_i|^2$$

yields

(2.20) $$\sum_i \|\nabla^2(\varphi_i\psi)\|^2 = \|\nabla^2\psi\|^2 + 4\sum_i\int|\underset{\sim}{\nabla}\varphi_i\cdot\underset{\sim}{\nabla}\psi|^2 +$$
$$+ \sum_i\int|\underset{\sim}{\nabla}\varphi_i|^2\,[\psi(-\nabla^2\psi^*) + \psi^*(-\nabla^2\psi)] -$$
$$- 2\sum_i\int\underset{\sim}{\nabla}\cdot(\nabla^2\varphi_i\underset{\sim}{\nabla}\varphi_i)\,|\psi|^2 + \sum_i \|\nabla^2\varphi_i\psi\|^2.$$

Repeated integration by parts shows that

$$\sum_i \int |\nabla\varphi_i|^2 [\psi(-\nabla^2\psi^*) + \psi^*(-\nabla^2\psi)] = \tag{2.21}$$

$$= \sum_i \int [\nabla\psi^* \cdot \nabla(\psi\nabla\varphi_i\cdot\nabla\varphi_i) + \nabla\psi\cdot\nabla(\psi^*\nabla\varphi_i\cdot\nabla\varphi_i)] =$$

$$= \sum_i \int [2|\nabla\psi|^2 |\nabla\varphi_i|^2 + (\psi\nabla\psi^* + \psi^*\nabla\psi)\cdot\nabla|\nabla\varphi_i|^2] =$$

$$= 2\int |\nabla\psi|^2 \sum_i |\nabla\varphi_i|^2 - \sum_i \int |\psi|^2 \nabla\cdot\nabla(\nabla\varphi_i\cdot\nabla\varphi_i).$$

Hence using $|\nabla\varphi_i\cdot\nabla\psi| \leqslant |\nabla\varphi_i||\nabla\psi|$ shows that the r.h.s. of (2.20) does not exceed

$$\|\nabla^2\psi\|^2 + 6\int|\nabla\psi|^2 \sum_i |\nabla\varphi_i|^2 - \sum_i \int |\psi|^2\nabla\cdot\nabla(\nabla\varphi_i\cdot\nabla\varphi_i) - \tag{2.22}$$

$$-2\sum_i \int \nabla\cdot(\nabla^2\varphi_i\nabla\varphi_i)|\psi|^2 + \sum_i \|\nabla^2\varphi_i\psi\|^2.$$

Inserting (2.19) shows that (2.22) equals

$$\|\nabla^2\psi\|^2 + 6\int|\nabla\psi|^2 \sum_i |\nabla\varphi_i|^2 + \sum_i \int |\psi|^2\nabla\cdot\nabla(\varphi_i\nabla^2\varphi_i) - \tag{2.23}$$

$$-2\sum_i \int \nabla\cdot(\nabla^2\varphi_i\nabla\varphi_i)|\psi|^2 + \sum_i \|\nabla^2\varphi_i\psi\|^2 =$$

$$= \|\nabla^2\psi\|^2 + 6\int|\nabla\psi|^2 \sum_i |\nabla\varphi_i|^2 + \sum_i \int |\psi|^2\nabla\cdot(\varphi_i\nabla(\nabla^2\varphi_i)) -$$

$$-\sum_i \int \nabla\cdot(\nabla^2\varphi_i\nabla\varphi_i)|\psi|^2 + \sum_i \|\nabla^2\varphi_i\psi\|^2 =$$

$$= \|\nabla^2\psi\|^2 + 6\int|\nabla\psi|^2 \sum_i |\nabla\varphi_i|^2 + \sum_i \int |\psi|^2 \varphi_i\nabla^4\varphi_i -$$

$$-\sum_i \int |\psi|^2 |\nabla^2\varphi_i|^2 + \sum_i \|\nabla^2\varphi_i\psi\|^2 \leqslant$$

$$\leqslant \|\nabla^2\psi\|^2 + 6\sup(\sum|\nabla\varphi_i|^2)(\psi - \nabla^2\psi) + \sup|\sum_i \varphi_i\nabla^4\varphi_i| \|\psi\|^2.$$

The rest of the proof mimics that of Theorem 2.1.

As in the case of quadratic forms, we can use uniform local relative bounds on V to derive global ones. Chernoff has proved similar results on the essential self-adjointness of Schrödinger and Dirac operators on $C_0^\infty(\mathbf{R}^n)$ [8]. However, a *uniform* local relative bound is not required for essential self-adjointness on $C_0^\infty(\mathbf{R}^n)$, but it is if one is considering essential self-adjointness on any core for $-\nabla^2$. For example, the Hamiltonian for the one-dimensional harmonic oscillator,

$$-\frac{d^2}{dx^2}+kx^2, \tag{2.24}$$

is essentially self-adjoint on $C_0^\infty(\mathbf{R})$, but it is not even defined on $D(-\nabla^2)$, for the latter set contains functions which are not in $D(|x|)$, *e.g.*, $(1+x^2)^{-1/2}$.

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JOHN D. MORGAN III, Department of Chemistry, University of California, Berkeley, California 94720, *USA,*
and Department of Physics,
Princeton University, Princeton,
N.J. 08540, *USA.*

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