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Scattering Length and the Spectrum of $-\Delta + V$

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Abstract. Given a non-negative, locally integrable function V on $\mathbb{R}^n$, we give a necessary and sufficient condition that $-\Delta + V$ have purely discrete spectrum, in terms of the scattering length of V restricted to boxes.

1 Introduction

It is a classical result of K. Friedrichs [F] that if $V \in L^1_{\text{loc}}(\mathbb{R}^n)$ and $V \geq 0$, then $-\Delta + V$ yields a positive self-adjoint operator on $L^2(\mathbb{R}^n)$, and its spectrum is discrete if $V(x) \to +\infty$ as $|x| \to \infty$. A. Molchanov [Mol] produced a necessary and sufficient condition for such an operator to have discrete spectrum. His condition takes the form

$$\inf_F \int_{Q_{b,\xi} \setminus F} V(x)\, dx \to \infty, \quad \text{as } |\xi| \to \infty, \tag{1.1}$$

for each $b \in (0, 1]$, where $Q_{b,\xi}$ is the n-dimensional cube of the form

$$Q_{b,\xi} = \Big\{ x \in \mathbb{R}^n : \xi_j - \frac{b}{2} \leq x_j \leq \xi_j + \frac{b}{2} \Big\}. \tag{1.2}$$

(We henceforth say $Q_{b,\xi}$ is the cube with sidelength b and center ξ.) In (1.1), F runs over the "negligible" subsets of $Q_{b,\xi}$, defined by the condition $\operatorname{cap} F \leq \gamma \operatorname{cap} Q_{b,\xi}$. In [Mol], γ was taken to be a particular (small) constant γ_n.

Recent important work of V. Maz'ya and M. Shubin [MS] provides a cleaner form for the necessary and sufficient condition. In particular, γ can be given any value in $(0, 1)$. Furthermore, they allow $\gamma = \gamma(b)$, possibly decaying to 0 as $b \to 0$, as long as $b^{-2}\gamma(b) \to \infty$.

Our purpose here is to produce an alternative formulation of a necessary and sufficient condition that $-\Delta + V$ have discrete spectrum (given $V \geq 0,\ V \in L^1_{\text{loc}}(\mathbb{R}^n)$). Our result is phrased in terms of "scattering length," a quantity $\Gamma(v)$ associated to integrable $v \geq 0$ that is somewhat parallel to the notion of capacity of a set. In fact, if K is a compact set satisfying a mild regularity condition,

$$\operatorname{cap} K = \lim_{r \to +\infty} \Gamma(r\chi_K), \tag{1.3}$$

where χ_K denotes the characteristic function of K. We will recall the definition of $\Gamma(v)$ in §2. Our main result is the following.

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Theorem 1.1 *Given $V \geq 0$, $V \in L^1_{\text{loc}}(\mathbb{R}^n)$, the following three conditions are equivalent.*

(1) *$-\Delta + V$ has purely discrete spectrum on $L^2(\mathbb{R}^n)$.*

(2) *Given $A \in (0, \infty)$, there exists $b = b(A) \in (0, 1]$ and $R \in (0, \infty)$ such that*

$$\Gamma(b^2 V_{b,\xi}) \geq Ab^2, \quad \text{for } |\xi| \geq R.$$

(3) *Given $A \in (0, \infty)$, there exists $b_0 = b_0(A) \in (0, 1]$ and $R \colon (0, b_0] \to (0, \infty)$ such that*

$$\Gamma(b^2 V_{b,\xi}) \geq Ab^2, \quad \text{for } b \in (0, b_0],\ |\xi| \geq R(b).$$

Here $V_{b,\xi}$ is a positive function supported on the unit cube $Q = Q_{1,0}$, given by

$$V_{b,\xi}(x) = V(bx + \xi), \quad x \in Q. \tag{1.4}$$

The rest of this paper is structured as follows. In §2 we define $\Gamma(v)$ for positive, integrable v and review some of its crucial properties. In §3 we prove that (2) $\Rightarrow$ (1) in Theorem 1.1, and in §4 we prove that (1) $\Rightarrow$ (3). Clearly (3) $\Rightarrow$ (2), so this will prove Theorem 1.1. There is one result in §4, Lemma 4.2, whose proof is presented in §5.

Remark In the formal limit $V = +\infty$ on $K = \mathbb{R}^n \setminus \Omega$, where one considers $-\Delta$ on $L^2(\Omega)$, with the Dirichlet boundary condition on $\partial\Omega$, the condition (3) of Theorem 1.1 becomes that for each $A \in (0, \infty)$, there exists $b_0 = b_0(A) \in (0, 1]$ and $R \colon (0, b_0] \to (0, \infty)$ such that

$$\operatorname{cap} K_{b,\xi} \geq Ab^2(\operatorname{cap} Q_{b,\xi}), \quad \forall\, b \in (0, b_0],\ |\xi| \geq R(b), \tag{1.5}$$

where $K_{b,\xi} = K \cap Q_{b,\xi}$. This coincides with one of the criteria (necessary and sufficient) for discreteness presented in [MS, Remark 2.7].

2 Scattering Length

Here we define the scattering length $\Gamma(v)$ of a positive integrable potential v and review some of its properties. Our material is taken from [T], which in turn was influenced by results on scattering length presented in [K, KL]. For simplicity we take $n \geq 3$.

To such v we associate the capacitory potential U_v and the scattering length $\Gamma(v)$ as follows. First assume that $v \in L^2(\mathbb{R}^n)$ and has support in a compact set K, as well as $v \geq 0$. We define U_v by

$$U_v(x) = \lim_{\varepsilon \searrow 0} (\varepsilon + v - \Delta)^{-1} v(x). \tag{2.1}$$

It is shown that this limit exists in $L^2_{\text{loc}}(\mathbb{R}^n)$ and satisfies

$$0 \leq U_v \leq 1, \quad v \leq w \Rightarrow U_v \leq U_w. \tag{2.2}$$

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The existence proof in [K, KL] involves producing the formula

$$U_v(x) = E_x\Big\{1 - \exp\Big(-\int_0^\infty v(b(\tau))\,d\tau\Big)\Big\}, \tag{2.3}$$

where E_x is expectation with respect to Wiener measure on Brownian paths b starting at x; see also [T, p. 292] for a derivation of this formula.

The function U_v solves the PDE

$$\Delta U_v = -v(1 - U_v). \tag{2.4}$$

It follows that $-\Delta U_v = \mu_v$ is a positive measure on $\mathbb{R}^n$. We set

$$\Gamma(v) = \int d\mu_v(x). \tag{2.5}$$

Some basic results on $\Gamma(v)$ include:

$$\begin{gathered} v \le w \Longrightarrow \Gamma(v) \le \Gamma(w), \\ \Gamma(v + w) \le \Gamma(v) + \Gamma(w), \\ v_n \nearrow v \Longrightarrow \Gamma(v_n) \nearrow \Gamma(v), \\ \Gamma(v) \le \|v\|_{L^1}. \end{gathered} \tag{2.6}$$

We also have

$$\|\nabla U_v\|^2_{L^2(\mathbb{R}^n)} = \int_{\mathbb{R}^n} U_v(x)\,d\mu_v(x) \le \Gamma(v), \tag{2.7}$$

and, for any ball $B \subset \mathbb{R}^n$,

$$\|U_v\|_{L^1(B)} \le \alpha(B)\Gamma(v). \tag{2.8}$$

These results are established in [T, Propositions 1.2–1.6]. They allow us to define U_v and $\Gamma(v)$ for positive $v \in L^1(\mathbb{R}^n)$, having

$$v_n \nearrow v, \;\; v_n \in L^2_{\mathrm{comp}}(\mathbb{R}^n) \Longrightarrow U_{v_n} \nearrow U_v, \;\; \Gamma(v_n) \nearrow \Gamma(v). \tag{2.9}$$

We now give two key estimates, established in [T], which connect scattering length to eigenvalue estimates. Suppose $v \ge 0$ is an integrable function supported on Q, the cube of sidelength 1 centered at 0. Let $\lambda_1(v) \in [0, \infty)$ denote the smallest eigenvalue of $-\Delta + v$, with the Neumann boundary condition, on $L^2(Q)$. The following result summarizes [T, Propositions 2.2–2.3].

Proposition 2.1 *There exists $C_n \in (0, \infty)$ such that*

$$\lambda_1(v) \ge C_n \Gamma(v). \tag{2.10}$$

Furthermore, there exist $E_n, \widetilde{C}_n \in (0, \infty)$ such that

$$\Gamma(v) \le E_n \Longrightarrow \lambda_1(v) \le \widetilde{C}_n \Gamma(v). \tag{2.11}$$

We refer to [T, pp. 295–297] for proofs of these results. We mention that (2.11) is proven by an apt choice of test function in the variational characterization of $\lambda_1(v)$, while (2.10) is proven by examining the decay rate for e^{-tL_N}, where L_N denotes $-\Delta + v$, with the Neumann boundary condition, on $L^2(Q)$.

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3 Sufficient Condition for Discrete Spectrum

The following result yields the implication (2) ⇒ (1) in Theorem 1.1.

Proposition 3.1 *Take $A \in (0, \infty)$ and let C_n be as in* (2.10). *Assume that there exists $b = b(A) \in (0, 1]$ and $R = R(A) \in (0, \infty)$ such that*

$$C_n \Gamma(b^2 V_{b,\xi}) \geq A b^2, \quad \text{for } |\xi| \geq R. \tag{3.1}$$

Then

$$\text{ess spec}(-\Delta + V) \subset [A, \infty). \tag{3.2}$$

Proof Let $Q_{b,\xi}$ denote the cube of edge b, center ξ, as in (1.2), and let $L_{b,\xi}$ denote the operator $-\Delta + V$ on $L^2(Q_{b,\xi})$, with the Neumann boundary condition. A standard argument involving Rellich's theorem shows that, if there exists $R = R(A)$ such that

$$\text{spec } L_{b,\xi} \subset [A, \infty), \quad \text{for } |\xi| \geq R, \tag{3.3}$$

then (3.2) holds. Now $L_{b,\xi}$ is unitarily equivalent to the operator

$$-b^{-2}\Delta + V_{b,\xi} = b^{-2}(-\Delta + b^2 V_{b,\xi}), \tag{3.4}$$

on $L^2(Q)$ (Q denoting the cube of edge 1, center 0), where

$$V_{b,\xi}(x) = V(bx + \xi), \quad x \in Q, \tag{3.5}$$

and one places the Neumann boundary condition on the operator (3.4). Now, by Proposition 2.1, the spectrum of this operator is bounded below by

$$C_n b^{-2} \Gamma(b^2 V_{b,\xi}), \tag{3.6}$$

so Proposition 3.1 is proven. ■

4 Necessary Condition for Discrete Spectrum

It is convenient to set up some notation. Given a cube $Q_\nu \subset \mathbb{R}^n$, we denote by

$$\lambda_D^{Q_\nu}(-\Delta + V), \quad \text{resp.,} \quad \lambda_N^{Q_\nu}(-\Delta + V), \tag{4.1}$$

the smallest eigenvalue of $-\Delta + V$ on $L^2(Q_\nu)$, where we impose, respectively, the Dirichlet or Neumann boundary condition on ∂Q_ν. As before, let $Q_{b,\xi}$ denote the cube of edge b, center ξ, as in (1.2). We continue to assume $V \geq 0$ and $V \in L^1_{\text{loc}}(\mathbb{R}^n)$.

Lemma 4.1 *If $-\Delta + V$ has discrete spectrum on $L^2(\mathbb{R}^n)$, then for each $b \in (0, 1]$,*

$$\lambda_D^{Q_{b,\xi}}(-\Delta + V) \longrightarrow +\infty, \quad \textit{as } |\xi| \to \infty. \tag{4.2}$$

Proof As is well known, $-\Delta + V$ has discrete spectrum on $L^2(\mathbb{R}^n)$ if and only if the set

$$X = \{u \in H^1(\mathbb{R}^n) : \|\nabla u\|_{L^2}^2 + \|V^{1/2}u\|_{L^2}^2 \le 1\} \tag{4.3}$$

is compact in $L^2(\mathbb{R}^n)$. In turn, such compactness implies

$$\int_{|x|\ge R} |u(x)|^2 \, dx \le \varepsilon(R), \quad \forall\, u \in X, \tag{4.4}$$

where $\varepsilon(R) \to 0$ as $R \to \infty$. If we restrict attention to $u \in H_0^1(Q_{b,\xi})$, this gives (4.2). ■

In the following lemma, $Q = Q_{1,0}$, the unit cube centered at 0.

Lemma 4.2 *There exists $A_n \in (0,\infty)$ and $B_n \colon [A_n,\infty) \to (0,\infty)$, such that $B_n(A) \to \infty$ as $A \to \infty$, and such that whenever $v \in L^1(Q)$ is non-negative and whenever $A \ge A_n$,*

$$\lambda_D^Q(-\Delta + v) \ge A \Longrightarrow \lambda_N^Q(-\Delta + v) \ge B_n(A). \tag{4.5}$$

Such a result is established in [Mol]; a proof is also given in [KS, Lemma 2.9]. For the convenience of the reader, we present yet another proof of Lemma 4.2 in §5. Granted the result, we deduce from Lemma 4.1 the following.

Corollary 4.3 *If $-\Delta + V$ has discrete spectrum on $L^2(\mathbb{R}^n)$, then, for each $b \in (0,1]$,*

$$\lambda_N^{Q_{b,\xi}}(-\Delta + V) \longrightarrow +\infty, \quad \textit{as } |\xi| \to \infty. \tag{4.6}$$

Note that the left side of (4.6) is equal to

$$b^{-2}\lambda_N^Q(-\Delta + b^2 V_{b,\xi}). \tag{4.7}$$

We are now ready to prove the implication (1) ⇒ (3) in Theorem 1.1. Given $A \in (0,\infty)$, pick $b_0 = b_0(A)$ so small that (2.11) applies, so that

$$\Gamma(v) \le b_0^2 A \Longrightarrow \lambda_N^Q(-\Delta + v) \le \widetilde{C}_n \Gamma(v). \tag{4.8}$$

Consequently, for $b \in (0, b_0]$,

$$\Gamma(b^2 V_{b,\xi}) \le Ab^2 \Rightarrow \lambda_N^Q(-\Delta + b^2 V_{b,\xi}) \le \widetilde{C}_n \Gamma(b^2 V_{b,\xi}) \le \widetilde{C}_n A b^2. \tag{4.9}$$

Now, by (4.6)–(4.7), we cannot have the bound $\lambda_N^Q(-\Delta + b^2 V_{b,\xi}) \le \widetilde{C}_n A b^2$ for large $|\xi|$, so consequently we cannot have the bound $\Gamma(b^2 V_{b,\xi}) \le Ab^2$ for large $|\xi|$. The proof of Theorem 1.1 is complete, modulo the proof of Lemma 4.2, which will be given in the next section.

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5 Proof of Lemma 4.2

Given non-negative $v \in L^1(Q)$, let us denote by L_D the operator $L = -\Delta + v$ on $L^2(Q)$ with the Dirichlet boundary condition and by L_N the operator with the Neumann boundary condition. We assume

$$\lambda = \lambda_D^Q(-\Delta + v), \tag{5.1}$$

the smallest eigenvalue of L_D, is large, and we want to estimate the smallest eigenvalue of L_N. We will estimate various "heat semigroups." For $x, y \in Q,\ t > 0$, set

$$\begin{aligned} p_D(t,x,y) &= e^{-tL_D}\delta_y(x), \quad p_N(t,x,y) = e^{-tL_N}\delta_y(x), \\ p_Q(t,x,y) &= e^{t\Delta_N}\delta_y(x), \quad p_0(t,x,y) = (4\pi t)^{-n/2}e^{-|x-y|^2/4t}. \end{aligned} \tag{5.2}$$

Here Δ_N denotes the Laplace operator on $L^2(Q)$, with the Neumann boundary condition. It will be convenient to note the following inequalities:

$$p_D(t,x,y) \le p_0(t,x,y), \quad p_N(t,x,y) \le p_Q(t,x,y). \tag{5.3}$$

We want to estimate $p_N(t,x,y)$, but first we will estimate $p_D(t,x,y)$. Let us fix $a \in (0,1)$ and set

$$\tau = \lambda^{-a}. \tag{5.4}$$

Using (5.3) we have

$$\|e^{-\tau L_D}\|_{\mathcal{L}(L^1,L^2)} \le (4\pi\tau)^{-n/4}, \quad \|e^{-\tau L_D}\|_{\mathcal{L}(L^2,L^\infty)} \le (4\pi\tau)^{-n/4}, \tag{5.5}$$

while (5.1) gives

$$\|e^{-\tau L_D}\|_{\mathcal{L}(L^2,L^2)} \le e^{-\tau\lambda}. \tag{5.6}$$

Hence

$$\|e^{-3\tau L_D}\delta_y\|_{L^\infty} \le C\tau^{-n/2}e^{-\tau\lambda} = C\lambda^{an/2}e^{-\lambda^{1-a}}. \tag{5.7}$$

In other words,

$$0 \le p_D(3\tau,x,y) \le C\lambda^{an/2}e^{-\lambda^{1-a}}, \quad \forall\, x,y \in Q. \tag{5.8}$$

Next, we estimate $V_y(t,x) = p_N(t,x,y) - p_D(t,x,y)$, for $t \in [0,3\tau]$. We have

$$(\partial_t - L)V_y = 0 \ \text{ on } \mathbb{R}^+ \times Q, \quad V_y(0,x) = 0, \tag{5.9}$$

and $x \in \partial Q \Longrightarrow V_y(t,x) = p_N(t,x,y)$. Hence

$$x \in \partial Q \Longrightarrow 0 \le V_y(t,x) \le p_Q(t,x,y). \tag{5.10}$$

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Let us define the set $\Omega_\tau \subset Q$ by

$$\Omega_\tau = \{y \in Q : \operatorname{dist}(y, \partial Q) \geq \tau^{1/3}\}. \tag{5.11}$$

It is clear that, if λ is sufficiently large, so τ is sufficiently small,

$$x \in \partial Q,\ y \in \Omega_\tau,\ t \in [0, 3\tau] \Rightarrow p_Q(t, x, y) \leq Ce^{-\lambda^{a/4}}, \tag{5.12}$$

so applying the maximum principle to (5.9)–(5.10) gives

$$V_y(t, x) \leq Ce^{-\lambda^{a/4}}, \quad \text{for } x \in Q,\ y \in \Omega_\tau,\ t \in [0, 3\tau], \tag{5.13}$$

and hence, by (5.8), if we take $a = 4/5$ and assume λ is sufficiently large,

$$0 \leq p_N(3\tau, x, y) \leq C\lambda^{2n/5}e^{-\lambda^{1/5}}, \quad \forall\, x \in Q,\ y \in \Omega_\tau. \tag{5.14}$$

Now, using the semigroup property of e^{tL_N} and the fact that $\|e^{-tL_N}\|_{\mathcal{L}(L^\infty, L^\infty)} \leq 1$, we deduce that

$$0 \leq p_N(t, x, y) \leq C\lambda^{2n/5}e^{-\lambda^{1/5}}, \quad \forall\, x \in Q,\ y \in \Omega_\tau,\ t \geq 3\tau. \tag{5.15}$$

In particular, if λ is large enough that $3\tau = 3\lambda^{-4/5} < 1$, the estimate (5.15) applies with $t = 1$. On the other hand, we can use (5.3) to obtain

$$p_N(1, x, y) \leq p_Q(1, x, y) \leq C, \quad \forall\, x \in Q,\ y \in Q \setminus \Omega_\tau. \tag{5.16}$$

It follows that

$$\begin{aligned} \int_Q p_N(1, x, y)\, dy &\leq C\lambda^{2n/5}e^{-\lambda^{1/5}} + C \operatorname{Vol}(Q \setminus \Omega_\tau) \\ &\leq C\lambda^{2n/5}e^{-\lambda^{1/5}} + C\lambda^{-4/15}. \end{aligned} \tag{5.17}$$

Of course $p_N(1, x, y) = p_N(1, y, x)$, so there is a similar bound on $\int_Q p_N(1, x, y)\, dx$. Hence we deduce that

$$\|e^{-L_N}\|_{\mathcal{L}(L^2, L^2)} \leq C\lambda^{2n/5}e^{-\lambda^{1/5}} + C\lambda^{-4/15} = \Phi(\lambda). \tag{5.18}$$

It follows that

$$\lambda_N^Q(-\Delta + v) \geq \log \frac{1}{\Phi(\lambda)}, \tag{5.19}$$

and Lemma 4.2 is proven.

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