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# Averaging methods in spectral theory of Schrödinger operators

## 1. INTRODUCTION

We shall discuss an eigenvalue problem in the context of perturbation theory. Given an operator A with a "nice" discrete spectrum $\{\lambda_k^0\}_{k=1}^\infty$ and a perturbation $L = A + B$, one is asked:

(I) to find the eigenvalues of L, $\{\lambda_k\}_1^\infty$ (Direct Problem),

(II) to recover perturbation B (of some given class), from the pertrubed eigenvalues (Inverse Problem).

The solution of problem (II) often requires a characterization of all "isospectral" pertrubations.

The classical operator for an eigenvalue problem is the regular Sturm-Liouville operator: $L = -\frac{d^2}{dx^2} + V(x)$ on [0,1] (see [1], [9], [10]) and its multivariable generalizations, i.e., Schrödinger operators $L = -\Delta + V(x)$ on the n-sphere $S_n$ ([3], [4], [12-14]) and the n-torus $T^n$ [2]. Another interesting example is the perturbation of the harmonic oscillator $A = \frac{1}{2}(-\partial^2 + x^2)$, ([5], [11]).

The perturbed eigenvalues $\{\lambda_k(L)\}$ can rarely be calculated explicitly. Most often, one is asked to find an approximate (asymptotic) formula for $\lambda_k$. Ideally, one would like to have formulae with sufficient data on the perturbation to solve the Inverse Problem.

Let us briefly review some known results. For regular Sturm-Liouville operators, $L = -\partial^2 + V(x)$, asymptotics of $\{\lambda_k\}$ were first derived by G. Borg [1];

$$\lambda_k \sim (\pi k)^2 + b_0 + \frac{b_1}{k^2} + \ldots \text{ as } k \to \infty, \tag{1.1}$$

where $b_0 = \int_0^1 V dx$, and $b_i$, $i = 1,2,\ldots$ depend on the Fourier coefficients of V. We note that (1.1) does not provide sufficient data to solve the

Inverse Problem. In fact, Sturm-Liouville operators have large "isospectral families", both in the periodic [9] and the two-point-boundary-value case [7].

The situation is different for multivariable operators, $-\Delta + V$ on $S_n$ or $T^n$, where it is believed that the only isospectral deformations of V are given by natural symmetries (rotations, translations, etc.). This is the so-called "spectral rigidity hypothesis" of V. Guillemin. Precise results of this nature were established for generic potentials on $T^n$ [2], some special (low degree) spherical harmonics on $S_n$ ([3], [4], [12]), and for anharmonic oscillators [5-6].

The purpose of the present paper is to outline an approach to the problem based on "averaging methods" as developed by several authors ([4], [12], [14]) in the context of the n-sphere Schrödinger theory and by the author [5-6] for anharmonic oscillators. We shall start with a general scheme and then specify it to Schrödinger operators.

## 2. PERTURBATION EXPANSION

Let $L = A + B$ be a "small" (relatively compact) perturbation of a self adjoint operator A with "nice" (integral) spectrum: spec $A \subseteq \{0,1,2,\ldots,\}$. The k-th eigenvalue of L is $\lambda_k \equiv \lambda_k(L) = k + \mu_k$ with "small" $\mu_k$. We want to derive an asymptotic expression

$$\mu_k \sim f(k), \text{ as } k \to \infty, \tag{2.1}$$

and relate it in some explicit way to the perturbation; in other words, to write f as a "functional of B". Thus we hope to recover B from asymptotics of spectral fluctuations $\{\mu_k\}_1^\infty$.

The standard eigenvalue perturbation yields the following expansion of $\mu_k$:

$$\mu_k \sim \mu_k^{(1)} + \mu_k^{(2)} + \ldots , \tag{2.2}$$

where

$$\left.\begin{array}{ll}\text{(1st order)} & \mu_k^{(1)} = \langle B\phi_k|\phi_k\rangle = \text{"diagonal B"},\\[2ex] \text{(2nd order)} & \mu_k^{(2)} = \langle (B-\mu_k^{(1)})(k-A)^{-1}(B-\mu_k^{(1)})\phi_k|\phi_k\rangle = \sum_{j\neq k}\dfrac{b_{kj}^2}{k-j}\,.\end{array}\right\} \quad (2.3)$$

Here $\{\phi_k\}_1^\infty$ represents a normalized system of eigenfunctions of A and $\{b_{kj}\}$ are matrix entries of B in the basis $\{\phi_k\}_1^\infty$. The numbers $\mu_k^{(1)}$ and $\mu_k^{(2)}$ give the first and second order corrections to the k-th eigenvalues.

The perturbation expansion (2.2) is well known and effectively used to construct higher order corrections of a fixed eigenvalue. However, it seems to be of little help in determining the large-eigenvalue asymptotic function f(k) to (2.1). We shall resort to a different approach motivated by [4] and [14].

Our goal is to replace a perturbation B in L = A + B by an operator $\bar{B}$, that commutes with A and is such that $A + \bar{B}$ is almost unitary equivalent to A + B, i.e.,

$$A + B = U(A + \bar{B})U^{-1} + \text{"small remainder R"}. \quad (2.4)$$

The main advantage of passing from A + B to $A + \bar{B}$ is that the operator $\bar{B}$ can be diagonalized jointly with A. Thus the k-th fluctuation $\bar{\mu}_k$ of $A + \bar{B}$ becomes the k-th eigenvalue of $\bar{B}$. If we could approximate $\bar{B}$ by an explicit "function of A", asymptotics (2.1) would immediately follow. This is shown to be the case in one of two examples below (anharmonic oscillator). In the other example (n-sphere Schrödinger), though $\bar{B}$ is not a "function of A" (because of multiplicities), the commutativity relation $[A;\bar{B}] = 0$ yields some valuable information on spectra that lead to a partial solution of the Inverse Problem.

Thus our method requires two steps

(i) explicit construction of $\bar{B}$ by "averaging",

(ii) justification of (2.4), including estimates on the remainder.

## 3. AVERAGING

The operator A of Section 2 with integral spectrum, spec $A = \{k\}_{k=0}^{\infty}$, generates a periodic unitary group, $e^{2\pi iA} = I$.

We denote by B(t) the conjugates of B, $e^{itA}\, B\, e^{-itA}$, and introduce the "first" and "second" order averages of B:

$$B_1 = \frac{1}{2\pi}\int_0^{2\pi} B(t)dt, \quad B_2 = \frac{1}{4\pi i}\int_0^{2\pi}\int_0^{t} [B(t); B(s)]ds\, dt, \tag{3.1}$$

where [ ; ] means the usual commutator of two operators. The meaning and motivation for (3.1) comes from the so-called "return operator" approach.

If we define the return operator

$$W := e^{2\pi i(A+B)} - I,$$

it can be shown that W admits the following expansion (see [4], [6])

$$W = 2\pi i\, B_1 - \frac{1}{2!}\,(4\pi^2 B_1^2 + 4\pi i\, B_2) + \dots\ . \tag{3.2}$$

Furthermore the following commutation relations hold

$$[A; B_1] = 0, \quad [A; B_2] = 4\pi[B; B_1].$$

In other words, A commutes with the first average, and commutes modulo l.o.t. with the second. As a corollary in some cases (see "anharmonic oscillator" below), both averages can be approximated by functions of A:

$$B_1 \approx f_1(A), \quad B_2 \approx f_2(A).$$

The explicit calculation of $f_1, f_2$ involves symbolic calculi and will be carried out in the next section.

The second step (ii) in our method is stated in the following

<u>Ansatz</u>: Operators L = A + B and $\bar{L} = A + \bar{B}$ are "almost unitary equivalent", i.e., there exist a skew symmetric Q, and unitary $U = e^{Q}$ such that

$$A + B = e^{Q}(A + \bar{B})e^{-Q} + \text{"small R"},$$

where the remainder R satisfies the estimate

$$|R| = \sqrt{R^{*}R} \leq \text{Const } A^{-\gamma}. \tag{3.3}$$

is the sense of comparison of selfadjoint operators.

We note that the operator Q is also constructed explicitly. In fact, to first order approximation, $Q = \frac{1}{4\pi}\int_0^{2\pi} (2\pi - t)B(t)dt$ (see [14]); the second order correction is more complicated (see [4]; [6]).

The Ansatz combined with symbolic calculi below yields an approximate relation $\bar{B} \approx f(A)$, (consequently $\mu_k \approx f(k)$) as well as the error estimates

$$|\mu_k - \bar{\mu}_k| = \mathcal{O}(k^{-\gamma}). \tag{3.4}$$

However the rigorous justification of all constructions, estimates, asymptotics, etc. can be provided only within a specific context.

## 4. SPECIFIC EXAMPLES

We shall consider two examples.

1°. The n-sphere Schrödinger operator: $L = -\Delta + V$ on $S_n$.

The spectrum of the Laplacian $-\Delta$ on $S_n$ is well known: k-th eigenvalue = $k(k+n-1)$ with multiplicity $d_k = \mathcal{O}(k^{n-1})$. The eigenfunctions are spherical harmonics of degree k. If we perturb $-\Delta$ by a potential V, the k-th eigenvalue splits into a cluster $\lambda_{kj} = k(k+n-1) + \mu_{kj}$ $(j = 1,\dots,d_k)$.

We set $A = \sqrt{-\Delta - (\frac{n-1}{2})^2}$ (so spec $A = \{0,1,\dots\}$), $B = \sqrt{-\Delta + V} - A$, and treat $\sqrt{L} = A + B$ as a perturbation of the above type. To calculate the principal symbols of A, B, $B_1,\dots$, the standard symbolic (pseudodifferential) calculus on $S_n$ is used (cf. [4]; [12-14]). Then

1) $\sigma_A = |\xi|$

2) $\sigma_B(x,\xi) = \sqrt{\xi^2 + V} - |\xi| = \frac{V}{2|\xi|} - \frac{1}{4}\frac{V^2}{|\xi|^3} + \text{l.o.t.}$

3) $\sigma_B(t) = \sigma_B \circ \exp tH$ (Egorov's Theorem). Here $\exp tH$ denotes the Hamilton flow in the phase-space (cotangent or cosphere bundle over $S_n$) of symbol $A = |\xi|$. In other words, $\exp tH$ is the geodesic flow on $S_n$.

Now we can calculate symbols of averages :

4) $\sigma_{B_1} = \frac{1}{2\pi}\int_0^{2\pi} \sigma_B \circ \exp tH\, dt = \frac{1}{2|\xi|}\tilde{V}(x,\xi) - \frac{1}{4|\xi|^3}\tilde{V}^2(x,\xi)$. Here $\tilde{V}$, $\tilde{V}^2$ are the Radon transforms of functions $V$ and $V^2$ on $S_n$.

5) $$\sigma_{B_2} = \frac{1}{4\pi}\int_0^{2\pi}\int_0^t \{\sigma_B \circ \exp tH; \sigma_B \circ \exp SH\}\, ds\, dt =$$

$$\frac{1}{4\pi|\xi|^3}\int_0^{2\pi}\int_0^t \{V\circ\exp tH; V\circ\exp sH\}\, ds\, dt + \text{l.o.t.}$$

As usual, $\{\cdot;\cdot\}$ means the Poisson bracket of two functions on $T^*(S_n)$.
Finally

$$\sigma_{\bar{B}} = \frac{1}{2|\xi|}\tilde{V} + \frac{1}{4|\xi|^3}\left[-V^2 + \frac{1}{\pi}\int_0^{2\pi}\int_0^t \{\cdot\,;\,\cdot\}\, ds\, dt\right] + \dots .$$

In a similar way, one obtains symbols of $\bar{L} = (A + \bar{B})^2$, the intertwining operator $Q$ et al. Combining symbolic calculations with standard elliptic estimates on the sphere one can establish the following

Theorem 4.1: Let $L = -\Delta + V$ be a Schrödinger operator on $S_n$ and $\{\lambda_{kj} = k(k+n-1) + \mu_{kj}\}_{j=1}^{d_k}$ denote its spectrum.

(i) If $V$ is even, then spectral fluctuations $\mu_{kj} = \mathcal{O}(1)$ as $k \to \infty$. Moreover, the sequence of measures $d\rho_k = \frac{1}{d_k}\sum_{j=1}^{d_k} \delta(\lambda-\mu_{kj})$ ($k$-th cluster distribution) converges to a continuous limit:

$$\lim_{k\to\infty} d\rho_k = \beta_o(\lambda)d\lambda \text{ on } \mathbb{R},$$

where $\beta_o(\lambda)$ is the distribution density of the Radon transform $\tilde{V}$ on the cosphere bundle,

$$\langle\phi|\beta_o\rangle = \int_{S^*(S_n)} \phi\circ\tilde{V}\, dS, \text{ for any testing } \phi \text{ on } \mathbb{R}.$$

(ii) If V is odd, $\mu_{kj} = O(k^{-2})$ and

$$\lim_{k\to\infty} \frac{1}{d_k} \sum_j \delta(\lambda - k^2\mu_{kj}) = \beta_o(\lambda)\, d\lambda.$$

Here $\beta_o$ is the distribution density of the function

$$\tilde{V}_2 = \tilde{V}^2 - \frac{1}{4\pi}\int_0^{2\pi} \{V_t;\, V_t^{(-1)}\}dt, \quad \text{on } S^*(S_n),$$

where $V_t = V\circ\exp tH$ and $V_t^{(-1)}$ stands for its antiderivative $\int_0^t V_s\, ds$.

Note that both functions $V_t$ and $V_t^{(-1)}$ are well defined (continuous) on $S^*(S_n)$, provided V is odd. Different parts of Theorem 4.1 were established in [4], [12], [14].

In the general "even plus odd" case we derive, as a corollary of Theorem 4.1, two terms in the approximate expansion of spectral fluctuations: $\mu_{kj} \approx \mu_{kj}^{(0)} + \frac{1}{k^2}\mu_{kj}^{(1)}$. Here $\{\mu_{kj}^{(0)}\}$ result from the "principal contribution" of the even part of V, whereas $\{\mu_{kj}^{(1)}\}$ are due to the odd part as well as higher order contributions of the even part of V. By analogy with [1] and [14], we conjecture that the expansion of $\mu_{kj}$ can be extended to higher powers of $k^{-2}$,

$$\mu_{kj} = \mu_{kj}^{(0)} + \frac{1}{k^2}\mu_{kj}^{(1)} + \ldots, \text{ as } k\to\infty, \text{ j-fixed}$$

and the limiting distributions of m-th order coefficients $\{\mu_{kj}^{(m)}\}_j$ should give higher order band-invariants of A. Weinstein [14].

Unfortunately, $\beta_o$ (and even higher $\beta_m$) is not sufficient to recover the potential V. This was done in special cases (low degree spherical harmonics V), combining $\beta_o$ and the classical "heat-invariants" of Munakshisundaram-Plejel (see [4], [12]).

Our next example proves to be better in this respect.

2°. Anharmonic oscillators: $L = \frac{1}{2}(-\partial^2 + x^2 - 1) + B(x)$ on $\mathbb{R}$.

As in the first example, the harmonic oscillator $A = \frac{1}{2}(-\partial^2 + x^2 - 1)$ has integral spectrum $\{0,1,\ldots\}$. The eigenfunctions are the Hermite functions. We consider a class of perturbations described in terms of their asymptotics at $\infty$,

$$B(x) \sim |x|^{-\alpha} V(x) \text{ as } x \to \infty,$$

with a trigonometric function $V(x)$.

The first two terms in the return-operator expansion (3.2) become

$$\int_0^{2\pi} B(t)dt - \frac{1}{2}\left[\int_0^{2\pi} B^2(t)dt + \int_0^{2\pi}\int_0^t [B(t); B(s)]\, ds\, dt\right]$$

To calculate symbols of averages, we observe that the Hamilton flow of symbol $A = \frac{1}{2}(x^2 + \xi^2)$ consists of rotations in the $(x,\xi)$ phase-plane

$$\exp tH = \begin{pmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{pmatrix}.$$

Thus

$$\sigma_{B_1} = \frac{1}{2\pi}\int_0^{2\pi} B(x\cos t + \xi \sin t)\, dt, \qquad (4.1)$$

$$\sigma_{B_2} = \frac{1}{4\pi}\left[\int_0^{2\pi} B^2(\ldots)dt - \int_0^{2\pi}\int_0^t \{\ldots;\ldots\}\, ds\, dt\right], \qquad (4.2)$$

Both integrals (4.1), (4.2) can be asymptotically evaluated by the stationary phase method (see [5]). It turns out that both symbols depend on the radial variable $r = \sqrt{x^2 + \xi^2}$ only. Precisely,

$$\sigma_{B_1} \sim C_0 r^{-(\alpha+\frac{1}{2})} \;\tilde{V}(r) + \frac{C_1}{r} \text{ as } r \to \infty, \tag{4.3}$$

$$\sigma_{B_2} \sim C_2 r^{-(2\alpha+1/2)} (V_{ev}^2 + V_{od}^2)^{\sim}(r) + C_3\, r^{-(\alpha+3/2)}\, \tilde{\tilde{V}}_{od}(r).$$

Here $\tilde{V}$ and $\tilde{\tilde{V}}$ denote the so-called even and odd "Radon transforms" of V:

$$\tilde{V} = \sum \frac{a_m}{\sqrt{\omega_m}} \cos\,(\omega_m r - \pi/4) \text{ for even } V = \sum a_m \cos \omega_m x,$$

$$\tilde{\tilde{V}} = \sum b_m \sqrt{\omega_m}\, \sin(\omega_m r - \pi/4) \text{ for odd } V = \sum b_m \sin \omega_m x.$$

As a corollary, the whole average operator $\bar{B}$ is approximated by a "function of A", rather of $\sqrt{2A}$, whose symbol is $r = \sqrt{x^2 + \xi^2}$ . Precisely,

$$\bar{B} \approx f_0(\;2A) + f_1(\sqrt{2A}) + f_2(\sqrt{2A}) \tag{4.4}$$

where

$$f_0 = C_0 r^{-(\alpha+1/2)} \tilde{V}_{ev}(r) + \frac{C_1}{r}\;;\; f_1 = C_2 r^{-(2\alpha+1/2)} (V_{ev}^2 + V_{od}^2)^{\sim}\;;$$

$$f_2 = C_3 r^{-(\alpha+3/2)} \tilde{\tilde{V}}_{od}(r). \tag{4.5}$$

From (4.4) we immediately get estimates and asymptotics of spectral fluctuations.

<u>Theorem 4.2</u>: Let L = A + B be an anharmonic oscillator on $\mathbb{R}$ with potential $B(x) \sim |x|^{-\alpha} V(x)$, as $x \to \infty$, and eigenvalues $\{\lambda_k = k + \mu_k\}_1^{\infty}$. Then spectral fluctuations are estimated as

$$\mu_k = O(k^{-\gamma}) \text{ with } \gamma = \begin{cases} \alpha/2 + 1/4 \text{ for even } V \\ \alpha/2 + 3/4 \text{ for odd } V. \end{cases}$$

Moreover, the sequence $\{\mu_k\}$ is asymptotic to

$$\mu_k \sim f_0(\sqrt{2k}) + f_1(\sqrt{2k}) + f_2(\sqrt{2k}) \text{ as } k \to \infty, \tag{4.6}$$

where functions $f_0$, $f_1$, $f_2$ are given by (4.5).

Notice that all three of the functions that appear in (4.6) have the form $r^{-\gamma}F(r)$ with a trigonometric factor $F(r)$ and (generically) distinct exponentials $\gamma$. This allows one to (uniquely!) solve the inverse problem: recover asymptotics of $B(x)$ from asymptotics of $\{\mu_k\}$. The key ingredient in the reconstruction procedure is the so-called "uniform distribution property" [8] of the sequence $\sqrt{2k}$ (mod T) or any tuple of quasiperiods $(T_1, T_2, \ldots)$. In particular, any periodic (almost periodic) function $F(r)$ can be reconstructed from its values at $\{\sqrt{2k}\}_{k=1}^{\infty}$. The details of the inversion procedure in the "even" and "odd" case are discussed in the papers [5,6]. Theorem 4.2 allows us to extend these results to a general "even plus odd" case.

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