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BARRY SIMON

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Semiclassical Analysis of Low Lying Eigenvalues

I. Non-degenerate Minima: Asymptotic Expansions (*)

by

Barry SIMON

Departments of Mathematics and Physics,
California Institute of Technology, Pasadena, California, 91125

ABSTRACT. — We consider eigenvalues of Schrödinger operators of the form $-\Delta + \lambda^2 h + \lambda g$ where $h \geq 0$ has finitely many minima, each of which is non-degenerate. We prove a folk theorem about the asymptotic behavior of the n th eigenvalue in the $\lambda \rightarrow \infty$ limit. We conclude with a few remarks about the extension to Riemannian manifolds because of the significance to Witten's proof of the Morse inequalities.

RÉSUMÉ. — On considère les valeurs propres d'opérateurs de Schrödinger de la forme $-\Delta + \lambda^2 h + \lambda g$ où $h \geq 0$ a un nombre fini de minima, tous non dégénérés. On démontre un résultat généralement admis sur le comportement asymptotique de la $n^{\text{ème}}$ valeur propre dans la limite où $\lambda \rightarrow \infty$. On conclut par quelques remarques sur l'extension du résultat à des variétés riemanniennes, en raison de son rôle dans la démonstration par Witten des inégalités de Morse.

1. INTRODUCTION

In this paper, we consider operators of the form

$$H(\lambda) = -\Delta + \lambda^2 h + \lambda g \tag{1}$$

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on $L^2(\mathbf{R}^n)$ and we want to know about the behavior of the n th eigenvalue, $E_n(\lambda)$, as $\lambda \rightarrow \infty$. If we set $g = 0$, $h = V$ and $\lambda = \hbar^{-1}$ (where \hbar is Planck's constant), then

$$\lambda^{-2}H(\lambda) = -\hbar^2\Delta + V$$

so that the $\lambda \rightarrow \infty$ (equivalently $\hbar \rightarrow 0$) limit is semiclassical. A typical example to keep in mind is the case $v = 1$, $g = 0$, $h = x^2(1-x)^2$ where it has been traditional to replace λ by β^{-2} and then scale

$$x \rightarrow \beta x, \quad -d^2/dx^2 \rightarrow -\beta^{-2}d^2/dx^2$$

so that $\lambda^{-1}H(\lambda)$ becomes

$$-\frac{d^2}{dx^2} + x^2 - 2\beta x^2 + \beta^2 x^4 \quad (2)$$

the so-called double well. Throughout, we make the following hypotheses on h , g :

(A1) h, g are C^∞

(A2) g is bounded below; $h \geq 0$

(A3) h has a finite number of zeros, $\{x^{(a)}\}_{a=1}^k$ and for some \mathbf{R} , $\inf_{|x| > \mathbf{R}} h(x) > 0$

(A4) At each zero, $x^{(a)}$, the matrix

$$A_{ij}^{(a)} \equiv \frac{1}{2} \frac{\partial^2 h}{\partial x_i \partial x_j} (x^{(a)}) \quad (3)$$

is strictly positive definite.

The smoothness is not really necessary except near the points $x^{(a)}$ and one only needs that $g(h+1)^{-1}$ be bounded below (rather than g). Condition (A4) is critical for the results to have the form they will; we hope to study the case where h vanishes on a manifold in a later paper in this series.

In this paper, we will identify the limit of $E_n(\lambda)/\lambda$ as $\lambda \rightarrow \infty$ and more generally discuss asymptotic series, $E_n(\lambda) \sim \sum_{k=-1} a_n^k \lambda^{-k}$. The corresponding

eigenvalues will be concentrated near the minimum points $x^{(a)}$. Another interesting regime is to look at eigenvalues with an energy in the range $\lambda^2(E_0 - \varepsilon, E_0 + \varepsilon)$ which has evoked considerable discussion in the quantum chemistry literature (see e. g. [10] [11]). Hence, we emphasize that we are dealing with « low lying eigenvalues » (indeed, for $-\hbar^2\Delta + V$, we are looking at eigenvalues of energy of the order \hbar ; the true classical limit should involve taking large quantum numbers so the energy is about E_0).

We emphasize that the behavior of $E_n(\lambda)$ is governed by ideas well known in the folk wisdom of theoretical physics. Our decision to formalize the folk theorems is based on several sources: First, Combes, Duclos and Seiler [3] have recently pointed out the lack of a proof of these folk results, and they have provided a proof in the one dimensional case. Their proof

is much more complicated than need be: They require control on the decay of the eigenfunctions of H , and some machinery is required for this. In fact, such decay is irrelevant to the asymptotic series, although in fairness, it should be emphasized that to discuss tunnelling (as Combes *et al.* promise to do in future papers), one does need this decay. However, it seems to us worth dispelling the impression that the asymptotic series are a technically hard problem—indeed, it is (especially for the leading behavior) quite a simple one.

We should mention several discussions prior to [3] of these and related problems (*). In Reed-Simon [14], the model, (2), is discussed and eigenvalue asymptotic series are proven. A class of related problems involve the asymptotics of Born-Oppenheimer curves for large nuclear separations ($1/R$ expansion). The main difference is that at « minima », h has singularities rather than quadratic behavior, so this $1/R$ expansion is technically harder in many ways than the problem we discuss here. Assuming stability (see below), Ahlrichs [1] proved an asymptotic expansion for the $1/R$ situation. A complete analysis using resolvent methods was provided first by Combes-Seiler [4] and later by Morgan-Simon [13] who used geometric ideas. In fact, our analysis here is very similar in spirit to that in [13], although we use an operator form of the IMS localization formula (see § 3) which provides a somewhat less involved strategy.

Our second motivation concerns the recent beautiful paper of Witten [21], who proves Morse inequalities by using the leading semiclassical eigenvalue asymptotics for certain Schrödinger operators on Riemannian manifolds. Given his clever choice of these operators, the inequalities are the result of a simple calculation and the eigenvalue asymptotics. It seemed to be worthwhile to provide a rigorous proof of the step in Witten's proof which is the « obvious » semiclassical result, and for this reason, in § 6 we sketch the situation on a manifold. Witten remarked in [21] that one could probably extend the proof in Reed-Simon [14] to handle the situation he needs: This is probably correct (although the multidimensions may provide difficulties), but the use of the IMS formula is much simpler.

Having described both motivation and previous literature, we turn to the first steps in the analysis. Let

$$H_a(\lambda) = -\Delta + \lambda^2 \sum_{i,j} A_{ij}^a(x - x^{(a)})_i(x - x^{(a)})_j + \lambda g(x^{(a)}) \quad (4)$$

where we emphasize that the constant $g(x^{(a)})$ rather than the function $g(x)$ appears. The point is that lower lying eigenvalues should be concentrated near some $x^{(a)}$ and near $x^{(a)}$, $H(\lambda)$ looks like $H_a(\lambda)$. The next step is the note

(*) See Notes added in proof.

that by scaling, $H_a(\lambda)/\lambda$ has eigenvalues independent of λ ; explicitly, let

$$(U^{(a)}(\lambda)f)(x) = \lambda^{v/2} f(\lambda^{1/2}(x - x^{(a)})) \tag{5}$$

and

$$K^a = -\Delta + g(x^{(a)}) + \sum_{i,j} A_{ij}^a x_i x_j \tag{6}$$

Then

$$H_a(\lambda) = \lambda U^{(a)}(\lambda) K^a U^{(a)}(\lambda)^{-1} \tag{7}$$

Let $e_1 \leq e_2 \leq \dots \leq e_n \leq \dots$ be the eigenvalues of $\bigoplus_{a=1}^k K^a$ counting multiplicity, so $\{e_i\}$ is just a renumbering in increasing order of the eigenvalues $\bigcup_a \left\{ g(x^{(a)}) + \sum_1^v (2n_i + 1)\omega_i^{(a)} \mid n_i = 0, \dots \right\}$ where $[\omega_i^{(a)}]^2$ are the eigenvalues of $A^{(a)}$. (This comes from the exact solution of K^a .) The leading behavior of $E_n(\lambda)$ is given by

THEOREM 1.1. — Let h, g obey hypotheses (A1-4). Fix n . Then for λ sufficiently large $H(\lambda)$ has at least n eigenvalues below its continuous spectrum and

$$\lim_{\lambda \rightarrow \infty} E_n(\lambda)/\lambda = e_n$$

We call this result « stability », since if one thinks of $H(\lambda)/\lambda$ as a kind of perturbation if $\bigoplus_a K^a$, then it is precisely the analog of stability in the sense used by Kato [9] (although since $s - \lim H(\lambda)/\lambda$ doesn't exist, it is not stability in the strict sense). In section 2, we prove the upper bound half of Thm. 1.1 by a simple choice of trial functions, and in section 3, we begin by recalling the IMS localization formula and apply it to get the lower bound half of Thm. 1.1. Given stability, the asymptotic expansion of $E_n(\lambda)$ to all orders is fairly standard perturbation theory: We provide the details in sections 4 and 5. 4 deals with the case where e_n is a simple eigenvalue of $\bigoplus_a K^a$, and 5 with the more technical case where there is degeneracy (warning: Do not confuse degeneracy of eigenvalues with non-degeneracy of the minima of h !). In section 6, we sketch the manifold version of Thm. 1.1.

In a second paper of the series [20], we discuss tunnelling: Explicitly,

if $E(\lambda)$ has an eigenvector $\psi(\lambda; x)$ which lives in more than one well as $\lambda \rightarrow \infty$, then there is always a second eigenvalue $E'(\lambda)$ with

$$|E'(\lambda) - E(\lambda)| = O(e^{-c\lambda})$$

and we identify c explicitly in some situations.

It is a pleasure to thank H. Dym and I. Sigal for the hospitality of the Weizmann Institute where some of this work was done, and R. Seiler and E. Witten for telling me of their work [3] and [21].

2. STABILITY: THE UPPER BOUND

The proof of the upper bound half of Thm. 1.1, viz that

$$\overline{\lim} E_n(\lambda)/\lambda \leq e_n \tag{8}$$

is essentially trivial. One uses eigenfunctions of $H_a(\lambda)$ cutoff at « large distances » (since we have made no growth assumptions on h) as trial functions for $H(\lambda)$. While one has considerable freedom on the cutoffs here, we will use cutoffs suitable for our considerations in the next section. Fix a function $j \in C_0^\infty$ with $0 \leq j \leq 1$ and $j(x) = 1$ (resp 0) if $|x| \leq 1$ (resp $|x| \geq 2$). Let

$$J_\lambda^{(a)}(x) = j(\lambda^{2/5}(x - x^a)) \tag{9}$$

$2/5$ is not essential; any number between $1/3$ and $1/2$ will do. We only consider λ so large, that the J_λ have disjoint supports

$$(i. e. \lambda \geq 4 [\min_{a \neq b} |x^a - x^b|]^{-5/2}).$$

In the next section, we will require J_0 defined by

$$J_0^2 = 1 - \sum_{a=1}^k J_a^2 \tag{10}$$

so

$$1 = \sum_{a=0}^k J_a^2 \tag{11}$$

The following norm estimate is made stronger than we need in this section where only expectation values enter, but we will need it in the next:

LEMMA 2.1. — $\|J_a(H(\lambda) - H_a(\lambda))J_a\| = O(\lambda^{4/5})$.

Proof. — By Taylor's theorem with remainder, on the support of J_a , $\lambda[g - g(x^a)]$ can be bounded by $c\lambda|x - x^a|$ which is $O(\lambda^{+3/5})$ and $\lambda^2[h - \sum A_{ij}^{(a)}(x - x^a)_i(x - x^a)_j]$ is bounded by $\lambda^2|x - x^a|^3$ which is $O(\lambda^{+4/5})$. ■

Remark. — For the actual vectors we use $(\psi, [H(\lambda) - H_a(\lambda)]\psi)$ is $O(\lambda^{-1/2})$.

Let φ_1, \dots , be the eigenvectors of $\bigoplus_a K^a$. Without loss we can choose eigenvectors so that each φ_n is associated to a single summand $a(n)$; we let

$$\psi_n^\lambda = J_\lambda^{a(n)} U^{a(n)}(\lambda) \varphi_n \quad (12)$$

Since each φ_n is a polynomial times a Gaussian, one easily sees that

$$(\psi_n^\lambda, \psi_m^\lambda) = \delta_{nm} + O(\exp(-D\lambda^{1/5})) \quad (13)$$

where the error estimate is *not* uniform in n, m . Moreover,

$$(U^a(\lambda)\varphi_n, (\nabla J_b)^2 U^a(\lambda)\varphi_n) = O(\exp(-D\lambda^{1/5}))$$

so using that when $H\eta = E\eta$, we have (from $[f, [f, H]] = -2(\nabla f)^2$) that

$$(f\eta, Hf\eta) = E(f\eta, f\eta) + (\eta, (\nabla f)^2 \eta)$$

we find that (applying also lemma 2.1)

$$(\psi_n^\lambda, H\psi_m^\lambda) = \lambda e_n \delta_{nm} + O(\lambda^{4/5}) \quad (14)$$

(13), (14), the Rayleigh-Ritz principle (see e. g. [14]) and the fact that by hypothesis (A3)

$$\inf \sigma_{\text{ess}}(H(\lambda)) \geq c\lambda^2$$

with $c > 0$, imply that

THEOREM 2.2. — Let hypothesis A hold. Fix n ; then for λ large, $H(\lambda)$ has at least n eigenvalues below its essential spectrum and (8) holds.

In the next section, we will show that $\lim E_n(\lambda)/\lambda \geq e_n$. Using this fact and (13), (14) we want to show that (at least in the nondegenerate case), the ψ_n^λ approach eigenvectors. For each n , pick ε_n with the property that for each m either $e_m = e_n$ or else $|e_m - e_n| > \varepsilon_n$. Let

$$P_n^\lambda = (2\pi i)^{-1} \oint_{|z - \lambda e_n| \leq \lambda \varepsilon_n} dz (z - H(\lambda))^{-1}$$

so that if e_n is a nondegenerate eigenvalue of $\bigoplus K^a$, then P_n^λ is the orthogonal projection onto the eigenvector corresponding to $E_n(\lambda)$. If e_n is degenerate, then P_n^λ is the projection onto the span of all eigenvectors with eigenvalues $E_m(\lambda)$ obeying $E_m(\lambda)/\lambda \rightarrow e_n$. Thus a vector in $\text{Ran } P_n^\lambda$ can be a linear combination of eigenvectors for eigenvalues which are distinct for all finite λ . The following is critical to higher order perturbation theory.

THEOREM 2.3. — $\|(1 - P_n^\lambda)\psi_n^\lambda\| \rightarrow 0$ as $\lambda \rightarrow \infty$.

Proof. — By induction in n . Fix k and suppose the theorem has been proven for all smaller $n < k$. In particular, if $e_l < e_k$, then by (13), Thm. 1.1,

and the fact that $(1 - P_i^\lambda)\psi_i^\lambda \rightarrow 0$, we conclude that $P_i^\lambda\psi_k^\lambda \rightarrow 0$. Thus, if E_Ω^λ is the spectral family for $H(\lambda)/\lambda$, $E_{(-\infty, e_k - \varepsilon)}^\lambda\psi_k^\lambda \rightarrow 0$ for all ε . The only way this is consistent with $(\psi_k^\lambda, [H(\lambda)\lambda^{-1}]\psi_k^\lambda) \rightarrow e_k$ is if $\|E_{(e_k - \varepsilon, e_k + \varepsilon)}^\lambda\psi_k^\lambda\| \rightarrow 1$ for all ε . ■

3. STABILITY: THE LOWER BOUND

The key to a simple proof of the lower bound part of Thm. 1.1 is a localization formula which has recently been very useful in the study of Schrödinger operators. It appears implicitly in work of Ismagilov [8] and Morgan [12], and explicitly in Morgan-Simon [13]. But it was I. M. Sigal [15] [16] who first appreciated its great power: We dub it the IMS localization formula; for the reader's convenience we begin with a statement and proof:

LEMMA 3.1 (IMS localization formula). — Let $\{J_a\}_{a=0}^k$ be any smooth partition of unity with $J_1, \dots, J_k \in C_0^\infty$ normalized by $\sum_0^k J_a^2 = 1$. Let V be any potential so that the form sum $H = -\Delta + V$ has form domain $Q(H_0) \cap Q(V_+)$. Then

$$H = \sum_{a=0}^k J_a H J_a - \sum_{a=0}^k (\nabla J_a)^2.$$

Remarks. — 1. The domain hypothesis is arranged so that J_a maps $Q(H)$ to itself.

2. The compactness of the support of J_1, \dots, J_k isn't very important, nor is the finiteness of k , but some restrictions to ensure that $\sum (\nabla J_a)^2$ is bounded is needed.

3. Having stated the lemma carefully, we ignore domain questions in the proof which are easy to provide.

Proof. — We have

$$J_a^2 H + H J_a^2 - 2J_a H J_a \equiv [J_a, [J_a, H]] = -2(\nabla J_a)^2$$

summing over a yields the lemma. ■

THEOREM 3.2. — $\liminf E_n(\lambda)/\lambda \geq e_n$.

Proof. — Fix r not an eigenvalue of $\oplus K^a$, say $e_n < r < e_{n+1}$. We will show that for λ large

$$H(\lambda) \geq r\lambda 1 + F_n(\lambda)$$

where 1 is the identity operator and F_n has rank at most n . From this it follows that $\liminf E_{n+1}(\lambda)/\lambda \geq r$. Let $P^{(1)}, \dots, P^{(k)}$ be the projections onto

all eigenvalues below $r\lambda$ for $H^a(\lambda)$, so the sum of the ranks of the $P^{(a)}$ is exactly n . Let $F^{(a)} = H^{(a)}P^{(a)}$. By the IMS formula we write

$$H = J^0 H J^0 + \sum_{a=1}^k J^a H^a J^a + \sum_{a=1}^k J^a (H - H^a) J^a - \sum (\nabla J_a)^2.$$

Now, by lemma 2.1, $\left\| \sum_a J^a (H - H^a) J^a \right\| = O(\lambda^{4/5})$ and $\left\| \sum (\nabla J_a)^2 \right\| = O(\lambda^{4/5})$.

Moreover,

$$J^a H^a J^a \geq J^a F^a J^a + \lambda e_n (J^a)^2$$

and, since $h^2 \geq O(\lambda^{-4/5})$ on $\text{supp } J^0$ we have that

$$J^0 H J^0 \geq (J^0)^2 [O(\lambda^{6/5}) - O(\lambda)] \geq \lambda e_n (J^0)^2$$

for λ large. Summing up and using $\sum_0^k (J^a)^2 = 1$, we obtain

$$H \geq \lambda e_n 1 - O(\lambda^{4/5}) + F_n$$

where $F_n = \sum J^a F^a J^a$ has rank at most n . Thus (15) is proven. ■

Note. — One can probably obtain Thm. 3.2 using the twisting trick à la Davies [22].

4. ASYMPTOTIC SERIES: SIMPLE CASE

In this section, our goal is to obtain asymptotic series if e_n is a simple eigenvalue of $\oplus K^a$. We will suppose:

(B) $h(x)$ and $g(x)$ are polynomially bounded, say $|h(x)| \leq C(1 + |x|^m)$ and $|g(x)| \leq C(1 + |x|^m)$.

Probably, one could get away with growth as fast as e^{ax^2} but who cares! Our main result is:

THEOREM 4.1. — Assume hypotheses (A) and (B). Let e_n be a simple eigenvalue of $\oplus K^a$. Let $E_n(\lambda)$ and $\gamma_n(\lambda)$ be the corresponding eigenvalue and eigenvector of $H(\lambda)$. Then

$$E_n(\lambda) \sim e_n \lambda + a_n^0 + a_n^1 \lambda^{-1} + \dots \tag{16}$$

in the sense that

$$E_n(\lambda) - e_n \lambda - \sum_{l=0}^m a_n^l \lambda^{-l} = O(\lambda^{-m-1})$$

and

$$[U^{a(n)}]^{-1}\gamma_n(\lambda) = \varphi_n + \lambda^{\frac{1}{2}}\varphi_n^{(1)} + \dots + \lambda^{-l/2}\varphi_n^{(l)} + \dots \tag{17}$$

in the sense that

$$\left\| [U^{a(n)}]^{-1}\gamma_n(\lambda) - \sum_{l=0}^m \lambda^{-l/2}\varphi_n^{(l)} \right\| = o(\lambda^{-(m+1)/2})$$

As we note at the end of the section, one has an explicit procedure for computing a_n^l and $\varphi_n^{(l)}$. Our methods follow those in [17] [2] [6], although alternately one could use Kato [9]. We define

$$\tilde{H}(\lambda) = \lambda^{-1}(U^a)^{-1}H(\lambda)(U^a)$$

so

$$\tilde{H}(\lambda) = K^a + V(\lambda)$$

with

$$V(\lambda)(x) = g(x_a + \lambda^{-\frac{1}{2}}x) - g(x_a) + \lambda[h(x_a + \lambda^{-\frac{1}{2}}x) - \lambda^{-1}\Sigma A^{(a)}xx]$$

Clearly $V(\lambda)$ has an asymptotic expansion about $\lambda = \infty$ of the form

$$V(\lambda)(x) = Q_n(\lambda, x) + R_n(\lambda, x)$$

where Q_n is a polynomial in $x, \lambda^{-\frac{1}{2}}$ of degree n and for n sufficiently large ($n \geq m$ where m is given in hypothesis (B) will do),

$$|R_n(\lambda, x)| \leq C_n[\lambda^{-\frac{1}{2}}|x|]^{n+1} \tag{18}$$

Moreover,

$$|Q_n(x, \lambda)| \leq D_n\lambda^{-\frac{1}{2}}(1 + |x|)^n \tag{19}$$

Below, we intend to prove (17) and (16) where the series is instead in $\lambda^{-\frac{1}{2}}$. The fact that all $\lambda^{-l/2}$ turns with l odd vanishing in (16) follows from noting that the operator obtained by changing the sign of $\lambda^{\frac{1}{2}}$ is unitarily equivalent to $\tilde{H}(\lambda)$ under changing the sign of x . Let $P(\lambda)$ be the projection

$$P(\lambda) = (2\pi i)^{-1} \oint_{|z - e_n| = \varepsilon} (z - \tilde{H}(\lambda))^{-1} dz \tag{20}$$

for ε so small that no other eigenvalue of $\oplus K^a$ is within ε of e_n . Then by Thm. 1.1, $P(\lambda)$ is rank one for λ small, and by Thm. 2.3, $P(\lambda)\tilde{\gamma}_n(\lambda) \rightarrow \varphi_n$. Thus $(\varphi_n, P(\lambda)\varphi_n) \rightarrow 1$ and so it is non-vanishing.

We claim it suffices to obtain an L^2 -asymptotic series for $P(\lambda)\varphi_n$ for

$$\lambda^{-1}E_n(\lambda) = (\tilde{H}(\lambda)\varphi_n, P(\lambda)\varphi_n)/(\varphi_n, P(\lambda)\varphi_n)$$

and

$$U^a(\lambda)^{-1}\gamma_n(\lambda) = (\varphi_n, P(\lambda)\varphi_n)^{-\frac{1}{2}}[P_n(\lambda)\varphi_n]$$

and moreover, $\tilde{H}(\lambda)\varphi_n$ has an L^2 asymptotic series as is easy to see. By (20), we only need an asymptotic series for $(\tilde{H}(\lambda) - z)^{-1}\varphi_n$ uniform for z in the relevant circle. Henceforth, we ignore this uniformity requirement which is easy to check throughout our proof. As a preliminary, we note:

LEMMA 4.2. — For each fixed m , $(1 + |x|)^m(K^a - z)^{-1}(1 + |x|)^{-m}$ is a bounded operator.

Proof. — This is a very general feature of Schrödinger operators and is discussed in [I9]. One can prove it by the Combes-Thomas method [5] or by a commutator analysis [I8]. Of course, if one prefers, for this harmonic oscillator case, many other methods special to the oscillator can be used. ■

Now we expand the geometric series

$$(\tilde{H}(\lambda) - z)^{-1}\varphi_n = \sum_{k=0}^m \psi_k + r_m$$

where

$$\psi_k = (-1)^k(K_a - z)^{-1}[V(K_a - z)^{-1}]^k\varphi_n$$

Write $\rho = (1 + |\lambda|)$ and then

$$r_n = (-1)^m(\tilde{H}(\lambda) - z)^{-1}(\rho^{-b}V)(\rho^b(K_a - z)^{-1}\rho^{-b}) \\ (\rho^{-b}V)(\rho^{2b}(K_a - z)^{-1}\rho^{-2b} \dots \rho^{(m+1)b}\varphi_n$$

By the lemma, each factor $(\rho^{kb}(K_a - z)^{-1}\rho^{-kb})$ is bounded.

By (18), (19) for suitable b , $\|\rho^{-b}V\| = O(\lambda^{-\frac{1}{2}})$ so $\|r_m\| = O(\lambda^{-(m+1)/2})$. Similarly, if

$$\psi'_k = (-1)^k(K_a - z)^{-1}[Q_m(\lambda)(K_a - z)^{-1}]^m\varphi_n$$

then

$$\|\psi_k - \psi'_k\| = O(\lambda^{-(m+1)/2})$$

Since ψ'_k is a polynomial in $\lambda^{-\frac{1}{2}}$, it clearly has the appropriate expansion.

This completes the proof of Thm. 4.1. Notice that each $\varphi_n^{(k)}$ is a polynomial times φ_n . The procedure for computing the a^l is easy: Use ordinary Rayleigh-Schrödinger theory to order $2l$ using a fictitious W as perturbation. Set $W = Q_{2l}$ and collect all terms of order λ^{-l} . Since Q_{2l} is a polynomial and K^a an oscillator, the sums over intermediate states are all finite.

5. ASYMPTOTIC SERIES: DEGENERATE CASE

THEOREM 5.1. — Let α be an eigenvalue of $\oplus K^a$ of multiplicity k and let $E_n(\lambda), \dots, E_{n+k-1}(\lambda)$ be the eigenvalues of $H(\lambda)$ which, when divided by λ , approach α . Then for $n \leq j \leq n + k - 1$:

$$E_j(\lambda) \sim \alpha\lambda + \sum_{k=0}^{j-n} a_k^{(j)}\lambda^{-k}$$

LEMMA 5.2. — Let $C(\lambda)$ be a $k \times k$ Hermitian matrix whose elements have asymptotic series in λ . Then the eigenvalues of C have asymptotic expansions.

Proof. — For any n , we can write $C(\lambda) = A_n(\lambda) + B_n(\lambda)$ where A_n is analytic and $B_n(\lambda) = O(\lambda^{-n})$ and hermitian. Since all operators are hermitian, the difference of the eigenvalue is $O(\lambda^{-n})$ and by standard theory [9] [14], those of A_n are analytic. ■

Proof of Thm. 5.1. — By Thm. 2.3, we have k suitable eigenvectors of some H^a , so that $(\varphi_i, P(\lambda)\varphi_j) \rightarrow \delta_{ij}$ where $P(\lambda)$ is the projection onto the span of eigenspaces associated to $E_n(\lambda), \dots, E_{n+k-1}(\lambda)$. As in the last section, $\Delta_{ij}(\lambda) = (\varphi_i, P(\lambda)\varphi_j)$ and $H_{ij}(\lambda) = (\varphi_i, H(\lambda)P(\lambda)\varphi_j)$ have asymptotic series (we defer the proof that no $\lambda^{l/2}$ —with l odd—enter), and $\Delta_{ij} = \delta_{ij} + O(\lambda)$ so $C(\lambda) = \Delta^{-\frac{1}{2}} H \Delta^{-\frac{1}{2}}$ has an asymptotic series and so the E_n have an asymptotic series.

All that remains is to show no odd $\lambda^{l/2}$ terms occur. If φ_i and φ_j live in different wells, then $|\Delta_{ij}(\lambda)| + |H_{ij}(\lambda)| = O(\lambda^{-N})$ for all N . If they live in the same well, they must have the same parity under $x - x^a \rightarrow -(x - x^a)$, and so, as in the last section, no $\lambda^{l/2}$ terms enter. ■

The situation for eigenvectors is more subtle:

DEFINITION. — We say the degeneracy is removed at finite order if no two of the asymptotic series for $E_j(\lambda); j = n, \dots, n + k - 1$ are identical. It is easy to prove that

THEOREM 5.3. — If the degeneracy is removed at finite order, then for each eigenvector $\psi_j(\lambda)$ there is $a(j)$ so that (1) $\|J_a \psi_j - \psi_j\| = O(\lambda^{-N})$ for all N (2) $[U^{a(j)}]^{-1} \psi_j$ has an asymptotic series to all orders.

As a corollary, we have the following interesting alternative which we improve (to replace $O(\lambda^{-N})$ by $O(e^{-c\lambda})$ for suitable c) in paper II:

COROLLARY 5.4. — Fix an eigenvalue $E_j(\lambda)$ which is simple for λ large (although perhaps not at $\lambda = \infty$). Either the corresponding eigenvector lives in a single well up to errors of order $O(\lambda^{-N})$ for all N , or else there is another eigenvalue $E'(\lambda)$ with $E' - E_j = O(\lambda^{-N})$ for all N .

If the eigenvalue degeneracy is not removed at finite order due entirely to a symmetry (as happens in the double well) it is again easy to get asymptotic series for eigenvectors to all orders. Otherwise this can be a difficult question, as shown by Example II.5.3 of [9].

Note. — Recently, Hunziker-Pillet [7] have found a definitive approach to degenerate perturbation theory which includes a non-Hermitian analog of lemma 5.2.

6. OPERATORS ON MANIFOLDS

In this final section, we consider operators of the form $L + \lambda^2 h + \lambda g$ acting on the p -forms, $\Lambda^p(M)$ on a Riemannian manifold, M . Here L is a Laplace Beltrami operator, $d^*d + dd^*$. Such operators arise in Witten's proof. There are three new elements:

- a) The IMS formula needs to be extended.
- b) L is not $-\Delta$ even in local coordinates. Actually, for Witten's proof, one can take the metric flat near critical points, and finesse this problem. Nevertheless, we discuss it below.
- c) h and g are « functions » in the sense of acting on forms at a point, but they may have non-trivial vectorial dependence. At the risk of considerable complication, one could probably accomodate general h, g ; here, we suppose that h acts as a multiple $h(x)$ of the identity matrix, i. e. that h doesn't have vectorial dependence. This is the case in Witten's proof.

Here is the solution of these problems:

- a) The IMS formula can be extended. Let $a^*(f)$ be wedge product with df and $a(f)$ its adjoint. Then,

$$\{ a^*(f), a(f) \} = |df|^2 \tag{21}$$

where $|\cdot|^2$ means the square of the length in the Riemann metric (transferred to 1-forms). By Lebnitz rule, if ω is a p -form and f a function, then

$$d(f\omega) = f d\omega + a^*(f)\omega$$

so if $M_f \omega \equiv f\omega$, then

$$[d, M_f] = a^*(f) \tag{22}$$

Taking adjoints,

$$[d^*, M_f] = -a(f) \tag{23}$$

Then, using (21)-(23):

$$[M_f, [M_f, L]] = -2|df|^2$$

From this, one immediately gets

$$L = \sum J_\alpha L J_\alpha - \sum_\alpha |dJ_\alpha|^2$$

and so the IMS formula.

- b) One defines H^a on $L^2(\mathbb{R}^n)$ by using an ON coordinate system at the point x_a and replacing L by $-\Delta$. Since the metric g_0 is not constant in this coordinate system, there are extra $[g_0 - g_0(x_a)] \times 2^{nd}$ derivative terms, and so $J_\alpha(H - H^a)J_\alpha \equiv 0$ is no longer a bounded operator. However, $0 = 0_1 + 0_2$ with $\|0_1\| = 0(\lambda^{4/5})$ and $\|L^{-\frac{1}{2}}0_2L^{-\frac{1}{2}}\| = 0(\lambda^{-2/5})$ so

$$H \geq r\lambda + F_n(\lambda) + c\lambda^{-2/5}H$$

which yields

$$H \geq r\lambda(1 - c\lambda^{-2/5})^{-1}1 + \tilde{F}_n(\lambda)$$

and so the necessary result.

c) As above, one reduces the study of $E_n(\lambda)/\lambda$ to that of the H^q which, upon diagonalizing $g(x^q)$, become sums of scalar valued operators.

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Notes added in proof

(1) Additional earlier papers on the one dimensional case include:

- (a) J. M. COMBES, *Seminar on Spectral and Scattering Theory* (ed. S. Kuroda), RIMS Publication 242, 1975, p. 22-38.
- (b) J. M. COMBES, The Born Oppenheimer Approximation, in *The Schrödinger Equation* (ed. W. Thirring and P. Urban), Springer, 1976, p. 22-38.
- (c) J. M. COMBES and R. SEILER, in *Quantum Dynamics of Molecules* (ed. G. Wooley), Plenum, 1980.
- (d) J. M. COMBES, P. DUCLOS and R. SEILER, in *Rigorous Atomic and Molecular Physics* (ed. G. Velo and A. Wightman), Plenum, 1981.

(2) A sketch of Reference 20 appears in B. SIMON, Instantons, Double Wells and Large Deviations, *Bull. AMS*, March, 1983 issue.

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