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Spectral properties of Schrödinger operators with matrix potentials

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Abstract. Using perturbation theory we prove self-adjointness of a non-relativistic Hamiltonian H with a wide class of matrix potentials. We also give a simple criterion based on the Molchanov theorem which guarantees that H has a purely discrete spectrum.

1. Introduction

We will study the self-adjoint operator H defined on the Hilbert space $\mathscr{H} = L^2(R^+)\otimes C^n$ by using the differential expression

$$h = -\mathrm{d}^2/\mathrm{d}x^2 + V(x) \tag{1}$$

where $v(x)$ is a real symmetric $n\times n$ matrix with elements $V_{ij}(x) = \tilde{V}_{ij}(x) - \beta_{ij}(x)/x^{\alpha_{ij}}$

$$\begin{aligned} &\tilde{V}_{ij}(x) \geq 0 \quad \text{for } x \geq 0, \qquad \tilde{V}_{ij} \in L_{\mathrm{loc}}(\mathbb{R}^+) \\ &\beta_{ij} \in L^{\infty}(\mathbb{R}^+); \qquad \alpha_{ij} \geq 0. \end{aligned} \tag{C1}$$

In § 1 the construction of H using the quadratic-form technique is described and a criterion of self-adjointness of H is formulated with the help of inequalities for matrix elements of V and for the exponents α_{ij}. The criterion is checked for a class of NN potentials (Reid 1968), that have been used for calculation of deuteron spectra.

In § 2 we give a condition based on the Molchanov theorem (Molchanov 1953) which guarantees that the spectrum of H is purely discrete and using it we show that the spectrum of H with $q\bar{q}$ confining potentials is of this kind.

We use the following notation

$$(a, b)_n = \sum_{i=1}^{n} a_i b_i \qquad a, b \in C^n,$$

$C_0^\infty(R^+)$ is the set of infinitely differentiable functions with compact support in R^+, $L^2(R^+)\otimes C^n$ is the Hilbert space of vector functions

$$u = (u_1, u_2, \ldots, u_n), \qquad u_i \in L^2(R^+),$$

with the scalar product

$$(u, v) = \int_0^\infty (u, v)_n \,\mathrm{d}x, \qquad u, v \in L^2(R^+)\otimes C^n.$$

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2. Self-adjointness

Let us define the following quadratic form

$$h: D(h)\times D(h)\to C$$

with the help of differential expression (1):

$$h(u, v)=(u, \hbar, v) \quad \text{for all } u, v\in D(h).$$

The domain $D(h)$ will be specified below in such a way that h be densely defined, symmetric, closed and below bounded. Then by Kato's theorem (Kato 1966), there is a unique self-adjoint below-bounded operator H such that:

(i) $D(h)\supset D(H)$ and $h(u, v)=(Hu, v)\forall u\in D(H)$ and all $v\in D(h)$;

(ii) $D(H)$ is a form-core for h;

(iii) if for some $v\in D(h)$, $w\in \mathcal{H}$ the equality $h(u, v)=(u, w)$ holds for all u belonging to a form-core of h, then $v\in D(H)$ and $Hv=w$.

H is called 'the operator associated with h'.

Thus our next task is finding $D(h)$ such that the form h has the above properties. The basic difficulty is the occurrence of the negative part of V_{ij}, that is, moreover, singular at origin. We overcome it by applying the perturbation theory approach. The splitting of h into the unperturbed part h_1 and the perturbation h_2 corresponds to the following decomposition of V (see (C1)):

$$V=V_1+V_2 \qquad (V_1)_{ij}=\tilde{V}_{ij}\delta_{ij}.$$

In fact we set

$$h=h_1+h_2$$

$$h_1(u, v)=\int_0^\infty [(u, v)_n+(V_1u, v)_n]\,\mathrm{d}x,$$

$$D(h_1)=\left\{u\in \mathcal{H},\ u_j\in D_0,\ 1\leqslant j\leqslant n \text{ and } \int_0^\infty (V_1u, u)_n\,\mathrm{d}x<\infty\right\}$$

$$h_2(u, v)=\int_0^\infty (V_2u, v)_n\,\mathrm{d}x,$$

$$D(h_2)=\left\{u\in \mathcal{H},\ \int_0^\infty (V_2u, u)_n\,\mathrm{d}x<\infty\right\}$$

where D_0 is the set of all $u_j\in L^2(R^+)$ such that

(i) u_j is absolutely continuous in $[0,\infty)$

(ii) $u_j\in L^2(R^+)$

(iii) $u_j(0)=0$.

It is clear that h_1 is densely defined, positive and closed. In order to show that the form h has the same properties it is sufficient to prove that h_2 is h_1 bounded with h_1 bound $a<1$, i.e. there are $a, b\in R$, $0\leqslant a<1$, $b>0$ such that

$$|h_2(u, u)|\leqslant ah_1(u, u)+b(u, u)$$

holds for all $u\in D(h_1)$.

Theorem 1. Suppose there is $a \in [0, 1)$ such that

$$\sum_i \tilde{V}_{ij}(x) \leqslant a\tilde{V}_{jj}(x), \qquad j = 1, 2, \ldots, n \tag{C2}$$

AE in $[0, \infty)$

$$\alpha_{ij} = \alpha_{ji} \in [0, 2). \tag{C3}$$

Then the form h_2 is h_1 bounded and the relative bound of h_2 WRT h_1 equals a.

To prove this theorem we will use the following lemma.

Lemma. For any $a > 0$, $\alpha \in [0, 2)$ there exist some $b \geqslant 0$ such that for all $u \in D_0$

$$\int_0^\infty x^{-\alpha}|u|^2 \,\mathrm{d}x \leqslant a \int_0^\infty |u'|^2 \,\mathrm{d}x + b \int_0^\infty |u|^2 \,\mathrm{d}x. \tag{2}$$

holds.

Proof. This assertion holds if D_0 is replaced by $C_0^\infty(R^+) \subset D_0$ (see Reed and Simon 1975 § X.5). Furthermore, for each $u \in D_0$ there is a sequence $\{u_n\} \in C_0^\infty(R^+)$ satisfying $\|u_n - u\| \to 0$, $\|u_n' - u'\| \to 0$ and $u_n(x) \to u(x)$ for all $x \geqslant 0$ (cf Kato 1966 VI.4). Then (2) follows by the Fatou lemma.

Proof of theorem 1. Let $u \in D(h_1)$. Then

$$\begin{aligned}
h_2(u, u) &= \left| \int_0^\infty \sum_i \sum_j (V_2)_{ij} u_i \bar{u}_i \,\mathrm{d}x \right| \\
&\leqslant \left| \int_0^\infty \sum_i (V_2)_{ii} |u_i|^2 \,\mathrm{d}x + 2 \int_0^\infty \sum_{j>i} (V_2)_{ij} \operatorname{Re}(u_i \bar{u}_j) \,\mathrm{d}x \right| \\
&\leqslant \sum_i \sum_j \int_0^\infty \|\beta_{ij}\|_\infty |u_i|^2 x^{-\alpha_{ij}} \,\mathrm{d}x + \int_0^\infty \sum_i |u_i|^2 \left(\sum_{i \neq j} (\tilde{V}_{ij}) \right) \mathrm{d}x \\
&\leqslant b \cdot \int_0^\infty (u; u)_n \,\mathrm{d}x + a \left\{ \int_0^\infty [(u'; u')_n + (u; V_1 u)_n] \,\mathrm{d}x \right\} \\
&= a h_1(u; u) + b(u; u).
\end{aligned}$$

Now the representation theorem can be applied to the form h and the domain of the self-adjoint operator H associated with h can be specified explicitly

Theorem 2. Let V fulfil the conditions (C1)–(C3) for some a, $0 \leqslant a < 1$, and let H be the operator associated with h. Then the set

$$M = \left\{ u \in \mathscr{H};\ u_j \in D_0,\ u_j' \text{ absolutely continuous in } [0; \infty) \right.$$

$$\left. \int_0^\infty (V_1 u, u)_n \,\mathrm{d}x < \infty,\ \ell u \in \mathscr{H} \right\}$$

is the domain of H and $Hu = \ell u$ for each $u \in M$.

Proof. As h_2 is h_1 bounded we have $D(h) = D(h_1)$ and so M is the set of all $u \in D(h)$ such that u' is absolutely continuous in $[0, \infty)$ and $\not{h}u \in \mathcal{H}$.

(a) Let $u \in D(H)$. By the representation theorem $u \in D(h)$ and

$$(Hu, v) = h(u, v) = \int_0^\infty \{(u', v')_n + (Vu, v)_n\}\, dx \qquad (+)$$

for all $v \in C_0^\infty(R^+) \otimes C^n$, since $C_0^\infty(R^+) \otimes C^n \subset D(h)$. According to (C1) all the functions $V_{ij}(x)$ belong to $L(a, b)$ if $0 < a < b$. Furthermore, u_j are continuous on $(0, \infty)$ and thus $Vu \in L(a, b) \otimes C^n$. The same holds for $w = Hu$ and so all the components of

$$z = \int_0^x (w - Vu)\, dx'$$

are absolutely continuous on any $[a, b] \subset (0, \infty)$. Then

$$\int_0^\infty (w - Vu, v)_n\, dx = -\int_0^\infty (z, v')_n\, dx.$$

By substituting into (+) one has for $i = 1, \ldots, n$

$$\int_0^\infty (z_i + u_i')\bar{v}_i'\, dx = 0 \quad \text{for } v_i \in C_0^\infty(R^+). \qquad (++)$$

Consider $P = i\, d/dx$ on D_0. This is a closed symmetric operator on $L^2(R^+)$ and its restriction $P_0 = P \upharpoonright C_0^\infty(R^+)$ fulfils $\bar{P}_0 = P$. (See proof of the lemma following theorem 1.) Now (++) can be rewritten as

$$z_i + u_i \in (\text{Ran } P_0)^\perp = \ker(P_0^+) = \text{Ker } P^+$$

and since $\text{Ker } P^+ = \{0\}$, we have $u' = -z$. Hence u' is absolutely continuous in $(0, \infty)$ and $u'' = -z' = Vu - Hu$. We have thus proved $D(H) \subset M$, $Hu = \not{h}u$ for all $u \in (H)$.

(b) Let $u \in M$. If we find $w \in \mathcal{H}$ such that $h(u, v) = (w, v)$ for all v in some core of h, then by the representation theorem $u \in D(H)$ and the proof will be completed. But it is known (see Kato 1966; § VI.4) that $C_0^\infty(R^+)$ is a core of h_i obtained from the differential expression

$$\not{h}_i = -d^2/dx^2 + \tilde{V}_{ii}$$

Now one sees that $C_0^\infty(R^+) \otimes C^n$ is a core of the form $h = h_1 + h_2$, as h_2 is h_1 bounded with h_1 bound less than one. So in equation $h(u, v) = (w, v)$ we can assume $v \in C_0^\infty(R^+) \otimes C^n$. Now for $u \in M$ one has $\not{h}u \in \mathcal{H}$ and $h(u, v) = (\not{h}u, v)$ for all $v \in C_0^\infty(R^+) \otimes C^n$.

Example. A static N–N potential

for the isospin $T = 0$, the total angular momentum $J = 1$ and for spin $S = 1$ an N–N interaction in the energy region 0–500 MeV can be described by the potential (Reid 1968)

$$V_{NN} = \begin{pmatrix} \alpha V_c & 2\sqrt{2}\alpha V_T \\ 2\sqrt{2}\alpha V_T & 6/x^2 + \alpha V_c - 2\alpha V_T - 3\alpha V_{LS} \end{pmatrix}$$

where

$$V_c = (-10.4\,e^{-x} + 105.5\,e^{-2x} - 3181.8\,e^{-4x} + 9924.3\,e^{-6x})x^{-1}$$

$$V_{LS} = (708.9\,e^{-4x} - 2713.1\,e^{-6x})x^{-1}$$

$$V_T = (1 + 3/x + 3/x^2)\,e^{-x} - (12/x + 3/x^2)\,e^{-4x}(-10/x) + (351.8\,e^{-4x} - 1673.5\,e^{-6x})x^{-1}.$$

In this potential there are terms which behave like $-1/x^3$ for $x \to 0^+$. It is known that Hamiltonians with such strongly singular potentials are not semibounded and so somehow we regularise these terms. Now if we take any regularisation of these singular terms which behaves like $-1/x^{2-\varepsilon}$ for some $\varepsilon > 0$, we can choose $\tilde{V}_{12} = 0$ so that (C2), (C3) will be fulfilled. By theorem 2 the Hamiltonian H_{NN} defined on $L^2(R^+) \otimes C^n$ by the differential expression $-d^2/dx^2 + V_{NN}$ is self-adjoint and below bounded, its domain being given by theorem 2.

3. Discrete spectrum

In this section we find conditions under which the operator H has a purely discrete spectrum. This is a very important question having direct practical applications. For instance, if we calculate meson masses in the non-relativistic quark model we have to work with such Hamiltonians.

In order to obtain such conditions, we use the perturbation theory once more. We have already shown that under conditions (C2), (C3) the form h_2 is h_1 bounded and its h_1 bound a is less than one. Therefore the set

$$h(\varkappa) = h_1 + \varkappa h_2; \qquad \varkappa \in C; \qquad |\varkappa| < 1/a$$

is a holomorphic class of the type b (see Kato 1966). The operators $H(\varkappa)$ associated with $h(\varkappa)$ constitute a holomorphic class of type B. Such a holomorphic class has the following stability property: the operators $H(\varkappa)$ have compact resolvent (i.e. purely discrete spectrum) either for all $\varkappa$, or for no $\varkappa$. Hence it is sufficient to establish conditions for purely discrete spectrum of $H_0 = H(0)$.

This operator corresponds to the differential expression $\ell_1 = -d^2/dx^2 + V_1$, where $(V_1)_{ij} = \tilde{V}_{ii}\delta_{ij}$. Obviously $H(0)$ equals the direct sum of 'scalar' operators $H_i(0)$ on $L^2(R^+)$ that are defined by expressions

$$\ell_{1i} = -d^2/dx^2 + \tilde{V}_{ii}(x).$$

So $H(0) = H_1(0) + H_2(0) + \ldots + H_n(0)$ and for its spectrum holds $\sigma(H(0)) = \bigcup_i \sigma(H_i(0))$.

It is evident that $H(0)$ has a purely discrete spectrum if and only if such a spectrum has the operator $H_i(0)$ for all $i = 1, \ldots, n$. But the operator $H_i(0)$ is the ordinary scalar Schrödinger operator with positive potentials and the theorem of Molchanov applies. Using it we obtain

Theorem 3. Let V fulfil conditions (C1)–(C3) for some $a \in [0, 1)$. Then H has purely discrete spectrum if and only if for each $i = 1, \ldots, n$ and for each $c > 0$ holds

$$\lim_{x \to \infty} \int_x^{x+c} \tilde{V}_{ii}(y)\,dy = \infty.$$

Example. In the non-relativistic limit the $q\bar{q}$ interaction can be described for $J=1$ by the following potential (Beavis 1979)

$$V_{q\bar{q}}=\begin{pmatrix} 2/x^2-1.4/x+2.5x & -1.2/x^3+0.2/x \\ -1.2/x^3+0.2/x & -1.1/x^3+6/x^2-1.3/x+2.5x \end{pmatrix}.$$

By performing a suitable regularisation that transforms the x^{-2} and x^{-3} terms to terms behaving like $x^{-2+\varepsilon}$ and choosing $\tilde{V}_{12}=0$ we find that that the Hamiltonian $H_{q\bar{q}}$ defined on $L^2(R^+)\otimes C^n$ by $-\mathrm{d}^2/\mathrm{d}x^2+V_{g\bar{g}}$ is again self-adjoint and below bounded. Further $\tilde{V}_{11}$ and $\tilde{V}_{22}$ contains the terms $2.5x$ and so theorem 3 implies that $H_{q\bar{q}}$ has a purely discrete spectrum.

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