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Spectrum and Continuum Eigenfunctions of Schrödinger Operators

BARRY SIMON*

Sherman Fairchild Visiting Scholar, California Institute of Technology, Pasedena, California 91125

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We consider Schrödinger operators $H = -\frac{1}{2}\Delta + V$ for a large class of potentials. V. We show that if $H\varphi = E\varphi$ has a polynomially bounded solution φ then E is in the spectrum of H. This is accomplished by proving that the spectrum of H as an operator on L^2 is identical to its spectrum as an operator on the weighted L^2 space, L^2_δ.

1. INTRODUCTION

In this paper, we want to discuss eigenfunctions of Schrödinger operators

$$H = -\tfrac{1}{2}\Delta + V \tag{1.1}$$

on $L^2(R^\nu)$. We will deal with a wide class of potentials; typically we will require that $V = V_+ - V_-$ with $V_\pm \geqslant 0$ and $V_+ \in K_\nu^{\mathrm{loc}}$, $V_- \in K_\nu$, where K_ν is the class discussed in [2]:

DEFINITION. If $\nu \geqslant 3$, we say $f \in K_\nu$ if and only if

$$\lim_{\alpha \downarrow 0} \sup_x \int_{|x-y| \leqslant \alpha} |x-y|^{-(\nu-2)} |f(y)|\, d^\nu y = 0.$$

If $\nu = 2$, we replace $|x-y|^{-(\nu-2)}$ by $\ln |x-y|^{-1}$ (and take $\alpha \leqq 1$). If $\nu = 1$, K_ν is the set of f's with

$$\sup_x \int_{|x-y| \leqslant 1} |f(y)|\, dy < \infty,$$

$f \in K_\nu^{\mathrm{loc}}$ if and only if $fg \in K_\nu$ for all $g \in C_0^\infty(R^\nu)$.

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This class is sufficiently large to include virtually all interesting V's which lead to H's which are bounded below. It is convenient since a Harnack inequality holds for such potentials [2].

We are interested in solutions, φ, of

$$H\varphi = E\varphi \tag{1.2}$$

(we will discuss the sense in which this holds below) and, in particular, for which E (1.2) has a polynomially bounded solution.

One direction is already well known. Generalized eigenfunction expansions of differential operators is a subject associated with Berezanski, Gårding, Gel'fand, Kac and Maurin (see Berezanski [3] for references); the implementation of their ideas for Schrödinger operators is described in Faris [5], Herbst–Sloan [6] and Kovalenko–Semonov [7] and reviewed in Simon [12]. *One* consequence of this theory is the following (see [7] or [12]).

THEOREM 1.1. *Let $V_+ \in K_\nu^{\text{loc}}$, $V_- \in K_\nu$ and let H be the associated L^2-Schrödinger operator. Then for every $\varepsilon > 0$, (1.2) has a distributional solution φ obeying*

$$|\varphi(x)| \leqslant C(1 + |x|)^{(1/2)\nu + \varepsilon} \tag{1.3}$$

for H-spectrally almost every E. In particular, the set of E for which (1.2) has a solution obeying (1.3) is dense in the spectrum of H.

Remarks. 1. If V obeys the above hypothesis, then H defines a closed quadratic form on $Q(-\Delta) \cap Q(V_+)$ (and $C_0^\infty(R^\nu)$ is a form core [10]) and the associated self-adjoint operator is what we mean by "the associated L^2-Schrödinger operator."

2. If A is a self-adjoint operator, we say something holds "A-spectrally almost everywhere" if the set Δ for which it holds has an associated spectral projection which is the identity.

Our goal in this paper is to consider the converse of this result, i.e., to show that if (1.2) has a solution obeying

$$|\varphi(x)| \leqslant C(1 + |x|)^N \tag{1.4}$$

for some N, then E is in the spectrum of H. Surprisingly, except for [13, 14], this appears not to have been discussed before. We note that if polynomial growth is replaced by exponential growth, the result is not true as consideration of the case $V = 0$ shows. We also note that if φ obeys (1.2) and

$$\int_{|x-y| \leqslant 1} |\varphi(y)|\, d^\nu y \leqslant C(1 + |x|)^N \tag{1.5}$$

then automatically (1.4) holds by a Harnak type inequality; see [2].

In Section 3, we will prove

THEOREM 1.2. *Let $V_+ \in K_\nu^{\text{loc}}$, $V_- \in K_\nu$ and $V \in L^2_{\text{loc}}$ and let H be the associated L^2-Schrödinger Operator. Suppose that* (1.2) *has a distributional sollution, φ, obeying* (1.4) *for some N. Then $E \in \operatorname{spec}(H)$.*

This, together with Theorem 1.1 immediately implies

THEOREM 1.3. *If V obeys the hypothesis of Theorem 1.2, then*

$$\operatorname{spec} H = \overline{\{E \mid (1.2) \text{ has a districutional solution obeying } (1.4)\}}.$$

Actually, the condition $V \in L^2_{\text{loc}}$ is only needed for a "nice" meaning to the expression "solution of (1.2)." If $V_+ \in K_\nu^{\text{loc}}$, $V_- \in K_\nu$, then (see Section 2) e^{-tH} defines a map with

$$|(e^{-tH}g)(x)| \leqslant Ce^{-ax^2} \tag{1.6}$$

for every $g \in C_0^\infty$, so that $(\varphi, e^{-tH}g)$ makes sense if φ obeys (1.4). In Section 2, we will prove

THEOREM 1.4. *Let φ obey* (1.4). *Let $V_+ \in K_\nu^{\text{loc}}$, $V_- \in K_\nu$, and suppose that φ "obeys* (1.2)*" in the sense that*

$$(\varphi, e^{-tH}g) = e^{-tE}(\varphi, g) \tag{1.7}$$

for every $g \in C_0^\infty$. Then $E \in \operatorname{spec}(H)$.

The basic methods we use in Section 2 involve another natural question which has not been previously considered. Let $L^2_\delta = \{f \mid (1+x^2)^{\delta/2} f \in L^2\}$ with the norm

$$\|f\|_\delta = \left(\int (1+x^2)^\delta \, |f(x)|^2 \, d^\nu x\right)^{1/2} \tag{1.8}$$

In Section 2, we will prove that for $g \in C_0^\infty$:

$$\|e^{-tH}g\|_\delta \leqslant Ce^{At} \|g\|_\delta$$

so that the semigroup e^{-tH} can be defined on L^2_δ. We denote its generator by H_δ. In Section 2, we will prove

THEOREM 1.5. *Let $V_- \in K_\nu$, $V_+ \in K_\nu^{\text{loc}}$. Then, for any δ*

$$\operatorname{spec}(H_\delta) = \operatorname{spec}(H). \tag{1.9}$$

For V's going to zero at infinity sufficiently rapidly H_δ have been extensively considered in the Agmon [1]–Kuroda [8] theory. For this case, results close to this appear, for example, in Reed–Simon [9].

The point is that (1.7) implies that $H_\delta \varphi = E\varphi$ in operator for suitable δ. Thus E is in the point spectrum of H_δ and so by (1.9) in spec (H). Thus Theorem 1.5 implies Theorem 1.4.

In Section 3, we prove Theorem 1.2 from Theorem 1.4 by proving C_0^∞ is an operator core for H_δ. In Section 4 we discuss H on the weighted space $L^2(\mathbb{R}^\nu, e^{-a|x|}\, d^\nu x)$, where the spectrum changes but, in particular, we prove that (1.4) for some N can be replaced by

$$|\varphi(x)| \leqslant C_0 e^{a|x|}$$

for *all* $a > 0$.

Some special cases of Theorems 1.1 and 1.3 can be found in [13, 14]. Babbitt calls our Theorem 1.3 "a tight rigging."

It is a pleasure to thank B. Souillard for raising the question of converses to Theorem 1.1.

2. Spectrum on Polynomially Weighted Spaces

The basic facts that we will use about Schrödinger semigroups are:

(i) exp $(-tH)$ has an integral kernel bounded by

$$C_\varepsilon t^{-(\nu+\varepsilon)} e^{tA} \tag{2.1}$$

for all ε, some A and C depending on ε.

(ii) If $H_0 = -\frac{1}{2}\Delta$ and $H' = H_0 + 2V$ and $(e^{-tH})(x, y)$ is the integral kernel for e^{-tH}, then

$$e^{-tH}(x, y) \leqslant [e^{-tH_0}(x, y)]^{1/2}\, [e^{-tH'}(x, y)]^{1/2}. \tag{2.2}$$

Claim (i) follows from the Dunford–Pettis theorem and the fact that the semigroup is bounded from L^1 to L^∞ with norm given by (2.1), [4, 11]. Fact (ii) is just the Schwartz inequality in path space [11].

From (2.2), we conclude that for $f \in C_0^\infty$, $f \geqslant 0$:

$$\begin{aligned}&(1 + x^2)^\delta\, e^{-tH}[(1 + x^2)^{-\delta} f]\\ &\quad \leqslant (e^{-tH'} f) 1/2 \{(1 + x^2)^{2\delta}\, e^{-tH_0}(1 + x^2)^{-2\delta} f\}^{1/2}\end{aligned}$$

pointwise, so that if $\|A\|_{\delta,\delta}$ is the norm if A is a map of L_δ^2 to itself, then

$$\|e^{-tH}\|_{\delta,\delta} \leqslant \|e^{-tH'}\|_{0,0}^{1/2}\, \|e^{-tH_0}\|_{2\delta,2\delta}^{1/2} \tag{2.3}$$

(this can also be proven by complex interpolation). Using the explicit integral kernel of e^{-tH_0} and the fact that

$$\|f * g\|_2 \leqslant \|f\|_2 \, \|g\|_1$$

(with $*$ convolution), one easily sees that for $\delta > 0$:

$$\|e^{-tH_0}\|_{2\delta, 2\delta} \leqslant 1 + Ct^{2\delta}$$

so that we have

PROPOSITION 2.1. *If $V_+ \in K_\nu^{\mathrm{loc}}$, $V_- \in K_\nu$, then e^{-tH} defines a bounded map of L_δ^2 to itself obeying*

$$\|e^{-tH}\|_{\delta,\delta} \leqslant Ce^{At}. \tag{2.4}$$

In many ways, the main result of this paper is

THEOREM 2.2 ($\equiv$ Theorem 1.5). *The generator, H_δ, of e^{-tH} on L_δ^2 obeys*

$$\operatorname{spec}(H_\delta) = \operatorname{spec}(H)$$

Proof. As a preliminary, we note that $Q(H) \subset Q(H_0)$ so

$$(H - z)^{-1}\vec{\nabla} \tag{2.5}$$

is bounded as an operator on L^2 for any $z \notin \operatorname{spec}(H)$.

Now, let $^-$ denote the normal conjugation and note that, with $A^t \equiv \overline{(A^*)}$ we have

$$H = H^* = \bar{H} = H^t$$

so that

$$H_\delta^t = H_{-\delta}$$

and thus

$$\{(H_\delta - z)^{-1}\}^t = (H_{-\delta} - z)^{-1}$$

so by interpolation, we see that if $z \notin \operatorname{spec}(H_\delta)$, then $z \notin \operatorname{spec}(H)$.

To prove the result, we only need to show that if $z \notin \operatorname{spec}(H)$, then $z \notin \operatorname{spec}(H_\delta)$. By the interpolation and duality argument, we can suppose that δ is positive integer. We give formal commutator manipulations which are easy to justify. Let $g=(1+x^2)^{\delta/2}$ and we proceed inductively in δ (which is assumed integral). Then, if $z \notin \operatorname{spec}(H)$:

$$\begin{aligned} g(H-z)^{-1}g^{-1} &= (H-z)^{-1} + [g,(H-z)^{-1}]g^{-1} \\ &= (H-z)^{-1} - \tfrac{1}{2}(H-z)^{-1}\Delta g(H-z)^{-1}g^{-1} \\ &\quad + (H-z)^{-1}\nabla\cdot(\nabla g)(H-z)^{-1}g^{-1} \end{aligned} \tag{2.6}$$

By induction in δ, $\Delta g(H-z)^{-1}g^{-1}$ and $\nabla g(H-z)^{-1}g^{-1}$ are bounded on L^2, so by (2.5), $g(H-z)^{-1}g^{-1}$ is bounded on L^2, i.e., $(H-z)^{-1}$ is bounded on L^2_δ. ∎

As noted before, this implies:

THEOREM 2.3 ($\equiv$ Theorem 1.4). *Let $V_+ \in K_\nu^{\mathrm{loc}}$, $V_- \in K_-$ and suppose $\varphi \in L^2_{-N}$ for some N obeys*

$$H_{-N}\varphi = E\varphi$$

then $E \in \operatorname{spec}(H)$.

In the next section, we will need a small extension of the above argument:

THEOREM 2.4. *Let $\delta>0$. Suppose that $\varphi \in L^2_\delta$ lies in $D(H_\delta)$. Then $\nabla\varphi \in L^2_\delta$.*

Proof. Let $g=(1+x^2)^{\delta/2}$. For simplicity suppose $-1 \notin \operatorname{spec}(H)$. Writing

$$g\nabla\varphi = g\nabla(H+1)^{-1}g^{-1}[g(H+1)\varphi]$$

and noting that $g(H+1)\varphi \in L^2$ by hypothesis we see that it suffices that $g\nabla(H+1)^{-1}g^{-1}$ is bounded on L^2. Since

$$[g,\nabla](H+1)^{-1}g^{-1} = -(\nabla g)(H+1)^{-1}g^{-1}$$

is bounded by Theorem 2.2, we see that it suffices that $\nabla g(H+1)^{-1}g^{-1}$ is bounded. But, by (2.6):

$$\begin{aligned} \nabla g(H+1)^{-1}g^{-1} &= \nabla(H+1)^{-1} - \tfrac{1}{2}\nabla(H+1)^{-1}(\Delta g)(H+1)^{-1}g^{-1} \\ &\quad + \nabla(H+1)^{-1}\nabla\cdot(\nabla g)(H+1)^{-1}g^{-1} \end{aligned}$$

and each term is bounded on L^2 since $\nabla(H+1)^{-1}$, $\nabla(H+1)^{-1}\nabla$ and $g(H+1)^{-1}g^{-1}$ are all bounded. ∎

3. Cores on Polynomially Weighted Spaces

To relate distributional solutions of (1.2) to operator solutions we will need the following result which follows the "semigroup version of Kato's inequality" [10]; we remark that because of the V_- possibility, this proof is new even in the case $\delta = 0$:

THEOREM 3.1. *Let $V_+ \in K_\nu^{\mathrm{loc}}$, $V_- \in K_\nu$, $V \in L^2_{\mathrm{loc}}$ and let $\delta \geqslant 0$. Then C_0^∞ is a core for H_δ.*

Proof. e^{-tH_δ} is bounded and e^{-zH} (for $\delta = 0$) is holomorphic, so by the Stein interpolation theorem, e^{-tH_δ} is a holomorphic semigroup so $\mathrm{Ran}\,(e^{-tH_\delta}) \subset D(H_\delta)$ and if $\varphi \in D(H_\delta)$, then $H_\delta e^{-tH_\delta}\varphi \to H_\delta \varphi$ in L^2_δ. Since $\mathrm{Ran}\,(e^{-tH_\delta}) \subset L^\infty$, we conclude that $L^\infty \cap D(H_\delta)$ is a core for H_δ. Let $g \in C_0^\infty$ with $0 \leqslant g \leqslant 1$ and $g \equiv 1$ near $x = 0$. Let $g_n(x) = g(x/n)$. Let $\varphi \in L^\infty \cap D(H_\delta)$. Then

$$g_n \varphi \to \varphi$$

in L^2_δ and

$$H(g_n\varphi) = g_n H\varphi + (\Delta g_n)\,\varphi + 2(\nabla g_n)\cdot \nabla g \to H\varphi$$

in L^2_δ since $\nabla\varphi \in L^2_\delta$ by Theorem 2.4.

As a result, $L^\infty \cap D(H_\delta) \cap$ (compact support) is a core for H_δ. Now mollify and use $V \in L^2_{\mathrm{loc}}$, $\varphi \in L^\infty$ to approximate by functions in C_0^∞. ∎

THEOREM 3.2 ($\equiv$ Theorem 1.2). *Let $V_+ \in K_\nu^{\mathrm{loc}}$, $V_- \in K_\nu$, $V \in L^2_{\mathrm{loc}}$. Let $\varphi \in L^2_{-\delta}$ for some $\delta > 0$ and obey*

$$(\varphi, Hg) = E(\varphi, g) \tag{3.1}$$

for all $g \in C_0^\infty$ (i.e., $H\varphi = E\varphi$ in distributional sense). Then $\varphi \in D(H_{-\delta})$, $H_{-\delta}\varphi = E\varphi$ and thus $E \in \mathrm{spec}\,(H_{-\delta}) \equiv \mathrm{spec}\,(H)$.

Proof. Since C_0^∞ is a core for H_δ, (3.1) holds for all $g \in D(H_\delta)$. Thus $\varphi \in D(H_\delta^*)$ but $H_\delta^* = H_{-\delta}$.

4. Spectrum on Exponentially Weighted Spaces

In this final section, we want to prove the following which generalizes Theorem 2.2:

THEOREM 4.1. *Let $V_+ \in K_\nu^{\mathrm{loc}}$, $V_- \in K_\nu$. Then there exists a D*

depending only on V so that if (1.2) *has a solution* (*in the sense* $(\varphi, e^{-tH}g) = e^{-tE}(\varphi, g)$ *for all* $g \in C_0^\infty$) *obeying*

$$\int e^{-2a|x|} |\varphi(x)|^2 \, d^\nu x < \infty \tag{4.1}$$

then

$$\operatorname{dist}(E, \operatorname{spec}(H)) \leqslant 2Da(|E|^{1/2} + 1) + [a^2 + \nu a]. \tag{4.2}$$

In particular, if (4.1) *holds for all* $a > 0$, *then* $E \in \operatorname{spec}(H)$.

Proof. As in Section 2, e^{-tH} defines an exponentially bounded semigroup on $L^2_{(a)} = \{ |f| \mid \int e^{-2a|x|} |f|^2 \, d^\nu x < \infty \}$. We need only show that if E fails to obey (4.2), and $E \notin \operatorname{spec}(H)$, then $g(H-E)^{-1} g^{-1}$ is bounded on L^2, where

$$g(x) = \exp(-a \sqrt{x^2 + 1})$$

Let $\varphi \in C_0^\infty$, let $\alpha = \| g(H-z)^{-1} g^{-1} \varphi \|$ (which is finite) and apply (2.6) to φ to get

$$\alpha \leqslant \|(H-z)^{-1}\| \, \|\varphi\| + Q\alpha$$

with

$$Q = \|(H-z)^{-1}\| \, \|[\Delta g] \, g^{-1}\|_\infty + 2 \, \|(H-z)^{-1} |\nabla| \| \, \| |\nabla g| \, g^{-1} \|_\infty .$$

But by elementary calculations

$$\|[\Delta g] \, g^{-1}\|_\infty \leqslant a^2 + \nu a,$$
$$\| |\nabla g| \, g^{-1}\|_\infty \leqslant a$$

and

$$\|(H-z)^{-1} \nabla\| \leqslant D[(|z| + 1)^{1/2} \, | \, [\operatorname{dist}(z, \operatorname{spec}(H))]^{-1},$$

where D is H-dependent. If $Q < 1$, we see that $g(H-z)^{-1} g$ is bounded. ∎

Notes added in proof.

1. J. Rauch has pointed out that we neglected to prove that $(H-z)^{-1}$ is the inverse to $H_\delta - z$. This can be proven as follows: by our semigroup definition of H_δ, it is true if Rez is very negative and thus by analyticity, and by the fact that the L^2 spectrum of H is a subset of R, the result is true for all z in the resolvent set of H.

2. A slightly stronger result than Theorems 1.2, 1.3 holds; namely if the eigenfunction is not in L^2, then E must lie in the essential spectrum of H. For our argument shows that if E is an isolated point of spec (H), the projection $P = \int_{|z-E|=\epsilon} (H-z)^{-1} \, dz/(-2\pi i)$ is bounded

from L^2_δ to L^2_δ and is the spectral projection for any H_δ. If its range is finite dimensional, then $P|L^2_\delta| = P|L^2|$ so any function in $P|L^2_\delta|$ is in L^2.

3. Yu. Orochko has kindly pointed out that I. Schnol (in *Dokl. Akad. Nauk.* **89** (1953), 411–413, and especially in *Math. Sb.* **42** (1957), 273–286) proved Theorems 1.2, 1.3 and 4.1 in case V is bounded below. His results appear on pages 176–183 of the English translation of I. M. Glazman's book "Direct Methods of the Qualitative Spectral Analysis *Pf* Differential Operators," Davey & Co., 1965. By using results from [2], one can extend Schnol's method to treat the general case discussed in this paper and the extension noted in Remark 2, above. Schnol's proof is more direct than ours.

REFERENCES

1. S. AGMON, Spectral properties of Schrödinger operators and scattering theory, *Ann. Scuola Norm. Pisa II*, **2** (1975), 151–218.
2. M. AIZENMAN AND B. SIMON, Brownian motion and Harnack's inequality for Schrödinger operators, *Comm. Pure Appl. Math.*, to appear.
3. J.M. BEREZANSKI, "Expansions in Eigenfunctions of Self-Adjoint Operators," Amer. Math. Soc., Providence, R. I., 1968.
4. R. CARMONA, Regularity properties of Schrödinger and Dirichlet semigroups, *J. Funct. Anal.* **33** (1979), 259–296.
5. W. FARIS, Perturbations and non-normalizable eigenvectors, *Helv. Phys. Acta* **44** (1971), 936–936.
6. I. HERBST AND A. SLOAN, Perturbation of translation invariant positivity preserving semigroups in $L^2(R^N)$, *Trans. Amer. Math. Soc.* **236** (1978), 325–360.
7. V. F. KOVANLENKO AND YU. SEMENOV, General theory of expansions in eigenfunctions for Schrödinger operators with strongly singular potentials, *Russian Math. Surveys* **33**, No. 3 (1978), 119–157.
8. S. KURODA, Scattering theory for differential operators, I, II, *J. Math. Soc. Japan* **25** (1973), 75–104; 222–234.
9. M. REED AND B. SIMON, "Methods of Modern Mathematical Physics, IV. Analysis of Operators," Academic Press, New York, 1978.
10. B. SIMON, Maximal and minimal Schrödinger operators and forms, *J. Oper. Theory* **1** (1979), 37–47.
11. B. SIMON, "Functional Integration and Quantum Physics," Academic Press, New York, 1979.
12. B. SIMON, Schrödinger Semigroups, in preparation.
13. D. BABBITT, Rigged Hilbert space and one particle Schrödinger operators, *Rep. Math. Phys.* **3** (1972), 37.
14. D. FREDRICKS, Tight riggings for a set of commuting observables, *Rep. Math. Phys.* **8** (1975), 277.