Self-Adjoint Perturbations in the Discrete Case

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1. Introduction

Let $A(t)$ be an analytic family of compact, self-adjoint operators on a Hilbert space $\mathcal{H}$, for $t \in I = (a, b)$, with $a < 0 < b$. For example, we might have

$$A(t) = ((H + tV)^2 + I)^{-1}, \tag{1.1}$$

where H is an unbounded, self-adjoint operator with discrete spectrum and V is a bounded self-adjoint operator. Let λ be an eigenvalue of $A(0)$.

More generally, $A(t)$ can be an analytic family of bounded self-adjoint operators on $\mathcal{H}$ with the property that λ is an isolated point of $\operatorname{Spec} A(0)$, and such that the λ-eigenspace of $A(0)$ is finite dimensional.

Let D be a closed disk centered at λ such that $\operatorname{Spec} A(0) \cap D = \{\lambda\}$. It follows tat, for $|t|$ sufficiently small, $\operatorname{Spec} A(t) \cap \gamma = \emptyset$, where $\gamma = \partial D$. For such t, we have orthogonal projections

$$P(t) = \frac{1}{2\pi i} \int\limits_{\gamma} (\zeta - A(t))^{-1} \, d\zeta, \tag{1.2}$$

depending analytically on t, such that $P(0)$ is the orthogonal projection of $\mathcal{H}$ onto the λ-eigenspace of $A(0)$. We want to analyze the range $\mathcal{H}(t)$ of $P(t)$ and the eigenvalues and eigenvectors of $A(t)|_{\mathcal{H}(t)}$.

In case the λ-eigenspace of $A(0)$ has dimension 1, then each $P(t)$ has rank 1, and it is straightforward to produce a power series for nontrivial $u(t) \in \mathcal{H}(t)$ and the associated eigenvalue $\lambda(t)$, satisfying $A(t)u(t) = \lambda(t)u(t)$. We record the calculation in §1. Actually, we concentrate on the case (1.1), but extensions to more general $A(t)$ are easily done. In §3 we show how results of §2 apply to radially symmetric operators of the form $H + tV$ acting on functions on $\mathbb{R}^n$, where $H = -\Delta + W$, and W and V are both radially symmetric, with V bounded and $W(x) \to +\infty$ as $|x| \to \infty$. In such a case, H has eigenspaces of dimension > 1, but $L^2(\mathbb{R}^n)$ splits into a direct sum of subspaces, invariant under $H(t)$, on which we have simple spectrum.

Generally, if the λ-eigenspace of $A(0)$ has dimension > 1, matters are more complicated. The space $\mathcal{H}(t)$ splits into a number of eigenspaces $\mathcal{H}_j(t)$ for $A(t)|_{\mathcal{H}(t)}$, with eigenvalues $\lambda_j(t)$. It is an important result of T. Kato that there is an orthonormal basis of $\mathcal{H}(t)$, consisting of eigenvectors of $A(t)$, and depending analytically on t, and the eigenvalues are hence also analytic in t. We discuss this in §4.

2. Perturbation of a simple eigenspace

Let us say

$$Hu = \lambda u, \tag{2.1}$$

and λ is a simple eigenvalue of H. Then, for small ε, $H+\varepsilon V$ has a simple eigenvalue $\lambda(\varepsilon)$, analytic in ε, such that $\lambda(0)=\lambda$, and an associated eigenvector $u(\varepsilon)$, analytic in ε. Here we produce recursion formulas for the power series. Let us write

$$\begin{aligned} \lambda(\varepsilon) &= \lambda + \varepsilon\mu(\varepsilon), \quad \mu(\varepsilon) = \mu_0 + \varepsilon\mu_1 + \cdots, \\ u(\varepsilon) &= u + \varepsilon v(\varepsilon), \quad v(\varepsilon) = v_0 + \varepsilon v_1 + \cdots. \end{aligned} \tag{2.2}$$

We set

$$(H+\varepsilon V)(u+\varepsilon v(\varepsilon)) = (\lambda + \varepsilon\mu(\varepsilon))(u+\varepsilon v(\varepsilon)), \tag{2.3}$$

expand in powers of ε, and compare like powers of ε to obtain formulas for μ_j and v_j. Of course, (2.3) defines $u+\varepsilon v(\varepsilon)$ only up to a scalar factor. One could normalize by requiring $\|u+\varepsilon v(\varepsilon)\|$ to be constant, but we find it convenient to use the following normalization:

$$v(\varepsilon) \perp u. \tag{2.4}$$

From (2.3) we get

$$(H-\lambda)v(\varepsilon) = \mu(\varepsilon)u - Vu + \varepsilon\mu(\varepsilon)v(\varepsilon) - \varepsilon V v(\varepsilon), \tag{2.5}$$

and applying the expansion (2.2) yields

$$\begin{aligned} \sum_{j\ge 0} \varepsilon^j (H-\lambda)v_j &= \mu_0 u - Vu + \sum_{j\ge 1} \varepsilon^j \mu_j u \\ &\quad + \sum_{k,\ell\ge 0} \varepsilon^{1+\ell+k}\mu_\ell v_k - \sum_{j\ge 1} V v_{j-1}\varepsilon^j. \end{aligned} \tag{2.6}$$

Equating multiples of ε^0 yields

$$(H-\lambda)v_0 = (\mu_0 - V)u. \tag{2.7}$$

For this to be solvable for v_0, we need the right side to be in the range of $H-\lambda$, i.e., $(\mu_0 - V)u \perp u$, or equivalently

$$\mu_0 = (Vu, u) \quad (\text{assuming } \|u\|_{L^2} = 1). \tag{2.8}$$

Then (2.7) is uniquely solvable for v_0 up to a scalar multiple of u. The normalization (2.4) gives $v_0 \perp u$, so

$$v_0 = (H-\lambda)^{-1}\big[(\mu_0 - V)u\big], \tag{2.9}$$

with $(H-\lambda)^{-1}$ integpreted as 0 on the span of u.

To treat higher powers of ε in (2.6), let us write

$$\sum_{k,\ell\geq 0} \varepsilon^{1+\ell+k}\mu_\ell v_k = \sum_{j\geq 1} \varepsilon^j w_j, \tag{2.10}$$

with

$$w_j = \sum_{k=0}^{j-1} \mu_{j-1-k} v_k, \quad \text{for} \quad j \geq 1. \tag{2.11}$$

Then equating factors of ε^j in (2.6) gives

$$(H-\lambda)v_j = \mu_j u + w_j - V v_{j-1}, \quad j \geq 1. \tag{2.12}$$

As with (2.7), we need the right side of (2.12) to be in the range of $H-\lambda$, or equivalently, orthogonal to u, which is to say

$$\mu_j = (V v_{j-1} - w_j, u), \tag{2.13}$$

as before assuming $\|u\|_{L^2} = 1$. Then (2.12) determines v_j uniquely up to a multiple of u, and again (2.4) requires $v_j \perp u$, so

$$v_j = (H-\lambda)^{-1}\big[\mu_j u + w_j - V v_{j-1}\big], \quad \text{for} \quad j \geq 1. \tag{2.14}$$

3. Rotationally symmetric Hamiltonians

Let

$$H = -\Delta + W, \tag{3.1}$$

where $\Delta = \partial_1^2 + \cdots + \partial_n^2$ is the Laplace operator on $\mathbb{R}^n$ and $W \in C^\infty(\mathbb{R}^n)$ satisfies

$$W(x) = W(|x|), \quad W(x) \to +\infty \ \text{ as } \ |x| \to \infty. \tag{3.2}$$

Then H has discrete spectrum as an unbounded self adjoint operator on $L^2(\mathbb{R}^n)$. Now assume

$$V \in C^\infty(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n), \quad V(x) = V(|x|), \tag{3.3}$$

and consider

$$H(\varepsilon) = H + \varepsilon V. \tag{3.4}$$

Each $H(\varepsilon)$ also has discrete spectrum. Since $SO(n)$ leaves each eigenspace of $H(\varepsilon)$ invariant, many of these eigenspaces have dimension > 1. However, the following observation greatly simplifies the study of the spectrum of $H(\varepsilon)$ and its eigenspaces. Namely, let

$$\{\varphi_{jk} : 1 \le j \le d_k, k \ge 0\} \tag{3.5}$$

be an orthonormal basis of $L^2(S^{n-1})$ such that, for each k, $\{\varphi_{jk} : 1 \le j \le d_k\}$ is an orthonormal basis for an eigenspace of Δ_S, the Laplace-Beltrami operator on S^{n-1}. Then

$$L^2(\mathbb{R}^n) = \bigoplus_{j,k} \mathcal{H}_{jk}, \tag{3.6}$$

where

$$\mathcal{H}_{jk} = \{f \in L^2(\mathbb{R}^n) : f(x) = \varphi_{jk}(\omega)\psi(r), \text{ for some } \psi\}, \tag{3.7}$$

where $x = r\omega,\ r = |x|,\ \omega \in S^{n-1}$. We see that

$$e^{itH(\varepsilon)} : \mathcal{H}_{jk} \longrightarrow \mathcal{H}_{jk}, \tag{3.8}$$

for each $t, \varepsilon \in \mathbb{R},\ k \ge 0,\ j \in \{1, \dots, d_k\}$. Thus the problem of analyzing the eigenvalues and eigenfunctions of $H(\varepsilon)$ can be reduced to analyzing these objects on each Hilbert space $\mathcal{H}_{jk}$. That this is a great simplification follows from:

Proposition 2.1. *For wach $k \geq 0,\ j \in \{1, \dots, d_k\}$,*

$$H\Big|_{\mathcal{H}_{jk}} \quad \textit{has simple spectrum.} \tag{3.9}$$

Proof. If (3.9) fails, there is an eigenvalue λ of H and orthonormal

$$u_i \in \mathcal{H}_{jk}, \quad u_i(x) = \varphi_{jk}(\omega)\psi_i(r), \quad i = 1, 2, \tag{3.10}$$

such that

$$Hu_i = \lambda u_i, \quad i = 1, 2. \tag{3.12}$$

Then $\psi_1(r)$ and $\psi_2(r)$ satisfy the same second-order, homogeneous ODE. Rather than finish off the proof with a purely ODE argument, we proceed as follows. Given each i, for no $r > 0$ can we have $\psi_i(r) = \psi_i'(r) = 0$. It follows that there exist $r_\nu \searrow 0$ such that $\psi_1(r_\nu) = a_\nu \neq 0$ and $\psi_2(r_\nu) = b_\nu \neq 0$. Hence

$$b_\nu u_1 - a_\nu u_2 = 0 \ \text{ on } |x| = r_\nu. \tag{3.13}$$

This would imply that $-\Delta + V$ would have λ as an eigenvalue when acting on functions on the ball $B_{r_\nu}(0)$ of radius r_ν centered at 0, with the Dirichlet boundary condition. But it is readily verified that the smallest eigenvalue of such operators tends to $+\infty$ as $r_\nu \searrow 0$, so we cannot have such u_1 and u_2. This proves Proposition 2.1.

Remark. We therefore see that each $H(\varepsilon)|_{\mathcal{H}_{jk}}$ has simple spectrum.

4. Kato's analyticity theorem – local version

As in §1, we assume $A(t)$ is an analytic family of bounded self-adjoint operators on a Hilbert space $\mathcal{H}$, for $t \in (a,b)$, $a < 0 < b$. We assume that λ is an isolated point of $\operatorname{Spec} A(0)$, and that the λ-eigenspace of $A(0)$ is finite dimensional. We have a small closed disk D about λ such that $\operatorname{Spec} A(0) \cap D = \{\lambda\}$ and such that, for $|t|$ small, $\operatorname{Spec} A(t) \cap \gamma = \emptyset$, where $\gamma = \partial D$, and we have the orthogonal projections

$$P(t) = \frac{1}{2\pi i} \int_\gamma (\zeta - A(t))^{-1}\, d\zeta, \tag{4.1}$$

with range $\mathcal{H}(t)$, depending analytically on t. We discuss the spectral behavior of $A(t)|_{\mathcal{H}(t)}$.

For this, it is useful to bring in the analytic family of unitary operators

$$U(t) : \mathcal{H}(0) \xrightarrow{\approx} \mathcal{H}(t), \tag{4.2}$$

defined by $U(t)u(0) = u(t)$, where

$$u'(t) = P'(t)u(t). \tag{4.3}$$

This construction was used in [K2]. It arose in [K1], in another setting, that of the quantum adiabatic theorem. See Appendix A for a discussion of how solving (4.3) with $u(0) \in \mathcal{H}(0)$ yields the unitary operators $U(t)$ in (4.2). As emphasized in Appendix A, this construction has a natural interpretation in terms of parallel transport of sections of the vector bundle associated to $\{P(t)\}$. Such a geometrical context was not considered in [K1] and [K2], but knowing the geometrical setting naturally leads one to the "Berry phase." See Appendix U of [T] for further discussion of this.

Having (4.2), we see that $A(t)|_{\mathcal{H}(t)}$ is unitarily equivalent to

$$B(t) : \mathcal{H}(0) \longrightarrow \mathcal{H}(0), \quad B(t) = U(t)^{-1} A(t) U(t), \tag{4.4}$$

an analytic family of self-adjoint operators on $\mathcal{H}(0)$. Note that $B(0) = \lambda I$. Let us write

$$B(t) = B_0(t) + \beta(t) I, \tag{4.5}$$

with

$$\beta(t) = \frac{1}{n} \operatorname{Tr} B(t) = \frac{1}{n} \operatorname{Tr} A(t)P(t), \tag{4.6}$$

where $n = \dim \mathcal{H}(0)$. We see that $\beta(t)$ is analytic in t, and

$$B_0(0) = 0, \quad \operatorname{Tr} B_0(t) = 0. \tag{4.7}$$

There are two cases to consider.

Case I. $B_0(t) \equiv 0$.
In this case, $B(t) = \beta(t)I$, and we are done. All the eigenvalues of $B(t)$ (hence of $A(t)|_{\mathcal{H}(t)}$) are $\beta(t)$, analytic in t. Picking an orthonormal basis $u_1, \dots, u_n$ of $\mathcal{H}(0)$, we get the orthonormal basis $u_1(t), \dots, u_n(t)$ of $\mathcal{H}(t)$ by solving $u_j'(t) = P_j'(t)u_j(t)$, and these are eigenvectors of $A(t)$, depending analytically on t.

Case II. $B_0(t)$ not identically 0.
In this case, there is a positive integer k such that

$$B_0(t) = t^k B_1(t), \tag{4.8}$$

where

$$B_1(t) : \mathcal{H}(0) \longrightarrow \mathcal{H}(0) \ \text{ is analytic in } t, \quad B_1(0) \neq 0. \tag{4.9}$$

Note that

$$\operatorname{Tr} B_1(0) = 0, \tag{4.10}$$

so the eigenspaces of $B_1(0)$ all have dimension $< n$.

Now we can apply the analysis of $A(t)$ described above to the analytic family of operators $B_1(t)$, about each eigenspace of $B_1(0)$, and continue. In view of the dimensional considerations, this must terminate after a finite number of steps, yielding an analytic, orthonormal family $u_1(t), \dots, u_n(t)$ of eigenvectors of $A(t)$, with eigenvalues $\lambda_j(t)$, such that $u_1(0), \dots, u_n(0)$ form an orthonormal basis of $\mathcal{H}(0)$ and $\lambda_j(0) = \lambda$.

The analysis just described works for sufficiently small t, so we call it a local analysis. Under appropriate conditions, one can proceed to a global analysis.

A. Parallel transport defined by families of orthogonal projections

Let $\mathcal{H}$ be a hilbert space (real or complex), M a smooth manifold, and $E = M\times\mathcal{H}$ the trivial vector bundle with fiber $\mathcal{H}$. Assume we have orthogonal projections

$$P_k(x) : \mathcal{H} \longrightarrow \mathcal{H}, \quad 1 \le k \le m, \tag{A.1}$$

depending smoothly of $x \in M$, with range $E_{k,x} \subset \mathcal{H}$, defining smooth vector bundles $E_k \to M$, such that $E = E_1 \oplus \cdots \oplus E_m$. Each E_k has a natural covariant derivative ∇^k, defined by

$$\nabla^k_X u(x) = P_k(x) D_X u, \quad \text{for} \ \ u \in C^\infty(M, E_k), \tag{A.2}$$

where X is a vector field on M and D is the standard flat covariant derivative on E. Let $\gamma(t)$ be a smooth path in M, and, for short, set $P_k(t) = P_k(\gamma(t))$. Now parallel transport anong γ for a section u of E_k over γ is defined by

$$u(t) = P_k(t)u(t), \quad P_k(t)u'(t) = 0. \tag{A.2A}$$

Differentiating the first of these equations and using the second, we get

$$u'(t) = P_k'(t)u(t). \tag{A.3}$$

We claim that (A.3) itself defines such parallel transport. To see this, we check that

$$u(0) \in E_{k,\gamma(0)} \Longrightarrow u(t) \in E_{k,\gamma(t)}, \tag{A.4}$$

when u solves (A.3). This is equivalent to

$$(I - P_k(t))u(t) \equiv 0, \quad \text{given} \ \ P_k(0)u(0) = u(0). \tag{A.5}$$

To see this, set $w(t) = (I - P_k(t))u(t)$, and compute

$$\begin{aligned} w'(t) &= \frac{d}{dt}(I - P_k(t))u(t) \\ &= u'(t) - P_k'(t)u(t) - P_k(t)u'(t) \\ &= P_k'(t)u(t) - P_k'(t)u(t) - P_k(t)P_k'(t)u(t) \\ &= -P_k'(t)w(t), \end{aligned} \tag{A.6}$$

since

$$\begin{aligned} P_k(t) = P_k(t)^2 &\Longrightarrow P_k'(t) = P_k'(t)P_k(t) + P_k(t)P_k'(t) \\ &\Longrightarrow P_k(t)P_k'(t) = P_k'(t)(I - P_k(t)). \end{aligned} \tag{A.6A}$$

Since $w(0) = 0$, we see that the ODE $w'(t) = -P_k'(t)w(t)$ yields $w(t) \equiv 0$. Having (A.5), we see that (A.3) plus $P_k(0)u(0) = u(0)$ implies the first identity in (A.2A).

Then differentiating this first identity and using (A.3) yields the second identity in (A.2A).

Now we can put the covariant derivatives ∇^k on E_k together to produce a new covariant derivative on E:

$$\widetilde{\nabla} = \nabla^1 \oplus \cdots \oplus \nabla^m, \tag{A.7}$$

typically different from the trivial covariant derivative D. Then $\widetilde{\nabla}$ defines a parallel transport, along a curve γ in M, for $\mathcal{H}$-valued functions, which preserves sections of each sub-bundle E_k. In fact, we go from (A.3) to

$$u'(t) = C(t)u(t), \quad C(t) = \sum_{k=1}^{m} P_k'(t)P_k(t). \tag{A.8}$$

Note that since $\sum_k P_k(t) = I$ and each $P_k(t) = P_k(t)^2$, we have

$$\begin{aligned} 0 &= \frac{d}{dt}\sum_{k=1}^{m} P_k(t)^2 \\ &= \sum_{k=1}^{m} \Big[P_k'(t)P_k(t) + P_k(t)P_k'(t)\Big]. \end{aligned} \tag{A.9}$$

Also

$$P_k(t)^* = P_k(t) \Longrightarrow P_k'(t)^* = P_k'(t), \tag{A.10}$$

so

$$C(t)^* = -C(t), \tag{A.11}$$

In other words, $C(t)$ in (A.8) is skew-adjoint for each t, so the solution operator acting on functions with values in $\mathcal{H}$ is

$$u(t) = U(t)u(0), \quad U(t) : \mathcal{H} \to \mathcal{H} \ \text{ is unitary, for each } t. \tag{A.12}$$

It follows that

$$U(t) : E_{k,\gamma(0)} \longrightarrow E_{k,\gamma(t)} \tag{A.13}$$

is unitary, for each $t \in \{1, \dots, m\}$.

Such results as discussed above can be found in Chapter 2, §4.4 of [K2], except for the differential geometric interpretation, which we pursue a little further here. Regarding the relation between the covariant derivatives D and $\widetilde{\nabla}$, parallel to (A.2) we have

$$\begin{aligned} \widetilde{\nabla}_X u &= \sum_{k=1}^{m} P_k(x)D_X(P_k(x)u) \\ &= \sum_k P_k(x)^2 D_X u + \sum_k P_k(x)(D_X P_k(x))u \\ &= D_X u + \Gamma_X u, \end{aligned} \tag{A.14}$$

for a smooth $\mathcal{H}$-valued function u on M. Thus we have the connection form

$$\Gamma_X = \sum_k P_k(x) D_X P_k(x), \tag{A.15}$$

or

$$\Gamma = \sum_{k=1}^{m} P_k \, dP_k. \tag{A.16}$$

Now the curvature of $\widetilde{\nabla}$ is given by

$$\Omega = d\Gamma + \Gamma \wedge \Gamma, \tag{A.17}$$

from which a calculation gives

$$\Omega = \sum_{k=1}^{m} P_k \, dP_k \wedge dP_k \, P_k. \tag{A.18}$$

The kth term in this sum is the curvature of the bundle E_k.

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