Singular Schrödinger Operators as Limits of Point Interaction Hamiltonians

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Abstract

In this paper we give results on the approximation of (generalized) Schrödinger operators of the form $-\Delta + \mu$ for some finite Radon measure μ on $\mathbf{R}^d$. For $d = 1$ we shall show that weak convergence of measures μ_n to μ implies norm resolvent convergence of the operators $-\Delta + \mu_n$ to $-\Delta + \mu$. In particular Schrödinger operators of the form $-\Delta + \mu$ for some finite Radon measure μ can be regularized or approximated by Hamiltonians describing point interactions. For $d = 3$ we shall show that a fairly large class of singular interactions can be regarded as limit of point interactions.

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1 Introduction

The dynamics of a quantum particle in $\mathbf{R}^d$ is usually specified by the unitary group generated on $L^2(\mathbf{R}^d)$ by a self–adjoint operator $-\Delta + V$ (referred to in the following as Hamiltonian or Schrödinger operator), where the function $V : \mathbf{R}^d \longrightarrow \mathbf{R}$ describes the interaction of the particle with the environment. Modelling such interaction requires often to extend our analysis to a wider class of Hamiltonians. Consider, e.g., a "quantum mechanical particle" interacting with a potential localized inside some closed subset N of $\mathbf{R}^d$ with Lebesgue measure zero. The corresponding Hamiltonian H must be a self–adjoint operator in $L^2(\mathbf{R}^d)$ and has to satisfy the following condition.

$$\begin{array}{c} C_0^\infty(\mathbf{R}^d \setminus N) \subset D(H) \quad \text{and} \\ Hf = -\Delta f, \quad f \in C_0^\infty(\mathbf{R}^d \setminus N), \\ \text{but} \quad H \not\equiv -\Delta. \end{array} \tag{1}$$

One can easily check that $Hf = H'f$ for every $f \in D(H) \cap D(H')$ if both H and H' are self–adjoint operators in $L^2(\mathbf{R}^d)$ and satisfy condition (1). Thus Hamiltonians describing an interaction taking place inside N do not differ from each other in the way they act on a vector but only because they have different domains. Potentials localized inside some closed set with Lebesgue measure zero are then characterized in a rather implicit way via the domain $D(H)$ of the corresponding Hamiltonian H.

Dependence of spectral and dynamical properties on the potential function was extensively analized since the early days of Quantum Mechanics. In the more general setting of Schrödinger operators with "singular potentials" new techniques are required to investigate the dependence of the above mentioned properties on the domains of the corresponding Hamiltonians.

In the following we list some additional problems one is faced by in the theory of "singular Schrödinger operators". First of all one wants to characterize the closed subsets N of $\mathbf{R}^d$ such that there exists a self–adjoint operator H in $L^2(\mathbf{R}^d)$ satisfying condition (1). This problem has been solved a long time ago: it immediately follows from Hedberg's theorem on the spectral synthesis in Sobolev spaces that there exists a self–adjoint operator H in $L^2(\mathbf{R}^d)$ satisfying condition (1) if and only if the c_2–capacity of N is strictly positive. Here for $j = 1, 2, \ldots,$ and every compact subset C of $\mathbf{R}^d$ the c_j–capacity

$c_j(C)$ of C is defined by

$$c_j(C) := \inf\{\| f \|_{H^j}^2 : f \in C_0^\infty(\mathbf{R}^d), \quad f(x) \geq 1 \quad \forall x \in C\}.$$

$\| \cdot \|_{H^j}$ denotes the norm in the Sobolev space $H^j(\mathbf{R}^d)$, i.e. the space of square integrable functions such that all partial derivatives up to order j are also square integrable. For an arbitrary Borel set B the c_j–capacity of B is defined by

$$c_j(B) := \sup c_j(C)$$

where the supremum is taken over all compact subsets C of B.

Further questions are, of course, how to construct and how to represent self–adjoint operators H in $L^2(\mathbf{R}^d)$ satisfying condition (1). One canonical idea is to use operators of the form $-\Delta + \mu$ for some measure μ; for convenience of the reader we shall recall the definition of such operators in the next section. When $d\mu = V\,dx$ for some function V then we have $-\Delta + \mu = -\Delta + V$, i.e. the class of operators of the form $-\Delta + \mu$ is fairly large and contains the class of all "usual" lower semi–bounded Schrödinger operators of the form $-\Delta + V$. If the measure μ is supported by the set N and $\mu \neq 0$ then the self–adjoint operator $-\Delta+\mu$ satisfies condition (1). Thus via the ansatz $H = -\Delta + \mu$ it is sometimes possible to replace the difficult problem to investigate the dependence of the spectral and dynamical properties of a system on the domain $D(H)$ of the corresponding Hamiltonian H by the problem to investigate the dependence on the measure μ. Actually after some preparatory work quite often it is possible to treat operators of the form $-\Delta+\mu$ in the same way as "usual Schrödinger operators", cf., e.g., [12]. We refer to [1], [5], [7], [9], [12], [14], [15], [16], [18], [22] and references given therein for results on the spectral and the scattering theory of operators of the form $-\Delta + \mu$.

There is no measure μ such that the operator $-\Delta + \mu$ satisfies condition (1) if the c_1–capacity of N equals zero, cf., e.g, [1]. Thus if $c_2(N) > 0$ but $c_1(N) = 0$, which for instance is true when the non–empty set N is discrete and $d = 2$ or $d = 3$, then one needs other methods for the construction of operators satisfying condition (1). Cf. [1], [3], [10], [13], [20], [21], [26] and references given therein for different ways to achieve this result.

In addition to the existence and the representation problem already mentioned above one is led to extremely interesting and difficult convergence problems when one investigates "singular Schrödinger operators".

Since such operators are regarded as idealizations of "usual Schrödinger operators" one wants to know whether it is possible to approximate "singular Schrödinger operators" by "usual" ones. For point interactions, i.e. when the set N is discrete, strong convergence results are available, cf. the monograph [4] by S.Albeverio, F.Gesztesy, R.Høegh–Krohn, H.Holden. We refer to [2], [6] and [24] for results in more general cases.

In the framework of "singular Schrödinger operators" relevant quantities are quite often explicitly computable, the most striking example being when the singular set N is finite, cf. the book [4] mentioned above; other solvable models have been presented, e.g., in [8] and [11]. One is then naturally led to analize an "inverse" convergence problem : how to approximate operators of the form $-\Delta + V$ for some function V, or even more generally operators of the form $-\Delta + \mu$ for some measure μ, by "singular Schrödinger operators" H_n, $n \in \mathbf{N}$, with the property that every H_n leads to a completely solvable theory.

When the dimension d of $\mathbf{R}^d$ equals one then one can easily get very strong convergence results. In fact, in the next section we shall prove that the operators $-\Delta + \mu_n$ converge in the norm resolvent sense to $-\Delta + \mu$ provided μ and every μ_n are finite Radon measures on $\mathbf{R}$, i.e. the difference of two finite positive measures on the Borel–σ –algebra of $\mathbf{R}$, and μ_n weakly converges to μ, i.e.

$$\int f \, d\,\mu_n \longrightarrow \int f \, d\,\mu$$

for all f in the space $C_b(\mathbf{R})$ of bounded continuous functions on $\mathbf{R}$. This implies that for every finite Radon measure μ on $\mathbf{R}$ the operator $-\Delta + \mu$ can be regularized, i.e. approximated in the norm resolvent sense, by operators of the form $-\Delta + V_n$ where all the V_n are C_0^∞–functions. Moreover it can also be approximated in the norm resolvent sense by operators of the form $-\Delta + \mu_n$ where for every $n \in \mathbf{N}$ the measure μ_n is a finite linear combination of Dirac–measures. We recall that one can easily and explicitly calculate all the spectral quantities and scattering data of operators of the form $-\Delta + \mu$ provided μ is a finite linear combination of Dirac measures. It is noteworthy that for every finite Radon measure μ on $\mathbf{R}$ the operator $-\Delta + \mu$ can be approximated via Monte Carlo methods, cf. Corollary 5. This fact might be interesting with a view to applications in the theory of random media, cf., e.g., the discussion of this point in [17]

In section 3 we shall concentrate on the much more difficult three– dimensional case. For a fairly large class of measures μ we shall prove that the operator $-\Delta + \mu$ can be approximated in the strong resolvent sense by operators describing point interactions which take place at only finitely many points; we refer to section 3 for the precise definition. Thus for a fairly large class of measures μ the operator $-\Delta + \mu$ can be approximated by operators with the property that one can easily and explicitly calculate all their spectral and scattering data. Our results in section 3 extend the results in [17].

2 One–dimensional results

In this section we shall concentrate on convergence results in the one– dimensional case. By Sobolev's embedding theorem, every element of the Sobolev space $H^1(\mathbf{R})$ has a unique continuous representative and for every $a > 0$ there exists a $b < \infty$ such that

$$\| f \|_\infty^2 \leq a \int | \nabla f |^2 dx + b \| f \|^2, \quad f \in H^1(\mathbf{R}). \tag{2}$$

We will denote a continuous function and its equivalence class with respect to some measure by the same symbol. In every case it will be clear from the context what is meant. Let μ be a finite Radon measure on $\mathbf{R}$. We put

$$\begin{aligned} D(\mathbf{D}^\mu) &:= H^1(\mathbf{R}), \\ \mathbf{D}^\mu(f,g) &:= \int \nabla \bar{f} \cdot \nabla g \, dx + \int \bar{f} \, g \, d\mu, \quad f, g \in H^1(\mathbf{R}). \end{aligned} \tag{3}$$

It is well known and easily checked that $\mathbf{D}^\mu$ is a lower semi–bounded closed quadratic form in $L^2(\mathbf{R})$. We shall denote by $-\Delta+\mu$ the self–adjoint operator associated with $\mathbf{D}^\mu$ in the sense of the representation theorem [25], Theorem VIII.15, i.e. $-\Delta + \mu$ is the unique self–adjoint operator in $L^2(\mathbf{R})$ such that

$$D(-\Delta + \mu) \subset D(\mathbf{D}^\mu), \tag{4}$$

$$((-\Delta + \mu) f, g) = \mathbf{D}^\mu(f,g), \quad f \in D(-\Delta + \mu), \quad g \in D(\mathbf{D}^\mu). \tag{5}$$

We shall show that weak convergence of the finite Radon measures μ_n to the finite Radon measure μ implies norm resolvent convergence of the operators $-\Delta+\mu_n$ to the operator $-\Delta+\mu$. To prove this result we need the two following lemmata. We shall denote by $\hat{\mu}$ the Fourier transform of μ.

Lemma 1 *Let μ_n, $n \in \mathbf{N}$, and μ be finite Radon measures on $\mathbf{R}$. Suppose that $\mu_n \longrightarrow \mu$ weakly. Then*

$$\sup_{n\in\mathbf{N}} \| \hat{\mu}_n \|_\infty < \infty.$$

Proof: Obviously for every finite Radon measure ν on $\mathbf{R}$

$$\nu(f) := \int f\, d\,\nu, \quad f \in C_b(\mathbf{R}),$$

defines a bounded linear functional on the Banach space $(C_b(\mathbf{R}), \| \cdot \|_\infty)$. Weak convergence of the measures μ_n implies pointwise boundedness of the associated bounded functionals μ_n. By the uniform boundedness principle, this implies that $C := \sup_{n\in\mathbf{N}} \| \mu_n \| < \infty$ where here $\| \mu_n \|$ denotes the operator norm of the functional μ_n. Since for every $n \in \mathbf{N}$ and every $x \in \mathbf{R}$

$$| \hat{\mu}_n(x) | = | \mu_n(e^{ix(\cdot)}) | \le \| e^{ix(\cdot)} \|_\infty \cdot \| \mu_n \| \le C$$

the lemma is proved. $\square$

Lemma 2 *Let μ_n, $n \in \mathbf{N}$, and μ be finite Radon measures on $\mathbf{R}$. Suppose that*

$$\mu_n \longrightarrow \mu \quad \textit{weakly.}$$

Then

$$\sup \Big| \int | f |^2 d\,\mu - \int | f |^2 d\,\mu_n \Big| \longrightarrow 0$$

where the suprema are taken over all $f \in H^1(\mathbf{R})$ such that $\| f \|_{H^1} = 1$.

Proof: It is well known that there exists a unique $J \in L^2(\mathbf{R})$ such that

$$\begin{aligned} \hat{J}(p) &= \frac{1}{\sqrt{1+p^2}} \quad \text{a.e,} && (6)\\ \int J(x-y)\, f(y)\, dy &= (-\Delta+1)^{-1/2} f(x) \quad \text{a.e.,} \quad f \in L^2(\mathbf{R}). \end{aligned}$$

Let $g \in H^1(\mathbf{R})$. We have

$$\begin{aligned}
|\int g\,d\nu\,| &= |\int(-\Delta+1)^{-1/2}(-\Delta+1)^{1/2}g\,d\nu\,| \\
&= |\int\int J(x-y)(-\Delta+1)^{1/2}g(y)\,dy\,\nu(dx)\,| \\
&= |\int\int J(x-y)\,\nu(dx)\,(-\Delta+1)^{1/2}g(y)\,dy\,| \\
&\leq \|\,J*\nu\,\|\,\|\,(-\Delta+1)^{1/2}g\,\| \\
&= \|\,\frac{1}{\sqrt{2\,\pi}}\,\hat{J}\cdot\hat{\nu}\,\|\,\|\,g\,\|_{H^1}
\end{aligned}$$

for every finite Radon measure ν on $\mathbf{R}$. In the third step it is justified to change the order of integration since

$$\begin{aligned}
\int\int|\,J(x-y)\,|\,|\,h(y)\,|\,dy\,|\,\nu\,|\,(dx) &\leq \int\|\,J(x-\,\cdot)\,\|\,\|\,h\,\|\,|\,\nu\,|\,(dx) \\
&= \int\|\,J\,\|\,\|\,h\,\|\,|\,\nu\,|\,(dx)<\infty
\end{aligned}$$

for every $h \in L^2(\mathbf{R})$. By (6), we now get that

$$|\int g\,d\,(\mu_n-\mu)\,| \leq \|\,g\,\|_{H^1}\left(\int\frac{1}{1+p^2}\,|\,\hat{\mu}_n(p)-\hat{\mu}(p)\,|^2dp\right)^{1/2}. \tag{7}$$

Since the sequence $\{\mu_n\}_{n\in\mathbf{N}}$ weakly converges to μ we have that $\hat{\mu}_n(p) \longrightarrow \hat{\mu}(p)$ for every $p \in \mathbf{R}$ and, by the previous lemma, $\sup_{n\in\mathbf{N}}\|\,\hat{\mu}_n-\hat{\mu}\,\|_\infty < \infty$. Thus we have

$$\int\frac{1}{1+p^2}\,|\,\hat{\mu}_n(p)-\hat{\mu}(p)\,|^2dp \longrightarrow 0. \tag{8}$$

Let $f \in H^1(\mathbf{R})$. It is well known that then also $|\,f\,|^2 \in H^1(\mathbf{R})$ and

$$\|\,|\,f\,|^2\|_{H^1} \leq 2\sqrt{2}\,\|\,f\,\|_{H^1}^2. \tag{9}$$

By (7), (8) and (9), the lemma is proved. □

Theorem 3 *Let μ_n, $n \in \mathbf{N}$, and μ be finite Radon measures on $\mathbf{R}$. Suppose that $\mu_n \longrightarrow \mu$ weakly. Then the operators $-\Delta+\mu_n$ converge to the operator $-\Delta+\mu$ in the norm resolvent sense.*

Proof: By Sobolev's inequality (2), we can choose $b < \infty$ such that

$$\mathbf{D}^{\mu}(f,f) + b \, \| f \|^2 \geq (1/2) \, \| f \|_{H^1}^2 \geq 0, \quad f \in H^1(\mathbf{R}). \tag{10}$$

By the previous lemma, there exists $n_0 \in \mathbf{N}$ such that for all $f \in H^1(\mathbf{R})$ and all $n \geq n_0$ the following holds:

$$\left| \int | f |^2 d\,\mu_n - \int | f |^2 d\,\mu \right| \leq (1/2) \, \| f \|_{H^1}^2$$

and therefore

$$\begin{aligned} \int | f |^2 d\,\mu_n &\geq \int | f |^2 d\,\mu - (1/2) \, \| f \|_{H^1}^2 \\ &\geq -\int | \nabla f |^2 dx - (b+1) \, \| f \|^2. \end{aligned}$$

Thus the lower semi–bounded closed quadratic forms $\mathbf{D}^{\mu_n}$, $n \in \mathbf{N}$, have a joint lower bound. Thus the theorem immediately follows from (10), the previous lemma and the following Theorem 4. □

Theorem 4 (cf, e.g., [25], Theorem VIII.25)
Let $\mathcal{E}_n$, $n \in \mathbf{N}$, and $\mathcal{E}$ be lower semi–bounded closed quadratic forms in some Hilbert space $\mathcal{H}$. Suppose that all the forms $\mathcal{E}_n$, $n \in \mathbf{N}$, and $\mathcal{E}$ have a common lower bound $c > -\infty$ and the same domain D, D is dense in $\mathcal{H}$ and

$$\sup | \mathcal{E}_n(f,f) - \mathcal{E}(f,f) | \longrightarrow 0$$

where the suprema are taken over all $f \in D$ such that $\mathcal{E}(f,f) + (1-c) \, \| f \|^2 = 1$. Let H_n, $n \in \mathbf{N}$, and H be the self–adjoint operator associated with $\mathcal{E}_n$, $n \in \mathbf{N}$, and $\mathcal{E}$, respectively. Then $H_n \longrightarrow H$ in the norm resolvent sense.

By Theorem 3, operators of the form $-\Delta + \mu$ can be regularized, i.e., approximated by operators of the form $-\Delta + V$, where V is some C_0^∞–function. In fact, let μ be a finite Radon measure on $\mathbf{R}$. Let $\mu_n := 1_{(-n,n)} \cdot \mu$ and $j_n(x) := n\, j(nx)$ for every $x \in \mathbf{R}$ for every $n \in \mathbf{N}$ where j is any C_0^∞–function such that $j \geq 0$ and $\int j \, dx = 1$. It is well known and easily seen that

$$\begin{aligned} V_n := j_n * \mu_n \in C_0^\infty(\mathbf{R}), \quad n \in \mathbf{N}, \\ V_n \,\mathrm{dx} \longrightarrow \mu \quad \text{weakly.} \end{aligned}$$

By Theorem 3, it follows that

$$-\Delta + V_n \longrightarrow -\Delta + \mu$$

in the norm resolvent sense.

On the other hand one can also explicitly give measures μ_n, $n \in \mathbf{N}$, such that μ_n is a finite linear combination of Dirac measures for every $n \in \mathbf{N}$ and

$$\mu_n \longrightarrow \mu \quad \text{weakly.}$$

By Theorem 3, it follows that

$$-\Delta + \mu_n \longrightarrow -\Delta + \mu$$

in the norm resolvent sense. We recall that for the approximands $-\Delta + \mu_n$ one can explicitly compute all the quantities one is interested in.

It is noteworthy that the finite linear combinations of Dirac measures in the above considerations can be randomly chosen, cf. the following corollary of Theorem 3. For a random variable X we shall denote by P_X its distribution, i.e. $P_X(B) = P(X \in B)$ for every Borel set B.

Corollary 5 *Let $\mu_\pm$ be positive measures on the Borel σ–algebra of $\mathbf{R}$ such that $c_\pm := \mu_\pm(\mathbf{R}) < \infty$. Let $X_j^\pm$, $j \in \mathbf{N}$, be pairwise independent random variables such that $c_\pm \, P_{X_j^\pm} = \mu_\pm$ for every $j \in \mathbf{N}$. Then almost surely we have*

$$-\Delta + c_+ \frac{1}{n} \sum_{j=1}^{n} \delta_{X_j^+} - c_- \frac{1}{n} \sum_{j=1}^{n} \delta_{X_j^-} \longrightarrow -\Delta + \mu$$

in the norm resolvent sense.

Proof: By the Theorem of Glivenko and Cantelli, almost surely the empirical distributions

$$\frac{1}{n} \sum_{j=1}^{n} \delta_{X_j}$$

of a sequence of pairwise independent random variables with joint distribution μ weakly converge to μ. Thus the corollary follows from Theorem 3. $\square$

3 Approximation via Hamiltonians describing point interactions

In this section we shall give results on the approximation of operators of the form $-\Delta + \mu$ in $L^2(\mathbf{R}^3)$ by Hamiltonians describing point interactions.

Since for $d > 1$ it is not true that every $f \in H^1(\mathbf{R}^d)$ has a continuous representative one needs some preparations for the definition of operators of the form $-\Delta + \mu$ and has to make some additional assumptions about the measure μ. A function $f : \mathbf{R}^d \longrightarrow \mathbf{C}$ will be called quasi continuous provided for every $\varepsilon > 0$ there exists an open set $U \subset \mathbf{R}^d$ such that $c_1(U) < \varepsilon$ and $f_{|\mathbf{R}^d \setminus U}$ is continuous. Every Lebesgue equivalence class $f \in H^1(\mathbf{R}^d)$ has a quasi continuous representative and if $\tilde{f}$ and f° are quasi continuous representatives of $f \in H^1(\mathbf{R}^d)$ then

$$c_1(\{x \in \mathbf{R}^d : \tilde{f}(x) \neq f^\circ(x)\}) = 0 \tag{11}$$

(cf., e.g., [19], [23]). In the following we shall denote by $\tilde{f}$ any quasi continuous representative of $f \in H^1(\mathbf{R}^d)$. By (11), the following statements will not depend on the special choice of the quasi continuous representative. Note that $c_1(B) > 0$ for every non–empty Borel set in $\mathbf{R}$ and therefore in the one–dimensional case the continuous functions are the only quasi continuous functions.

In the following let N be a non–empty closed subset of $\mathbf{R}^d$ and $\gamma : N \longrightarrow \mathbf{R}$ a bounded continuous function such that $\gamma \not\equiv 0$. Let m be a finite positive measure on the Borel σ–algebra of N such that $\mathrm{supp}(m) = N$, i.e., $m(U \cap N) > 0$ for every open subset U of $\mathbf{R}^d$ with $U \cap N \neq \emptyset$, and m belongs to the Kato class. We recall that for $d \geq 3$ this means that

$$\lim_{\varepsilon \downarrow 0} \sup_{x \in N} \int_{B_N(x,\varepsilon)} \frac{1}{|\, x - y\,|^{d-2}}\, m(dy) = 0 \tag{12}$$

where $B_N(x, \varepsilon) := \{y \in N : |\, x - y\,| < \varepsilon\}$. It is well known that under this assumption $m(B) = 0$ if $c_1(B) = 0$ and for every $a > 0$ there exists a $b > \infty$ such that

$$\int_N |\, \tilde{f}\,|^2 dm \leq a \int |\, \nabla f\,|^2 dx + b\, \|\, f\,\|^2, \quad f \in H^1(\mathbf{R}^d). \tag{13}$$

Thus, by the Kato–Lax–Milgram–Nelson Theorem, the quadratic form $\mathbf{D}^{\gamma m}$, defined by

$$\begin{aligned} D(\mathbf{D}^{\gamma m}) &:= H^1(\mathbf{R}^d), \\ \mathbf{D}^{\gamma m}(f,g) &:= \int \nabla \bar{f} \cdot \nabla g \, dx + \int_N \overline{\tilde{f}} \, \tilde{g} \, \gamma \, dm, \quad f,g \in H^1(\mathbf{R}^d), \end{aligned}$$

is lower semi–bounded and closed in $L^2(\mathbf{R}^d)$. We shall denote by $-\Delta + \gamma\, m$ the self–adjoint operator in $L^2(\mathbf{R}^d)$ associated with $\mathbf{D}^{\gamma m}$ in the sense of (4). One can easily show that this definition is equivalent to the one we have given in [12].

We can rewrite $-\Delta + \gamma\, m$ as $-\Delta - \frac{1}{\alpha}\, \mu$ where

$$\alpha := -\alpha_0 \operatorname{sgn}(\gamma), \quad \alpha_0 := \frac{1}{\int |\gamma| \, dm}, \quad \mu := \frac{|\gamma|\, m}{\int |\gamma| \, dm}. \tag{14}$$

Note that $|\alpha| \equiv \alpha_0$ and α is continuous on the set $\{\gamma \neq 0\} := \{x \in N : \gamma(x) \neq 0\}$ and $\mu(\{\gamma = 0\}) = 0$. We shall denote by $J : H^1(\mathbf{R}^d) \longrightarrow L^2(N, \mu)$ the mapping defined by

$$Jf := \tilde{f}_{|N} \quad \mu\text{–a.e.}, \quad f \in H^1(\mathbf{R}^d).$$

By (13), the operator J is bounded. Let $\lambda > 0$. We put $G^\lambda := (-\Delta + \lambda)^{-1}$. It is well known that there exists a unique continuous function on $\mathbf{R}^d \setminus \{0\}$ (on $\mathbf{R}$ when $d = 1$), which will be also denoted by G^λ, such that

$$G^\lambda f(x) = \int G^\lambda(x-y)\, f(y)\, dy \quad \text{a.e,} \quad f \in L^2(\mathbf{R}^d). \tag{15}$$

When $d = 3$ then

$$G^\lambda(x) = \frac{1}{4\pi\, |x|}\, e^{\sqrt{\lambda}\,|x|}, \quad x \in \mathbf{R}^3 \setminus \{0\}. \tag{16}$$

We put

$$G^\lambda_\mu h(x) := \int G^\lambda(x-y)\, h(y)\, \mu(dy) \tag{17}$$

whenever the expression on the right hand side is defined. By our results in [12], (17) defines an operator from $L^2(N,\mu)$ to $H^1(\mathbf{R}^d)$, JG^λ_μ is an integral operator in $L^2(N,\mu)$ with kernel $G^\lambda(x-y)$ and for all sufficiently large $\lambda > 0$

$$\| \frac{1}{\alpha}\, JG^\lambda_\mu \|_{2,2} < 1, \tag{18}$$

where here $\| T \|_{p,q}$ denotes the norm of T as an operator from $L^p(N,\mu)$ to $L^q(N,\mu)$ for $1 \leq p, q \leq \infty$. It is well known and easily follows from the Kato property and the finiteness of the measure μ that $JG_\mu^\lambda h$ has a continuous representative for every $h \in L^\infty(N,\mu)$ and

$$\| \frac{1}{\alpha} JG_\mu^\lambda \|_{\infty,\infty} \longrightarrow 0, \quad \lambda \longrightarrow \infty. \tag{19}$$

In the following let $\lambda > 0$ be such that both $\| \frac{1}{\alpha} JG_\mu^\lambda \|_{2,2} < 1$ and $\| \frac{1}{\alpha} JG_\mu^\lambda \|_{\infty,\infty} < 1$.

By our results in [12],

$$(-\Delta + \gamma m + \lambda)^{-1} f = G^\lambda f + G_\mu^\lambda \left(1 - \frac{1}{\alpha} JG_\mu^\lambda\right)^{-1} \frac{1}{\alpha} JG^\lambda f, \quad f \in L^2(\mathbf{R}^d).$$

Thus for every $f \in L^2(\mathbf{R}^d)$ we have

$$(-\Delta + \gamma m + \lambda)^{-1} f = G^\lambda f - G_\mu^\lambda \sigma \tag{20}$$

where $\sigma \in L^2(N,\mu)$ denotes the unique solution of the equation

$$\alpha \sigma - JG_\mu^\lambda \sigma = JG^\lambda f \quad \mu\text{–a.e} \tag{21}$$

By (18),

$$\left(1 - \frac{1}{\alpha} JG_\mu^\lambda\right)^{-1} = \sum_{n=0}^{\infty} \left(\frac{1}{\alpha} JG_\mu^\lambda\right)^n .$$

By (19) and (21), this implies that σ has a representative which is bounded and continuous on $\{\gamma \neq 0\}$ provided $G^\lambda f$ has a bounded continuous representative. Since, by Sobolev's embedding theorem, every $f \in H^2(\mathbf{R}^d)$ has a bounded continuous representative when $d \leq 3$ it follows that σ has a representative which is bounded and continuous on $\{\gamma \neq 0\}$ when $d \leq 3$.

In the following we shall consider the case when $d = 3$. We want to approximate $-\Delta + \gamma m$ by Hamiltonians describing point interactions which take place at only finitely many points. First we recall some definitions. Let $\lambda > 0$ and Y a non–empty finite subset of $\{\gamma \neq 0\}$. We shall denote by $\Gamma_{Y,\alpha}^\lambda$ the $|Y| \times |Y|$–matrix such that

$$\left(\Gamma_{Y,\alpha}^\lambda\right)_{xy} := \left(|Y|\, \alpha(x) + \frac{\sqrt{\lambda}}{4\pi}\right) \delta_{xy} - G^\lambda(x-y)\,(1 - \delta_{xy}). \tag{22}$$

Obviously the matrix $\Gamma^\lambda_{Y,\alpha}$ is invertible for all sufficiently large $\lambda > 0$. There exists a unique self–adjoint extension $H_{Y,\alpha}$ of the operator $-\Delta_{| C_0^\infty(\mathbf{R}^3\setminus Y)}$ such that λ is in the resolvent set $\rho(H_{Y,\alpha})$ of $H_{Y,\alpha}$ and

$$\begin{aligned} & (H_{Y,\alpha}+\lambda)^{-1} f \\ = \;& G^\lambda f + \Big(\underline{G}^\lambda(\cdot - Y), (\Gamma^\lambda_{Y,\alpha})^{-1}\underline{G}^\lambda f(Y)\Big) \quad \text{a.e.}, \; f \in L^2(\mathbf{R}^3), \end{aligned} \tag{23}$$

for every $\lambda > 0$ such that the matrix $\Gamma^\lambda_{Y,\alpha}$ is invertible, cf. [4], (II 1.1.33). Here $\underline{G}^\lambda(\cdot - Y)$ and $\underline{G}^\lambda f(Y)$ denote the vector in $\mathbf{C}^{|Y|}$ such that $\Big(\underline{G}^\lambda(\cdot - Y)\Big)_y = G^\lambda(\cdot - y)$ and $\Big(\underline{G}^\lambda f(Y)\Big)_y = G^\lambda f(y)$ for every $y \in Y$, respectively, and $(\, ,\,)$ denotes the scalar product in $\mathbf{C}^{|Y|}$. One says that $H_{Y,\alpha}$ describes point interactions which take place at the points of Y where for every $y \in Y$ the strength of the interaction equals $|Y|\,\alpha(y)$.

For every $n \in \mathbf{N}$, every $n \times n$–matrix Γ and all $1 \le p, q \le \infty$ we shall denote by $\|\,\Gamma\,\|_{p,q}$ the norm of Γ as an operator from $(\mathbf{C}^n, \|\cdot\|_p)$ to $(\mathbf{C}^n, \|\cdot\|_q)$.

Lemma 6 *Let $\lambda > 0$. Let $\{Y_n\}_{n\in\mathbf{N}}$ be a sequence of non–empty finite subsets of $\{\gamma \neq 0\}$ such that*

$$|Y_n| \longrightarrow \infty, \quad n \longrightarrow \infty$$

and

$$\sup_{n\in\mathbf{N}} \frac{1}{|Y_n|} \sup_{x\in Y_n} \sum_{y \in Y_n\setminus\{x\}} G^\lambda(x-y) < \alpha_0. \tag{24}$$

Then there exists a finite constant C and an $n_0 \in \mathbf{N}$ such that the matrix $\Gamma^\lambda_{Y_n,\alpha}$ is invertible and

$$\| \left(\frac{1}{|Y_n|}\,\Gamma^\lambda_{Y_n,\alpha}\right)^{-1} \|_{2,2} < 1 \tag{25}$$

for all $n \ge n_0$.

Proof: We choose a, $0 < a < \alpha_0$, such that the left hand side of (24) is less than a and decompose the matrices $\frac{1}{|Y_n|}\Gamma^\lambda_{Y_n,\alpha}$ as

$$\frac{1}{|Y_n|}\Gamma^\lambda_{Y_n,\alpha} = D_n + R_n$$

where D_n and R_n is a diagonal and an off–diagonal matrix, respectively. Obviously D_n is invertible for all sufficiently large n and

$$\| (D_n)^{-1} \|_{2,2} \longrightarrow \frac{1}{\alpha_0}. \tag{26}$$

By the Schur test, we have

$$\| R_n \|_{2,2} \leq \sup_{x \in Y_n} \frac{1}{|Y_n|} \sum_{y \in Y_n \setminus \{x\}} G^\lambda(x-y) < a. \tag{27}$$

By (26) and (27), the lemma is proved. □

Theorem 7 *Let N be a closed non–empty subset of $\mathbf{R}^3$ and m a finite positive measure on the Borel σ–algebra of N such that supp$(m) = N$ and m belongs to the Kato class. Let $\gamma : \mathbf{R}^3 \longrightarrow \mathbf{R}$ be a bounded continuous function and $\gamma \not\equiv 0$. Let α, α_0 and μ be defined by (14). Let $\lambda > 0$ be chosen such that the equation (21) has a unique solution σ and σ a representative – in the following also denoted by σ – which is bounded and continuous on the set $\{\gamma \neq 0\}$ (by our previous considerations every sufficiently large $\lambda > 0$ has this property).*

Suppose that there exists a sequence $\{Y_n\}_{n \in \mathbf{N}}$ of non–empty finite subsets of $\{\gamma \neq 0\}$ such that $|Y_n| \longrightarrow \infty$ and the following holds:

(i)

$$\frac{1}{|Y_n|} \sum_{y \in Y_n} f(y) \longrightarrow \int_N f \, d\, \mu$$

for every bounded continuous function $f : N \longrightarrow \mathbf{C}$.

(ii)

$$\sup_{n \in \mathbf{N}} \frac{1}{|Y_n|} \sup_{x \in Y_n} \sum_{y \in Y_n \setminus \{x\}} G^\lambda(x-y) < \alpha_0.$$

(iii)

$$\sup_{y \in Y_n} \frac{1}{|Y_n|} \sum_{y' \in Y_n \setminus \{y\}} \sigma(y')\, G^\lambda(y-y') - \left(G_\mu^\lambda \sigma\right)(y) \longrightarrow 0$$

for $n \longrightarrow \infty$.

Then $H_{Y_n,\alpha} \longrightarrow \Delta + \gamma\, m$ in the strong resolvent sense where the operators $H_{Y,\alpha}$ are defined by (23).

Proof: Observe that the explicit expression for the resolvent of $H_{Y_n,\alpha}$ can be written as

$$(H_{Y_n,\alpha} + \lambda)^{-1} f = G^\lambda f + \sum_{y \in Y_n} q_y G^\lambda(\cdot - y) \quad \text{a.e}, \quad f \in L^2(\mathbf{R}^3), \tag{28}$$

where the q_y's are the solutions of

$$\left(|Y_n|\, \alpha(y) + \frac{\sqrt{\lambda}}{4\,\pi} \right) q_y - \sum_{y' \in Y_n \setminus \{y\}} q_{y'}\, G^\lambda(y - y') = G^\lambda f(y). \tag{29}$$

Let $f, g \in L^2(\mathbf{R}^3)$. Since $-\Delta + \gamma\, m$ and the $H_{Y_n,\alpha}$ are self–adjoint operators it suffices to show that $I_n \longrightarrow 0$ where

$$\begin{array}{rcl} I_n & := & (g, (H_{Y_n,\alpha} + \lambda)^{-1} f - (-\Delta + \gamma\, m + \lambda)^{-1} f) \\ & = & \sum_{y \in Y_n} q_y G^\lambda g(y) - \int \sigma(z)\, G^\lambda g(z)\, \mu(dz) \\ & = & \frac{1}{|Y_n|} \sum_{y \in Y_n} (|Y_n|\, q_y - \sigma(y))\, G^\lambda g(y) + \\ & & + \frac{1}{|Y_n|} \sum_{y \in Y_n} \sigma(y) G^\lambda g(y) - \int \sigma(z)\, G^\lambda g(z)\, \mu(dz). \end{array} \tag{30}$$

Since, by the hypothesis, the difference of the last two terms on the right hand side of this equation tends to zero we have only to show that

$$\frac{1}{|Y_n|} \sum_{y \in Y_n} (|Y_n|\, q_y - \sigma(y))\, G^\lambda g(y) \longrightarrow 0.$$

Since the continuous function $G^\lambda g$ is bounded we have only to show that

$$\frac{1}{|Y_n|} \| \underline{v}^{(n)} \|_1 \longrightarrow 0 \tag{31}$$

where $\underline{v}^{(n)}$ denotes the vector in $\mathbf{C}^{|Y_n|}$ such that $(\underline{v}^{(n)})_y = |Y_n|\, q_y - \sigma(y)$ for every $y \in Y_n$.

Subtracting equation (21) evaluated in $y \in Y_n$ from (29) we get

$$
\begin{aligned}
0 \;=\; & \left(\alpha(y) + \tfrac{\sqrt{\lambda}}{4\,\pi\,|Y_n|}\right)\,(|Y_n|\,q_y - \sigma(y)) - \\
& - \tfrac{1}{|Y_n|}\,\textstyle\sum_{y' \in Y_n \setminus \{y\}} |Y_n|\,q_{y'} G^{\lambda}(y - y') + \\
& + \textstyle\int \sigma(z)\,G^{\lambda}(z - y)\,\mu(dz) + \tfrac{\sqrt{\lambda}}{4\,\pi\,|Y_N|}\,\sigma(y) \\
= \; & \left(\alpha(y) + \tfrac{\sqrt{\lambda}}{4\,\pi\,|Y_n|}\right)(|Y_n|\,q_y - \sigma(y)) - \\
& - \tfrac{1}{|Y_n|}\,\textstyle\sum_{y' \in Y_n \setminus \{y\}} (|Y_n|\,q_{y'} - \sigma(y'))\; G^{\lambda}(y - y') - \\
& - \tfrac{1}{|Y_n|}\,\textstyle\sum_{y' \in Y_n \setminus \{y\}} \sigma(y')\,G^{\lambda}(y - y') + \\
& + \textstyle\int \sigma(z)\,G^{\lambda}(z - y)\,\mu(dz) + \tfrac{\sqrt{\lambda}}{4\,\pi\,|Y_n|}\,\sigma(y).
\end{aligned}
\tag{32}
$$

Equation (32) can be rewritten as

$$\frac{1}{|Y_n|}\Gamma^{\lambda}_{Y_n,\alpha} \cdot \underline{v}^{(n)} = \underline{w}^{(n)} \tag{33}$$

where for every $y \in Y_n$

$$(\underline{w}^{(n)})_y := \frac{1}{|Y_n|} \sum_{y' \in Y_n \setminus \{y\}} \sigma(y')\,G^{\lambda}(y - y') - \left(G^{\lambda}_{\mu}\sigma\right)(y) - \frac{\sqrt{\lambda}}{4\,\pi\,|Y_n|}\,\sigma(y).$$

By the hypothesis, we have that

$$\|\,\underline{w}^{(n)}\,\|_{\infty} \longrightarrow 0.$$

Thus, by (33) and (31), we have only to show that for every sufficiently large $n \in \mathbf{N}$ the matrix $\Gamma^{\lambda}_{Y_n,\alpha}$ is invertible and

$$\frac{1}{|Y_n|}\,\|\left(\frac{1}{|Y_n|}\Gamma^{\lambda}_{Y_n,\alpha}\right)^{-1}\|_{\infty,1} \leq C \tag{34}$$

for some finite constant C which does not depend on n.

Since obviously $\|\,\Gamma\,\|_{\infty,1} \leq n\|\,\Gamma\,\|_{2,2}$ for every $n \times n$–matrix Γ for every $n \in \mathbf{N}$ the inequality (34) follows from Lemma 6. □

Example 8 Let $N = [0,1] \times [0,1] \times \{0\}$, $\gamma \equiv 1$ and m the area measure on N. For every $n \in \mathbf{N}$ we subdivide N into $n \times n$ squares with equal side length and denote by Y_n the set of the $n \times n$ middle points of these squares. It is easily verified that the hypothesis of theorem 7 is satisfied with this choice of N, γ, m and Y_n, $n \in \mathbf{N}$.

Example 9 Let N be a compact C^1–submanifold of $\mathbf{R}^3$ with dimension 2 such that N is orientable by some normal vector field $\mathbf{n}$. Let m be the area measure on N and $\gamma : N \longrightarrow \mathbf{R}$ a continuous function such that $\gamma \not\equiv 0$. Then the operator $-\Delta + \gamma\, m$ equals the Laplacian with boundary conditions

$$\frac{\partial f}{\partial \mathbf{n}_+} - \frac{\partial}{\partial \mathbf{n}_-} = \gamma\, f \quad m\text{–a.e.},$$

cf. [12]. Via some standard procedures, the investigation of this example can be reduced to the investigation of the previous Example 8 and we get that the operator $-\Delta + \gamma\, m$ can be approximated in the strong resolvent sense by operators of the form $H_{Y_n,\alpha}$ for suitably chosen finite sets Y_n.

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