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Spectral properties of Schrödinger operators with matrix potentials: II

Petr Šeba

Nuclear Centre, Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, Prague 8, Czechoslovakia

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Abstract. We describe the discrete and continuous spectrum of Schrödinger operators with matrix potentials in the one- and three-dimensional configuration space.

1. Introduction

Schrödinger operators with matrix potentials $V(x) = \{V_{ij}(x)\}$ are often used in various parts of quantum physics, e.g. the quark-antiquark interaction in the non-relativistic limit (Beavis 1979) or the nucleon-nucleon interaction (Landau and Lifshitz 1974, Reid 1968), etc. It is therefore important to know as much as possible about their spectra. But, unlike the scalar case, very little is known about the spectra of such operators.

The aim of this paper is to give a quick orientation about the character of $\sigma(H)$ for a Schrödinger operator H with a given matrix potential in the one- and three-dimensional configuration space. This represents a continuation of our previous work (Šeba 1984) where self-adjointness of such operators was investigated.

We describe the continuous spectrum in § 2. Section 3 discusses the discrete spectrum in the case of small coupling.

2. The continuous spectrum

2.1. The three-dimensional case

Consider the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3) \otimes C^n$ of vector functions

$$v = (v_1, \dots, v_n) \quad v_i \in L^2(\mathbb{R}^3) \quad i = 1, 2, \dots, n$$

with the scalar product

$$(u, v) = \int_{\mathbb{R}^3} (u, v)_n(x) d^3x \quad (u, v)_n(x) = \sum_{i=1}^n u_i(x) \overline{v_i(x)}$$

and the Schrödinger operator H defined by

$$H = -\Delta + V(x)$$

where $V(x)$ is a real symmetric matrix with elements $V_{ij}(x)$. We assume that the functions $V_{ij}(x)$ are locally square integrable and that

$$\lim_{|x| \rightarrow \infty} V_{ij}(x) = V_{ij}(\infty)$$

does exist and is finite for all $i, j = 1, 2, \dots, n$.

For the essential spectrum of H , theorem 1 holds (see below).

Theorem 1.

$$\sigma_{\text{ess}}(H) = [\mu, \infty)$$

where

$$\mu = \min(\lambda_1, \lambda_2, \dots, \lambda_n)$$

and $\lambda_1, \dots, \lambda_n$ are eigenvalues of the constant matrix $V(\infty) = \{V_{ij}(\infty)\}$.

Proof. We use the method of Dirichlet decoupling. Denote by H_D the operator $-\Delta + V(x)$ with the Dirichlet boundary condition at the surface of the sphere $|x| = R$. Then H_D is a self-adjoint operator in \mathcal{H} which decouples the regions $|x| < R$ and $|x| > R$. We have

$$H_D = H_{D,\text{in}} \oplus H_{D,\text{out}}$$

where $H_{D,\text{in}}$ is the operator $-\Delta + V$ defined on $L^2(B_R) \otimes C^n$ by the Dirichlet boundary condition at $|x| = R$ ($B_R = \{x \in R^3; |x| \leq R\}$), and $H_{D,\text{out}}$ is the same operator defined on $L^2(R^3 \setminus B_R) \otimes C^n$ by the Dirichlet boundary condition at $|x| = R$.

$H_{D,\text{in}}$ is an operator with compact resolvent and its essential spectrum is empty. Therefore

$$\sigma_{\text{ess}}(H_D) = \sigma_{\text{ess}}(H_{D,\text{out}}).$$

Using the same method as described in Pearson (1984), we get for $\text{Im } z \neq 0$ that

$$(H - z)^{-1} - (H_D - z)^{-1}$$

is compact (cf also Povzner 1953, Birman 1962). Weyl's theorem tells us that

$$\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_D)$$

and we have finally

$$\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_{D,\text{out}})$$

for all $R > 0$.

$\sigma_{\text{ess}}(H_{D,\text{out}})$ can easily be obtained. The constant unitary matrix U which diagonalises $V(\infty)$:

$$UV(\infty)U^{-1} = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$$

if applied to $H_{D,\text{out}}$ yields

$$UH_{D,\text{out}}U^{-1} = -\Delta + W(x)$$

where $W(x) = UV(x)U^{-1}$ is an almost diagonal matrix for R large. Choosing R sufficiently large we can make the non-diagonal elements of W small enough while the diagonal elements fulfil

$$\lim_{|x| \rightarrow \infty} W_{ii}(x) = \lambda_i \quad i = 1, 2, \dots, n.$$

Therefore we have

$$\sigma_{\text{ess}}(H) = [\mu, \infty).$$

Remark 1. If $\lim_{|x| \rightarrow \infty} V_{ij}(x)$ exists but is not finite for some i, j , we cannot obtain the lower boundary of $\sigma_{\text{ess}}(H)$ using the eigenvalues of the matrix $V(\infty)$. In this case we have to use a somewhat different method. We denote $\lambda_i(x)$, $i = 1, 2, \dots, n$ as the eigenvalues of the matrix $V(x)$ and we assume that

$$\lim_{|x| \rightarrow \infty} \lambda_i(x) = \lambda_i^*$$

exists for all i . Then

$$\sigma_{\text{ess}}(H) = [\mu, \infty)$$

where

$$\mu = \min(\lambda_1^*, \lambda_2^*, \dots, \lambda_n^*).$$

We note that some of the numbers λ_i^* can be infinite. If we have for instance $\lambda_i^* = \infty$ for all $i = 1, 2, \dots, n$, then $\sigma_{\text{ess}}(H)$ is empty and H is an operator with compact resolvent (cf Šeba 1984).

2.2. The one-dimensional case

We now have $\mathcal{H} = L^2(\mathbb{R}) \otimes C^n$ and

$$H = -\frac{d^2}{dx^2} + V(x).$$

We assume that the limits

$$\lim_{x \rightarrow \infty} V_{ij}(x) = V_{ij}(\infty)$$

$$\lim_{x \rightarrow -\infty} V_{ij}(x) = V_{ij}(-\infty)$$

exist and are finite for all $i, j = 1, 2, \dots, n$.

Matrices $V(\infty)$ and $V(-\infty)$ must not commute in the general case. Nevertheless we get the following.

Theorem 2.

$$\sigma_{\text{ess}}(H) = [\mu, \infty)$$

where

$$\mu = \min(\lambda_1^+, \lambda_2^+, \dots, \lambda_n^+, \lambda_1^-, \lambda_2^-, \dots, \lambda_n^-)$$

and λ_i^\pm , $i = 1, 2, \dots, n$ are eigenvalues of $V(\pm\infty)$.

Proof. The proof is similar to that of theorem 1. Let H_D be the self-adjoint operator given by the differential expression

$$-\frac{d^2}{dx^2} + V(x)$$

and by the Dirichlet boundary conditions at the points $x = \pm R$. Then

$$H_D = H_1 \oplus H_2 \oplus H_3$$

where H_1, H_2, H_3 are defined on $L^2(-\infty, -R) \otimes C^n, L^2(-R, R) \otimes C^n, L^2(R, \infty) \otimes C^n$ by $-\text{d}^2/\text{d}x^2 + V(x)$ and by the Dirichlet conditions at the boundary points. H_2 is an operator with compact resolvent and this implies

$$\sigma_{\text{ess}}(H_D) = \sigma_{\text{ess}}(H_1) \cup \sigma_{\text{ess}}(H_3).$$

Moreover

$$(H - z)^{-1} - (H_D - z)^{-1}$$

is an operator of finite rank for $\text{Im } z \neq 0$. Weyl's theorem gives

$$\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_D)$$

and therefore

$$\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_1) \cup \sigma_{\text{ess}}(H_3).$$

Using the same arguments as in the proof of theorem 1 we get

$$\sigma_{\text{ess}}(H_1) = \min(\lambda_1^-, \lambda_2^-, \dots, \lambda_n^-)$$

$$\sigma_{\text{ess}}(H_3) = \min(\lambda_1^+, \lambda_2^+, \dots, \lambda_n^+).$$

If $\lim_{x \rightarrow \pm\infty} V_{ij}(x)$ exists but is not finite for some i, j , we can describe $\sigma_{\text{ess}}(H)$ by the method indicated in remark 1.

3. The discrete spectrum

We investigate the one-dimensional case first. It is a well known fact that a one-dimensional scalar attractive potential binds at least one bound state, no matter how small the coupling is. We show that this remains true also for matrix potentials.

In the following we restrict ourselves to matrices $V(x)$ with elements

$$V_{ij}(x) \in C_0^\infty(\mathbb{R}) \quad i, j = 1, 2, \dots, n.$$

(This restriction is not essential but makes the computations simpler.)

We know from § 2 that $\sigma_{\text{ess}}(H) = [0, \infty)$ in this case and we will further investigate negative eigenvalues of the operator H_λ :

$$H_\lambda = -\frac{\text{d}^2}{\text{d}x^2} + \lambda V(x) \quad \lambda > 0$$

for small coupling constant λ .

We define the corresponding Birman-Schwinger operator K_α through its kernel

$$K_\alpha(x, y) = |V|^{1/2}(x) \frac{\exp(-\alpha|x-y|)}{2\alpha} |V|^{1/2}(y) \quad \alpha > 0$$

where

$$V(x) = U(x)|V(x)|$$

is the polar decomposition of the potential $V(x)$ and

$$V^{1/2}(x) = U(x)|V|^{1/2}(x)$$

so that

$$V^{1/2}(x)|V|^{1/2}(x) = V(x).$$

Following Simon (1976) we investigate the operator K_α further because there is a close connection between negative eigenvalues of H_λ and eigenvalues of K_α .

Lemma 1. $E_\lambda < 0$ is an eigenvalue of H_λ if and only if -1 is an eigenvalue of λK_α with $\alpha^2 = -E_\lambda$.

Proof. For the resolvent $(H_\lambda + \alpha^2)^{-1}$,

$$(H_\lambda + \alpha^2)^{-1} = R_0(\alpha) - \lambda R_0(\alpha) V^{1/2} (1 + \lambda |V|^{1/2} R_0(\alpha) V^{1/2})^{-1} |V|^{1/2} R_0(\alpha)$$

where

$$R_0(\alpha) = \left(-\frac{d^2}{dx^2} + \alpha^2 \right)^{-1}$$

is an integral operator with kernel

$$R_0(x, y) = \frac{\exp(-\alpha|x-y|)}{2\alpha}.$$

We see that $(H_\lambda + \alpha^2)^{-1}$ has a pole at $\alpha = \alpha_0$ if and only if -1 is an eigenvalue of λK_{α_0} .

This lemma makes it possible to determine, for a given λ , the eigenvalues of H_λ with the help of those of K_α . Namely, if $\nu(\alpha)$ is an eigenvalue of K_α then any solution $\alpha_\lambda > 0$ of

$$\lambda \nu(\alpha) = -1 \tag{1}$$

corresponds to the eigenvalue

$$E_\lambda = -\alpha_\lambda^2$$

of H_λ .

In order to investigate the spectrum of K_α we decompose this operator as follows:

$$K_\alpha = L_\alpha + M_\alpha$$

where L_α and M_α are Hilbert-Schmidt operators with kernels

$$L_\alpha(x, y) = (1/2\alpha) |V|^{1/2}(x) V^{1/2}(y)$$

$$M_\alpha(x, y) = (1/2\alpha) |V|^{1/2}(x) [\exp(-\alpha|x-y|) - 1] V^{1/2}(y).$$

Moreover M_α is analytic for α near 0 and we have

$$\|\lambda M_\alpha\| < 1$$

for α near 0 and λ small enough. Using the fact that

$$(1 + \lambda M_\alpha)^{-1}$$

exists and is bounded for these α and λ we get

$$(1 + \lambda K_\alpha)^{-1} = [1 + \lambda (1 + \lambda M_\alpha)^{-1} L_\alpha]^{-1} (1 + \lambda M_\alpha)^{-1}.$$

Thus -1 is an eigenvalue of λK_α if and only if -1 is an eigenvalue of the finite rank operator

$$\lambda (1 + \lambda M_\alpha)^{-1} L_\alpha.$$

We denote the eigenvalues and eigenvectors of $(1 + \lambda M_\alpha)^{-1} L_\alpha$ as $\xi_n(\lambda, \alpha)$ and $\chi_n(\lambda, \alpha)$:

$$(1 + \lambda M_\alpha)^{-1} L_\alpha \chi_n = \xi_n \chi_n. \tag{2}$$

Inserting

$$\chi_n(\lambda, \alpha, x) = (1/2\alpha)(1 + \lambda M_\alpha)^{-1} |V|^{1/2}(x) \mathbf{b}_n$$

where $\mathbf{b}_n \in C^n$ is a constant vector, we get from (2)

$$Z\mathbf{b}_n = \xi_n \mathbf{b}_n$$

where Z is the constant matrix

$$Z = (1/2\alpha) \int_{\mathbf{R}} V^{1/2}(x) [(1 + \lambda M_\alpha)^{-1} |V|^{1/2}](x) dx.$$

Decomposing Z we get for small λ

$$Z = (1/2\alpha)A - (\lambda/2\alpha)B(\alpha) + O(\lambda^2)$$

where

$$A = \int_{\mathbf{R}} V(x) dx \quad A_{ij} = \int_{\mathbf{R}} V_{ij}(x) dx$$

and

$$B(\alpha) = \int_{\mathbf{R}} V^{1/2}(x) (M_\alpha |V|^{1/2})(x) dx.$$

Denote by μ_i and \mathbf{a}_i the eigenvalues and eigenvectors of the matrix A :

$$A\mathbf{a}_i = \mu_i \mathbf{a}_i$$

and suppose for simplicity that all the eigenvalues μ_i are non-degenerate. The standard perturbation theory can now be applied and we have for $\xi_i(\lambda, \alpha)$

$$\xi_i(\lambda, \alpha) = (1/2\alpha)\mu_i - (\lambda/2\alpha)(\mathbf{a}_i, B(\alpha)\mathbf{a}_i)_n + O(\lambda^2).$$

Decomposing further $B(\alpha)$:

$$B(\alpha) = B_0 + B_1\alpha + B_2\alpha^2 + \dots$$

we find for the solution of (1)

$$\alpha_\lambda = -(\lambda/2)\mu_i + (\lambda^2/2)(\mathbf{a}_i, B_0\mathbf{a}_i)_n + O(\lambda^3) \quad (3)$$

where

$$B_0 = -\frac{1}{2} \int_{\mathbf{R}} \int_{\mathbf{R}} V(x) |x-y| V(y) dx dy.$$

We note that only positive α_λ corresponds to an eigenvalue of H_λ , while negative α_λ corresponds to a resonance of H_λ (Baumgärtel *et al* 1978, Lakaev 1980).

We see from (3) that to any negative eigenvalue $\mu_i < 0$ of A there is exactly one eigenvalue E_λ of H_λ for which

$$(-E_\lambda)^{1/2} = -(\lambda/2)\mu_i - \lambda^2/4 \int_{\mathbf{R}} \int_{\mathbf{R}} |x-y| (\mathbf{a}_i, V(x)V(y)\mathbf{a}_i)_n dx dy + O(\lambda^3). \quad (4)$$

Let us now examine what happens if 0 is an eigenvalue of A . (We suppose again that 0 is a simple eigenvalue.) Let

$$A\mathbf{a}_0 = 0$$

for some $\mathbf{a}_0 \neq 0$. Then

$$\begin{aligned} & -\frac{1}{2} \left(\mathbf{a}_0, \int_{\mathbf{R}} \int_{\mathbf{R}} V(x)|x-y|V(y) \, dx \, dy \, \mathbf{a}_0 \right)_n \\ &= \lim_{\alpha \rightarrow 0^+} \left(\mathbf{a}_0, \int_{\mathbf{R}} \int_{\mathbf{R}} V(x)V(y) \frac{\exp(-\alpha|x-y|)^{-1}}{2\alpha} \, dx \, dy \, \mathbf{a}_0 \right)_n \\ &= -\lim_{\alpha \rightarrow 0^+} (1/2\alpha)(\mathbf{a}_0, A^2 \mathbf{a}_0)_n + \lim_{\alpha \rightarrow 0^+} \sum_{i,j,k} \int_{\mathbf{R}} \int_{\mathbf{R}} \frac{\exp(-\alpha|x-y|)}{2\alpha} \\ & \quad \times V_{ik}(x) V_{kj}(y) (\mathbf{a}_0)_i \overline{(\mathbf{a}_0)_j} \, dx \, dy. \end{aligned}$$

The first term clearly vanishes. For the second one we find, with the help of the fact that for the Fourier transform of $(1/2\alpha) \exp(-\alpha|x|)$

$$\mathcal{F}[(1/2\alpha) \exp(-\alpha|x|)](p) = 1/(p^2 + \alpha^2)$$

that

$$\begin{aligned} & \lim_{\alpha \rightarrow 0^+} \sum_{i,j,k} \int_{\mathbf{R}} \int_{\mathbf{R}} (1/2\alpha) \exp(-\alpha|x-y|) V_{ik}(x) V_{kj}(y) (\mathbf{a}_0)_i \overline{(\mathbf{a}_0)_j} \, dx \, dy \\ &= \lim_{\alpha \rightarrow 0^+} \sum_{i,j,k} \int_{\mathbf{R}} 1/(p^2 + \alpha^2) \mathcal{F}(V_{ik})(p) \mathcal{F}(V_{kj})(p) (\mathbf{a}_0)_i \overline{(\mathbf{a}_0)_j} \, dp \\ &= \int_{\mathbf{R}} (1/p^2) (\mathbf{a}_0, \mathcal{F}(V)^2(p) \mathbf{a}_0)_n \, dp \geq 0 \end{aligned}$$

where $(\mathcal{F}V)(p)$ is the matrix with elements

$$(\mathcal{F}V)_{ij}(p) = \mathcal{F}(V_{ij})(p).$$

The non-positivity of $(\mathbf{a}_0, B_0 \mathbf{a}_0)_n$ implies that there is also, for $(\mathbf{a}_0, B_0 \mathbf{a}_0)_n \neq 0$, an eigenvalue of H_λ which corresponds to the eigenvalue 0 of A .

Summarising all the above results, we get the following.

Theorem 3. Let $H_\lambda = -d^2/dx^2 + \lambda V(x)$ be a one-dimensional Schrödinger operator with a matrix potential $V(x)$

$$V(x) = \{V_{ij}(x)\} \quad V_{ij}(x) \in C_0^\infty(\mathbf{R}) \quad i, j = 1, 2, \dots, n.$$

Using the potential $V(x)$ we introduce two constant matrices A and B , defined by

$$\begin{aligned} A = \{A_{ij}\} & \quad A_{ij} = \int_{\mathbf{R}} V_{ij}(x) \, dx \\ B = \{B_{ij}\} & \quad B_{ij} = \sum_k \int_{\mathbf{R}} V_{ik}(x) |x-y| V_{kj}(y) \, dx \, dy. \end{aligned}$$

Let A have k non-positive eigenvalues $\mu_1, \mu_2, \dots, \mu_k$ with multiplicities n_1, n_2, \dots, n_k . Then the operator H_λ has, for $\lambda > 0$ and small enough, precisely $n_1 + n_2 + \dots + n_k$ negative eigenvalues (counting multiplicity) $E_{i,j}$ and

$$(-E_{i,j}(\lambda))^{1/2} = -(\lambda/2)\mu_i - (\lambda^2/4)\nu_{ij} + O(\lambda^3) \quad i = 1, 2, \dots, k \quad j = 1, 2, \dots, n_i$$

where ν_{ij} are the eigenvalues of the matrix $P_i B P_i$ and P_i are eigenprojectors corresponding to μ_i .

Remark 2.

(i) The theorem remains valid also for matrices V with elements V_{ij} fulfilling a weaker condition:

$$\int_{\mathbf{R}} (1 + |x|^2) |V_{ij}(x)| dx < \infty.$$

The proof does not change in this case. But it seems that the theorem remains valid also if

$$\int_{\mathbf{R}} (1 + |x|) |V_{ij}(x)| dx < \infty$$

(cf Klaus 1977). For

$$\int_{\mathbf{R}} (1 + |x|) |V_{ij}(x)| dx = \infty$$

infinitely many eigenvalues occur. The ground-state behaviour in the scalar case is investigated in Blankenbecler *et al* (1977).

(ii) The min-max principle (Reed and Simon 1978) implies that the number of negative eigenvalues of H_λ is monotone, increasing in λ . Therefore the number $N(V)$ of negative eigenvalues of

$$H = -\frac{d^2}{dx^2} + V(x)$$

satisfies

$$n_1 + n_2 + \dots + n_k \leq N(V).$$

On the other hand if $\lambda_{\min}(x)$ is the smallest eigenvalue of $V(x)$, then

$$H \geq \left(-\frac{d^2}{dx^2} + \lambda_{\min}(x) \right) \otimes I$$

and we have

$$N(V) \leq nN(\lambda_{\min})$$

where $N(\lambda_{\min})$ is the number of negative eigenvalues of the operator

$$-\frac{d^2}{dx^2} + \lambda_{\min}(x)$$

on $L^2(\mathbf{R})$.

There are various estimates for the number $N(\lambda_{\min})$ (Lakaev 1980, Newton 1983). By using the simplest one we get

$$n_1 + n_2 + \dots + n_k \leq N(V) \leq n \left\lceil 1 + \int_{\mathbf{R}} |x\lambda_{\min}(x)| dx \right\rceil$$

where $\lceil c \rceil$ denotes the integer part of c .

Example. In order to illustrate theorem 3 let us consider the operator H_α with

$$V(x) = \begin{pmatrix} -\exp(-|x|) & \exp(-\alpha|x|) \\ \exp(-\alpha|x|) & -\exp(-2|x|) \end{pmatrix} \quad \alpha > 0.$$

Then

$$A = \begin{pmatrix} -2 & 2/\alpha \\ 2/\alpha & -1 \end{pmatrix}$$

and theorem 3 tells us that H_λ has exactly one negative eigenvalue, for $\lambda > 0$ and small, if $\alpha < \sqrt{2}$, and exactly two eigenvalues if $\alpha > \sqrt{2}$.

Let us now briefly discuss the three-dimensional case. For the Birman-Schwinger kernel we get

$$K_\alpha(x, y) = (1/4\pi) |V|^{1/2}(x) \frac{\exp(-\alpha|x-y|)}{|x-y|} |V|^{1/2}(y) \quad x, y \in \mathbb{R}^3.$$

The operator K_α is analytic for α near 0 and we have

$$\|\lambda K_\alpha\| < 1$$

for λ small enough. Using lemma 1 we find that H_λ has no eigenvalues for small λ . This corresponds to the well known fact that in the scalar case a one-dimensional attractive potential binds a single bound state no matter how small the coupling, while a three-dimensional potential that is too shallow has no bound states.

Using the same method as in remark 2 we get a simple upper bound for the number of negative eigenvalues of H_λ in three dimensions, but we will not do it here.

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