Université Paris-Saclay • M2 Analyse Modélisation Simulation
Introduction to spectral theory (2016-2017, 1er semestre)

Stéphane Nonnenmacher

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Problem : Negative eigenvalues of a Schrödinger operator

We consider the Schrödinger operator $A = -\Delta + V$ acting on $\mathcal{H} = L^2(\mathbb{R}^d)$, with a potential function $V \in L^\infty(\mathbb{R}^d, \mathbb{R})$.

1. Recall the domain $D(A) \subset L^2(\mathbb{R}^d)$ on which A is selfadjoint. Describe the quadratic form q_A associated with A, including its domain $Q(A) = D(q_A)$.

2. We assume $V \in L^\infty(\mathbb{R}^d)$ has a compact support. Explain why the essential spectrum $\sigma_{\text{ess}}(A) = \mathbb{R}_+$. We want to show that $\sigma_{\text{disc}}(A)$ is finite.

   Let $B \subset \mathbb{R}^d$ be an open ball containing the support of V. We define the sesquilinear form
   $$q_B(\psi, \psi) = \int_{\mathbb{R}^d} \left(|\nabla\psi(x)|^2 + V(x)|\psi(x)|^2 \right) dx\,,$$
   of domain $D(q_B) = H^1(B \cup (\mathbb{R}^d \setminus \overline{B}))$.

   (a) Show that q_B is a closed form. We call A_B the associated self-adjoint operator. Show that $D(q_B) = H^1(B) \oplus H^1(\mathbb{R}^d \setminus \overline{B})$. Deduce that A_B can be decomposed as the sum of two independent selfadjoint operators.

   (b) Show that A_B admits at most a finite number of negative eigenvalues.

   (c) Show the inclusion $H^1(\mathbb{R}^d) \subset D(q_B)$. Using the max-min principle for the operators A and A_B, show that $\mu_n(A_B) \leq \mu_n(A)$ for any $n \geq 1$.
   Hint : use the form domain in the max-min principle.

   (d) Deduce that A admits at most a finite number of negative eigenvalues.

3. From now on, we assume that V is continuous with compact support. We will consider the family of *semiclassical* Schrödinger operators
   $$A_h = -h^2\Delta + V(x),$$
   where $h \in (0, 1]$ is called "Planck's constant".
   Using question 2, show that for any $h \in (0, 1]$ the number $N(h)$ of negative eigenvalues of A_h is finite. We want to study the behaviour of $N(h)$, in the limit $h \to 0+$ (called the semiclassical limit).

   To simplify the notations, we restrict ourselves to the dimension $d = 2$. We assume that the support of V is contained in the unit square $S = (0, 1) \times (0, 1)$.

(a) Our strategy is to approximate the function V by functions constant over small squares. For any integer $j \geq 1$, let us divide the square S into j^2 *disjoint* open squares

$$S_j(\boldsymbol{m}) \stackrel{\text{def}}{=} (\frac{m_1-1}{j}, \frac{m_1}{j}) \times (\frac{m_2-1}{j}, \frac{m_2}{j}), \qquad \boldsymbol{m} = (m_1, m_2) \in \{1, \ldots, j\}^2,$$

and call their (disjoint) union $S_j \stackrel{\text{def}}{=} \bigcup_m S_j(\boldsymbol{m})$. What is the boundary of S_j? Draw a sketch of ∂S_j.

(b) Using these squares, we define the functions $V_j^{\pm}$ as follows :

$$\forall x \in S_j(\boldsymbol{m}), \quad \begin{cases} V_j^-(x) & = V_{j,\boldsymbol{m}}^- \stackrel{\text{def}}{=} \inf_{x \in S_j(\boldsymbol{m})} V(x) \\ V_j^+(x) & = V_{j,\boldsymbol{m}}^+ \stackrel{\text{def}}{=} \sup_{x \in S_j(\boldsymbol{m})} V(x) \end{cases} ; \quad \forall x \in \mathbb{R}^2 \backslash S_j, \quad V_j^{\pm}(x) = 0.$$

We want to show that V_j^+ and V_j^- are good approximations of V_- when j is large. For this, take $\varepsilon > 0$ arbitrary small. Show that there exists $j_0 = j_0(\varepsilon) \in \mathbb{N}$ such that, $\forall j \geq j_0$, we have

$$(1) \qquad \|V_j^+ - V\|_{L^1(\mathbb{R}^2} \leq \varepsilon, \quad \|V_j^- - V\|_{L^1(\mathbb{R}^2} \leq \varepsilon$$

(c) *Notation* : for any real valued function $f(x)$, its *negative part* is defined as $f_-(x) = \max(0, -f(x))$.
Show that the negative parts $(V_j^+)_-$ and $(V_j^+)_-$ are good approximations of V_- when j is large, in the sense of (1).

(d) We introduce two quadratic forms :

$$q_j^{\pm}(\psi, \psi) = \int \left(h^2 |\nabla\psi(x)|^2 + V_j^{\pm}(x)|\psi(x)|^2\right) dx\,, \qquad \text{of respective domains}$$

$$D(q_j^+) = H_0^1(S_j \cup \mathbb{R}^2 \setminus \overline{S}), \quad D(q_j^-) = H^1(S_j \cup \mathbb{R}^2 \setminus \overline{S}).$$

Show that q_j^+ can be split as the sum of $j^2 + 1$ quadratic forms, acting on functions defined respectively on $S_{j,\boldsymbol{m}}$, $\boldsymbol{m} \in \{1, \ldots, j\}^2$, and on $\mathbb{R}^2 \setminus \overline{S}$.
Call A_j^+ the operators associated with the forms $q_j^{\pm}$. Show that A_j^+ can be represented as a sum of j^2 selfadjoint operators $A_{j,\boldsymbol{m}}^+$ acting on $S_j(\boldsymbol{m})$, plus an operator A^+ acting on $\mathbb{R}^2 \setminus B$. Describe the operators $A_{j,\boldsymbol{m}}^+$, A^+, including their domains.

(e) Same question for q_j^- and its associated operator A_j^-, split into $A_{j,\boldsymbol{m}}^-$ and A^-

4. We now want to obtain quantitative informations on the spectra of the operators $A_{j,\boldsymbol{m}}^{\pm}$ and $A^{\pm}$.

(a) Taking $\boldsymbol{m}_0 = (1, 1)$, compute explicitly the spectrum of the Dirichlet Laplacian on the square $S_j(\boldsymbol{m}_0)$. Deduce the spectrum of the operator $A_{j,\boldsymbol{m}_0}^+$. Compute the spectrum of $A_{j,\boldsymbol{m}}^+$ for each $\boldsymbol{m} \in \{1, \ldots, j\}^2$.
Hint : notice that the squares $S_j(\boldsymbol{m})$ are all isometric to each other.

(b) We want to show that $\sigma(A^+) = \mathbb{R}^+$. For any $\lambda > 0$, construct a sequence of L^2-normalized states $(\psi_n \in H^2(\mathbb{R}^2))_{n\geq 1}$, such that ψ_n are supported in the left half-space $\mathbb{R}^2_- = \{(x,y) \in \mathbb{R}^2,\ x < 0\}$, and satisfy $\|(-\Delta - \lambda)\psi_n\| \overset{n\to\infty}{\to} 0$. Deduce that the Laplacian $(-\Delta_{\mathbb{R}^d \setminus S})$ on $\mathbb{R}^d \setminus S$, with Neumann or Dirichlet boundary conditions, admits for spectrum $\mathbb{R}^+$. Conclude.
Hint : you may take for ψ_n truncated plane waves.

(c) Describe the spectrum of the operator A_j^+.

(d) Compute similarly the spectra of $A^-_{j,\boldsymbol{m}}$, A^-, and A^-_j.

(e) We call $N_j^\pm(h)$ the number of negative eigenvalues of $A_j^\pm$. Show that these numbers are finite.

(f) Apply the max-min principle (again, using form domains) to compare the μ_n's of the operators A_j^+, A_j^- and A. Deduce that $N_j^+(h)$, $N_j^\pm(h)$ and $N(h)$ satisfy, for any $h \in (0,1]$, the inequalities

$$N_j^+(h) \leq N(h) \leq N_j^-(h)\,. \tag{2}$$

(g) We want to obtain an asymptotic expression of $N_j^+(h)$ and $N_j^-(h)$, when $h \to 0$. For this aim, we will admit the following asymptotics for the number of integer lattice points in large quarter-disks :

$$\#\{(n_1,n_2) \in \mathbb{N}^2,\ n_1^2 + n_2^2 \leq \lambda\} \sim \frac{\pi\lambda}{4}, \quad \text{when } \lambda \to \infty\,.$$

Use this expression to estimate the number of negative eigenvalues of the operators $A^\pm_{j,m}$ when $h \searrow 0$. Deduce the following asymptotics for $N_j^\pm(h)$:

$$N_j^\pm(h) \sim \frac{1}{4\pi h^2}\int_{\mathbb{R}^2} (V_j^\pm)_-(x)\,dx \quad \text{when } h \searrow 0.$$

(h) Using the inequalities (2) and the approximation (1), deduce the following asymptotics for the negative eigenvalues of A :

$$N(h) \sim \frac{1}{4\pi h^2}\int_{\mathbb{R}^2} V_-(x)\,dx \quad \text{when } h \searrow 0.$$

This type of asymptotics is called a (semiclassical) Weyl's formula.

Exercise : Rank 1 perturbation of a Schrödinger operator

Our base Hilbert space is $\mathcal{H} = L^2(\mathbb{R})$. Consider a potential function $V \in L^1_{\rm loc}(\mathbb{R}, [1, \infty))$. We consider the following sesquilinear form :

$$q(\varphi, \psi) = \int_{\mathbb{R}} \bar{\varphi}'(x)\psi'(x)\, dx + \int_{\mathbb{R}} V(x)\, \bar{\varphi}(x)\psi(x)\, dx\,,$$

defined on the domain $D(q) = \{\psi \in H^1(\mathbb{R}),\ \sqrt{V}\psi \in L^2(\mathbb{R})\}$. We call q_0 the restriction of q on the domain $D(q_0) = \{\psi \in D(q),\ \psi(0) = 0\}$.

1. (a) Show that q and q_0 are closed sesquilinear forms.
   (b) Let A, A_0 be respectively the operators associated with q and q_0.
   (c) Recall why A and A_0 are selfadjoint.
   (d) In the case where $V \in L^\infty(\mathbb{R})$, describe the domains $D(A)$ and $D(A_0)$. *Hint* : Apply the integration by parts separately on $\mathbb{R}_-$ and $\mathbb{R}_+$.
   (e) Show that and that the spectra of A and A_0 are included in the interval $[1, \infty)$.
2. We want to compare the operators A and A_0.
   (a) Show that there exists a unique $\phi \in D(q)$ such that $q(\phi, \psi) = \psi(0)$ for all $\psi \in D(q)$, and explain why $\phi(0) \neq 0$.
   Hint : apply Riesz's theorem on the appropriate Hilbert space.
   (b) Denote $K = \{\psi \in D(q),\ q(\varphi_0, \psi) = 0 \text{ for all } \varphi_0 \in D(q_0)\}$. Show that K is a one-dimensional subspace, and is spanned by ϕ.
   Hint : for any $\psi \in D(q)$, show that $\psi_0 \stackrel{\text{def}}{=} \psi - \frac{\psi(0)}{\varphi(0)}\varphi$ belongs to $D(q_0)$.
   (c) Let $f \in L^2(\mathbb{R})$. Set $\psi \stackrel{\text{def}}{=} A^{-1}f$ and $\psi_0 \stackrel{\text{def}}{=} A_0^{-1}f$. Justify that these states are well-defined. Show that $\psi - \psi_0 \in K$.
   (d) Deduce that the difference $A^{-1} - A_0^{-1}$ is a rank one operator. Show that this operator must be a multiple of the orthogonal projector π_ϕ on the state ϕ, namely $A^{-1} - A_0^{-1} = c\pi_\phi$ for some constant $c = c_V \in \mathbb{R}$.
   Hint : notice that $A^{-1} - A_0^{-1}$ is symmetric.
3. We will now treat more explicitly the case where the potential $V = 1$.
   (a) Using the defining formula $q(\phi, \psi) = \psi(0)$, compute the Fourier transform $\hat{\phi}(\xi)$ of the state $\phi \in D(q)$ defined in 2(a). Using contour integrals, give the explicit formula for $\phi(x)$.
   (b) Write the action of A on f as a multiplication operator in Fourier space, and then as a convolution operator acting on f.
   (c) From this expression and the condition $A_0^{-1}f \in D(A_0) \subset D(q_0)$, compute explicitly the constant $c = c_{V=1}$ for this case.
   (d) What are the spectra of A and A_0 for this case ? *Hint* : notice that A_0^{-1} is a compact perturbation of A^{-1}.