

Asymptotics for the Eigenvalues of the Harmonic Oscillator with a Quasi-Periodic Perturbation

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Abstract

We consider operators of the form $H + V$ where H is the one-dimensional harmonic oscillator and V is a zero-order pseudo-differential operator which is quasi-periodic in an appropriate sense (one can take V to be multiplication by a periodic function for example). It is shown that the eigenvalues of $H + V$ have asymptotics of the form $\lambda_n(H + V) = \lambda_n(H) + W(\sqrt{n})n^{-1/4} + O(n^{-1/2} \ln(n))$ as $n \rightarrow +\infty$, where W is a quasi-periodic function which can be defined explicitly in terms of V .

1 Introduction

The one-dimensional harmonic oscillator is the operator

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

where α is a positive parameter. We can consider H as an unbounded self-adjoint operator acting on $L^2(\mathbb{R})$. The determination of the spectrum of H is a classical problem — virtually any introductory book on quantum mechanics has a section devoted to this topic. In particular H has a compact resolvent and hence a discrete spectrum. Furthermore, the eigenvalues of H are simple and can be enumerated as

$$\lambda_n(H) = \alpha(2n + 1), \quad n \in \mathbb{N}_0.$$

A normalised eigenfunction corresponding to $\lambda_n(H)$ can be chosen as

$$\phi_n(x) = \frac{\alpha^{1/4}}{\sqrt{n!2^n\sqrt{\pi}}} e^{-\alpha x^2/2} \mathcal{H}_n(\sqrt{\alpha}x), \quad (1)$$

where \mathcal{H}_n is the n -th Hermite polynomial.

The purpose of this paper is to study the large n asymptotics of the eigenvalues of the perturbed operator $H + V$ when V is a self-adjoint quasi-periodic pseudo-differential operator of order 0. More precisely, we assume V can be written in the form

$$V = \sum_{\mathbf{a} \in \Lambda} V_{\mathbf{a}} U_{\mathbf{a}} \quad (2)$$

where $\Lambda \subset T^*\mathbb{R} \cong \mathbb{R}^2$ is a countable discrete index set and, for each $\mathbf{a} = (a_x, a_\xi) \in T^*\mathbb{R}$, we define $U_{\mathbf{a}}$ to be the unitary operator on $L^2(\mathbb{R})$ given by

$$U_{\mathbf{a}}\phi(x) = e^{ia_x a_\xi/2} e^{ia_x x} \phi(x + a_\xi). \quad (3)$$

The $V_{\mathbf{a}}$'s are just complex coefficients.

Since $U_{\mathbf{a}}^* = U_{-\mathbf{a}}$ for any $\mathbf{a} \in T^*\mathbb{R}$, the condition that V is self-adjoint can be rewritten as the requirement

$$\mathbf{a} \in \Lambda \implies -\mathbf{a} \in \Lambda \quad \text{and} \quad V_{-\mathbf{a}} = \overline{V_{\mathbf{a}}}, \quad \mathbf{a} \in \Lambda.$$

We will also assume the $V_{\mathbf{a}}$'s satisfy the following condition (essentially a regularity assumption);

$$\sum_{\mathbf{a} \in \Lambda} |\mathbf{a}|^3 |V_{\mathbf{a}}| < +\infty. \quad (4)$$

In particular, this condition ensures that the right hand side of (2) is absolutely convergent in operator norm, making V a well defined bounded operator. Since H has a compact resolvent the same must then be true for $H + V$; it follows that the spectrum of $H + V$ also consists of discrete eigenvalues.

Remark. If we take $\Lambda = \{(\omega m, 0) \mid m \in \mathbb{Z}\}$ then V is the operator of multiplication by a function with period ω whose m -th Fourier coefficient is simply $\omega^{1/2} V_{(\omega m, 0)}$. Condition (4) becomes a standard regularity requirement (that the function V should be a ‘‘bit more’’ than C^3).

In general we may consider V to be a zero-order pseudo-differential operator with Weyl-symbol $\sum_{\mathbf{a} \in \Lambda} V_{\mathbf{a}} e^{i(a_x x + a_\xi \xi)}$ (n.b., $U_{\mathbf{a}}$ is the operator with Weyl-symbol $e^{i(a_x x + a_\xi \xi)}$). If Λ is a rational periodic lattice then V will be a periodic operator (in the sense that it commutes with a specific translation operator). Taking Λ to be an irrational periodic lattice, or an irregular discrete set, leads to a generalisation of such periodic operators; when we apply ‘‘quasi-periodic’’ to V we mean this particular type of generalisation.

If $\mathbf{0} \in \Lambda$ then the corresponding term in V is $V_{\mathbf{0}}$ times the identity operator and will thus cause a simple shift in the spectrum of H by $V_{\mathbf{0}}$. This term is included in the statement of the main result (Theorem 1.1 below) but thereafter we shall assume $V_{\mathbf{0}} = 0$. We also set $\Lambda' = \Lambda \setminus \{\mathbf{0}\}$; since Λ is discrete, $T^*\mathbb{R} \setminus \Lambda'$ contains a neighbourhood of $\mathbf{0}$.

Define a metric $|\cdot|_\alpha$ on $T^*\mathbb{R}$ by $|\mathbf{a}|_\alpha = (\alpha^{-1}a_x^2 + \alpha a_\xi^2)^{1/2}$. This metric is equivalent to the usual metric $|\cdot|$ so condition (4) can be rewritten as

$$\sum_{\mathbf{a} \in \Lambda'} |\mathbf{a}|_\alpha^p |V_{\mathbf{a}}| < +\infty \quad \text{for all } p \leq 3. \quad (5)$$

The main result of the paper is the following.

Theorem 1.1. *Suppose V given by (2) satisfies (4) (or equivalently (5)). Then the eigenvalues of the operator $H + V$ satisfy*

$$\lambda_n(H + V) = \alpha(2n+1) + V_{\mathbf{0}} + W(\sqrt{n})n^{-1/4} + O(n^{-1/2} \ln(n))$$

as $n \rightarrow \infty$, where $W : \mathbb{R} \rightarrow \mathbb{R}$ is the quasi-periodic function defined by

$$W(\lambda) = \frac{2^{1/4}}{\sqrt{\pi}} \sum_{\mathbf{a} \in \Lambda'} V_{\mathbf{a}} |\mathbf{a}|_\alpha^{-1/2} \cos\left(\sqrt{2} |\mathbf{a}|_\alpha \lambda - \frac{\pi}{4}\right). \quad (6)$$

The presence of the quasi-periodic function W means the first order asymptotics given by Theorem 1.1 contain considerably more information about the operator V than one might expect (c.f. the simple power type asymptotics for the case when V is given as multiplication by an element of C_0^∞ ([PS]) or for the operator $-d^2/d\theta^2 + V(\theta)$ on S^1 (see Theorem 4.2 in [MO])). In particular we note that if V is given as multiplication by a periodic function, knowledge of the first order asymptotics of $\lambda_n(H + V)$ allows the Fourier coefficients of V to be ‘‘half’’ determined (the values of $V_{(-m\omega,0)} + V_{(m\omega,0)}$, $m \in \mathbb{N}$, can be determined from W).

It is likely that there exists a full asymptotic expansion for $\lambda_n(H + V)$, involving further terms with quasi-periodic functions multiplying increasingly negative powers of n . Judging by numerical evidence (for example with the potential $V(x) = \cos(x)$) the second term in the asymptotics is $O(n^{-3/4})$. This order (even as an improvement of the remainder estimate in Theorem 1.1) appears to involve reasonable subtle cancellation effects within the series giving the second term of the asymptotics; no attempt to deal with this analysis is made here.

Remark. With an obvious modification to the definition of W and a remainder estimate of $O(n^{-1/3} \ln(n))$, Theorem 1.1 also holds for operators V of the form

$$V = \int_{T^*\mathbb{R}} V_{\mathbf{a}} U_{\mathbf{a}} d^2 \mathbf{a} \quad \text{where } V_{\mathbf{a}} \text{ satisfies } \int_{T^*\mathbb{R}} (|\mathbf{a}|_\alpha^{-3/2} + |\mathbf{a}|_\alpha^3) |V_{\mathbf{a}}| d^2 \mathbf{a} < +\infty.$$

In this case V is a pseudo-differential operator of order zero whose Weyl-symbol has Fourier transform $2\pi V_{\mathbf{a}}$. The $|\mathbf{a}|_\alpha^3$ term in the condition on $V_{\mathbf{a}}$ is then a regularity condition, while the $|\mathbf{a}|_\alpha^{-3/2}$ term is a generalisation of quasi-periodicity.

The proof of Theorem 1.1 is given in Section 4 using standard ideas to express the eigenvalues of $H + V$ in terms of a series involving the resolvent of H and the operator V . The non-triviality of Theorem 1.1 is contained in technical results used to establish the convergence of these series. These results are obtained in Sections 2 and 3; estimates for the elements $\langle V\phi_k, \phi_{k'} \rangle$ of the matrix of V with respect to the eigenbasis $\{\phi_k \mid k \in \mathbb{N}_0\}$ are obtained in the former and are then combined to give resolvent estimates in the latter.

Notation. We use C to denote any positive real constant whose exact value is not important but which may depend only on the things it is allowed to in a given problem. Appropriate function type notation is used in places to make this clearer whilst subscripts are added if we need to keep track of the value of a particular constant (e.g. $C_1(V)$ etc.).

We use $\|T\|$, $\|T\|_1$ and $\|T\|_2$ to denote the operator, trace class and Hilbert-Schmidt norms of the operator T respectively.

2 Estimates for Matrix Elements

The aim of this section is to obtain the necessary estimates for the matrix elements $\langle V\phi_k, \phi_{k'} \rangle$ for all $k, k' \in \mathbb{N}_0$. In turn these will be estimated via

$$U_{\mathbf{a}}^{k,k'} := \langle U_{\mathbf{a}}\phi_k, \phi_{k'} \rangle \quad (7)$$

defined for all $\mathbf{a} \in T^*\mathbb{R}$ and $k, k' \in \mathbb{N}_0$. Since the operator $U_{\mathbf{a}}$ is unitary we immediately get

$$|U_{\mathbf{a}}^{k,k'}| \leq 1. \quad (8)$$

To obtain more precise estimates we can use the following special function identity (see 7.377 on page 844 of [GRJ]) to find an explicit formula for $U_{\mathbf{a}}^{k,k'}$; for any $0 \leq k \leq k'$ and $y, z \in \mathbb{C}$ we have

$$\int_{\mathbb{R}} e^{-x^2} \mathcal{H}_k(x+y) \mathcal{H}_{k'}(x+z) dx = 2^{k'} \sqrt{\pi} k! z^{k'-k} L_k^{(k'-k)}(-2yz), \quad (9)$$

where $L_k^{(k'-k)}$ is the generalised Laguerre polynomial.

Lemma 2.1. *For any $0 \leq k \leq k'$ and $\mathbf{a} \in T^*\mathbb{R} \setminus \{\mathbf{0}\}$ we have*

$$U_{\mathbf{a}}^{k,k'} = \sqrt{\frac{k!}{k'!}} (\sqrt{2}\rho e^{i\theta})^{k'-k} e^{-\rho^2} L_k^{(k'-k)}(2\rho^2)$$

for some $\theta \in \mathbb{R}$, where

$$\rho = \frac{1}{2} \left(\frac{a_x^2}{\alpha} + \alpha a_{\xi}^2 \right)^{1/2} = \frac{1}{2} |\mathbf{a}|_{\alpha}. \quad (10)$$

Proof. Introduce the complex number

$$\omega = \frac{\sqrt{\alpha} a_\xi}{2} - i \frac{a_x}{2\sqrt{\alpha}}.$$

From (7), (3) and (1) we get

$$\begin{aligned} U_{\mathbf{a}}^{k,k'} &= \langle U_{\mathbf{a}} \phi_k, \phi_{k'} \rangle \\ &= \frac{\sqrt{\alpha} 2^{-(k+k')/2}}{\sqrt{k!k'!\pi}} e^{ia_x a_\xi/2} \int_{\mathbb{R}} e^{ia_x x} e^{-\alpha(x+a_\xi)^2/2} e^{-\alpha x^2/2} \\ &\quad \mathcal{H}_k(\sqrt{\alpha}(x+a_\xi)) \mathcal{H}_{k'}(\sqrt{\alpha}x) dx \\ &= \frac{2^{-(k+k')/2}}{\sqrt{k!k'!\pi}} e^{\omega^2 - \alpha a_\xi^2/2 + ia_x a_\xi/2} \int_{\mathbb{R}} e^{-x^2} \mathcal{H}_k(x - \omega + \sqrt{\alpha}a_\xi) \mathcal{H}_{k'}(x - \omega) dx \\ &= \sqrt{\frac{k!}{k'!}} 2^{(k'-k)/2} (-\omega)^{k'-k} e^{\omega^2 - \alpha a_\xi^2/2 + ia_x a_\xi/2} L_k^{(k'-k)}(-2\omega(\omega - \sqrt{\alpha}a_\xi)) \end{aligned}$$

where the last line follows from (9). Now $|\omega| = \rho$ while

$$\omega^2 - \frac{\alpha a_\xi^2}{2} + \frac{ia_x a_\xi}{2} = \frac{\alpha a_\xi^2}{4} - \frac{a_x^2}{4\alpha} - \frac{\alpha a_\xi^2}{2} - \frac{ia_x a_\xi}{2} + \frac{ia_x a_\xi}{2} = -|\omega|^2$$

and

$$-2\omega(\omega - \sqrt{\alpha}a_\xi) = -2\omega(-\bar{\omega}) = 2|\omega|^2.$$

The result follows. ■

Throughout the remainder of this section we will assume $\mathbf{a} \in T^*\mathbb{R} \setminus \{\mathbf{0}\}$ is fixed and $\rho > 0$ is given by (10).

Laguerre polynomials can be expressed in terms of the confluent hypergeometric function; using 22.5.54 in [AS] we get

$$L_k^{(k'-k)}(2\rho^2) = \binom{k'}{k} M(-k, k' - k + 1, 2\rho^2).$$

The confluent hypergeometric function can, in turn, be written as a pointwise absolutely convergent series of Bessel functions; from 13.3.7 in [AS] we get

$$\begin{aligned} M(-k, k' - k + 1, 2\rho^2) &= (k' - k)! e^{\rho^2} (\rho^2(k' + k + 1))^{-(k'-k)/2} \\ &\quad \sum_{j=0}^{\infty} A_j \left(\frac{\rho}{(k' + k + 1)^{1/2}} \right)^j J_{k'-k+j}(2\rho\sqrt{k' + k + 1}), \end{aligned}$$

where

$$A_0 = 1, \quad A_1 = 0, \quad A_2 = \frac{1}{2}(k' - k + 1) \tag{11}$$

and, for $j \geq 2$,

$$(j+1)A_{j+1} = (j+k'-k)A_{j-1} - (k'+k+1)A_{j-2}. \quad (12)$$

It follows from Lemma 2.1 that

$$U_{\mathbf{a}}^{k,k'} = e^{i(k'-k)\theta} \sqrt{F_{k',k}} \sum_{j=0}^{\infty} A_j \left(\frac{\rho}{(k'+k+1)^{1/2}} \right)^j J_{k'-k+j}(2\rho\sqrt{k'+k+1}), \quad (13)$$

where

$$F_{k',k} := \frac{k'!}{k!} \left(\frac{2}{k'+k+1} \right)^{k'-k}.$$

The next two results give estimates for the constants appearing in (13).

Lemma 2.2. *Suppose $k' \geq 2$ and $0 \leq k' - k \leq k'^{2/3}$. Then*

$$|A_j| \leq (k'+k+1)^{j/3}.$$

Proof. Set $m = k' - k$ and $n = k' + k + 1$ so

$$0 \leq m \leq k'^{2/3} \leq (k'+k+1)^{2/3} = n^{2/3}$$

while $k' \geq 2$ and $k \geq 0$ so $n \geq 3$.

We have $A_0 = 1 = n^0$, $A_1 = 0 \leq n^{1/3}$ and $m, 1 \leq n^{2/3}$ so $A_2 = \frac{1}{2}(m+1) \leq n^{2/3}$. Now let $J \geq 2$ and suppose the result hold for $j \leq J$. Since

$$A_{J+1} = \frac{J+m}{J+1}A_{J-1} - \frac{n}{J+1}A_{J-2}$$

we then get

$$|A_{J+1}| \leq \frac{J+m}{J+1}n^{(J-1)/3} + \frac{n}{J+1}n^{(J-2)/3} = n^{(J+1)/3} \frac{(J+m)n^{-2/3} + 1}{J+1}.$$

Now $mn^{-2/3} \leq 1$ while

$$\begin{aligned} n \geq 3 &\implies n^{-2/3} \leq 3^{-2/3} \leq \frac{1}{2} \\ &\implies J(1 - n^{-2/3}) \geq 1 \quad (\text{as } J \geq 2) \\ &\implies 1 + Jn^{-2/3} \leq J. \end{aligned}$$

Thus $(J+m)n^{-2/3} + 1 \leq J+1$. Therefore $|A_{J+1}| \leq n^{(J+1)/3}$ and the result follows by induction. \blacksquare

Lemma 2.3. *If $0 \leq k \leq k'$ then $F_{k',k} \leq 1$.*

Proof. We have

$$F_{k',k} = \frac{k'(k' - 1) \dots (k + 1)}{\frac{1}{2}(k' + k + 1) \dots \frac{1}{2}(k' + k + 1)},$$

where the numerator and denominator both contain $k' - k$ terms. Now set $m = \frac{1}{2}(k' - k - 1)$ and $n = \frac{1}{2}(k' + k + 1)$ so $m \leq n$ while

$$F_{k',k} = \frac{(n + m)}{n} \frac{(n + m - 1)}{n} \dots \frac{(n - m + 1)}{n} \frac{(n - m)}{n}.$$

If $k' - k$ is odd this can be rearranged as

$$F_{k',k} = \frac{(n + m)(n - m)}{n^2} \frac{(n + m - 1)(n - m + 1)}{n^2} \dots \frac{n}{n},$$

while if $k' - k$ is even we get

$$F_{k',k} = \frac{(n + m)(n - m)}{n^2} \frac{(n + m - 1)(n - m + 1)}{n^2} \dots \frac{(n + \frac{1}{2})(n - \frac{1}{2})}{n^2}.$$

The result now follows from the fact that

$$\frac{(n + m')(n - m')}{n^2} = \frac{n^2 - m'^2}{n^2} \leq 1$$

for any $0 \leq m' \leq n$. ■

Next we obtain some estimates for the Bessel functions appearing in (13).

Lemma 2.4. *For any $x, \varepsilon > 0$ and $n \in [0, x/2]$*

$$|\{\theta \in [0, \pi] \mid |x \cos(\theta) - n| < \varepsilon\}| \leq \frac{4\pi}{3} \frac{\varepsilon}{x}.$$

Proof. Set $\delta = \varepsilon/x$, $y = n/x$ and $\Omega_{y,\delta} = \text{Cos}^{-1}([y - \delta, y + \delta])$; we need to show that $|\Omega_{y,\delta}| \leq 4\pi\delta/3$.

Now set $\theta_0 = \text{Cos}^{-1}(y)$ and let $\ell(\theta)$ denote the affine function with $\ell(0) = 1$ and $\ell(\theta_0) = y$. It is easy to see that $|\cos(\theta) - y| \geq |\ell(\theta) - y|$ which implies $|\Omega_{y,\delta}| \leq 2\delta/|L|$ where L is the gradient of $\ell(\theta)$. On the other hand, $y \in [0, \frac{1}{2}]$ so the minimum value for $|L|$ occurs when $y = 1/2$; hence $1/|L| \leq 2 \text{Cos}^{-1}(1/2) = 2\pi/3$ and the result follows. ■

Lemma 2.5. *For any $n \in \mathbb{N}_0$ and $x \geq 2n$ we have $|J_n(x)| \leq 4x^{-1/2}$.*

Surely this estimate (or an improvement) lies in a book somewhere!

Proof. Define a function by $f(\theta) = x \sin(\theta) - n\theta$ so we have the following integral representation for the Bessel function J_n (see 9.1.21 in [AS]);

$$J_n(x) = \frac{1}{\pi} \int_0^\pi \cos(f(\theta)) d\theta. \quad (14)$$

Now set

$$\Omega_0 = \{\theta \in [0, \pi] \mid |f'(\theta)| < x^{1/2}\} \quad \text{and} \quad \Omega_1 = [0, \pi] \setminus \Omega_0$$

so $J_n(x) = (I_0 + I_1)/\pi$ where $I_k = \int_{\Omega_k} \cos(f(\theta)) d\theta$ for $k = 0, 1$. Lemma 2.4 gives

$$|I_0| \leq |\Omega_0| \leq \frac{4\pi}{3} x^{-1/2}. \quad (15)$$

On the other hand

$$I_1 = \left[\frac{\sin(f(\theta))}{f'(\theta)} \right]_{\partial\Omega_1} + \int_{\Omega_1} \frac{f''(\theta)}{(f'(\theta))^2} \sin(f(\theta)) d\theta.$$

Now $f''(\theta) = -x \sin(\theta) \leq 0$ on $[0, \pi]$ while $(f'(\theta))^2 > 0$ on Ω_1 . Thus

$$\left| \int_{\Omega_1} \frac{f''(\theta)}{(f'(\theta))^2} \sin(f(\theta)) d\theta \right| \leq - \int_{\Omega_1} \frac{f''(\theta)}{(f'(\theta))^2} d\theta = \left[\frac{1}{f'(\theta)} \right]_{\partial\Omega_1}.$$

Furthermore $f'(\theta)$ is decreasing on $[0, \pi]$ so Ω_0 consists of a single interval. Hence $\partial\Omega_1 \setminus \{0, \pi\}$ contains at most 2 points. Since $f(0) = 0$ and $f(\pi) = -n\pi$ we then get

$$|I_1| \leq \left| \left[\frac{\sin(f(\theta))}{f'(\theta)} \right]_{\partial\Omega_1} \right| + \left[\frac{1}{f'(\theta)} \right]_{\partial\Omega_1} \leq 6 \max_{\theta \in \Omega_1} \frac{1}{|f'(\theta)|} \leq 6x^{-1/2}. \quad (16)$$

Combining (15), (16) we now get

$$|J_n(x)| \leq \frac{1}{\pi} (|I_0| + |I_1|) \leq \frac{1}{\pi} \left(\frac{4\pi}{3} + 6 \right) x^{-1/2} \leq 4x^{-1/2},$$

completing the result. ■

Lemma 2.6. *Suppose $k' \geq 2$, $0 \leq k' - k \leq \rho(k' + k + 1)^{1/2}$ and $2\rho \leq (k' + k + 1)^{1/6}$. Then*

$$|U_{\mathbf{a}}^{k, k'}| \leq (4(2\rho)^{-1/2} + \frac{1}{2}(2\rho)^2) (k' + k + 1)^{-1/4}.$$

Before starting, note that as a clear consequence of (14) we have

$$|J_n(x)| \leq 1. \quad (17)$$

Proof. Since $2, k \leq k'$

$$k' - k \leq \frac{1}{2}(k' + k + 1)^{2/3} \leq \frac{1}{2}\left(\frac{5}{2}\right)^{2/3} k'^{2/3} \leq k'^{2/3}.$$

Now combining (13) with (11), (17) and Lemmas 2.2 and 2.3 we get

$$\begin{aligned} |U_{\mathbf{a}}^{k,k'}| &\leq \sqrt{F_{k',k}} \sum_{j=0}^{\infty} |A_j| \frac{\rho^j}{(k' + k + 1)^{j/2}} |J_{k'-k+j}(2\rho\sqrt{k' + k + 1})| \\ &\leq |J_{k'-k}(2\rho\sqrt{k' + k + 1})| + \sum_{j \geq 2}^{\infty} \rho^j (k' + k + 1)^{-j/6} \\ &\leq |J_{k'-k}(2\rho\sqrt{k' + k + 1})| + \frac{1}{2}(2\rho)^2 (k' + k + 1)^{-1/3}, \end{aligned}$$

where the last line follows from the hypothesis that $\rho(k' + k + 1)^{-1/6} \leq 1/2$. Lemma 2.5 can now be used to estimate the remaining Bessel function term. \blacksquare

Main estimate

The next result is the main estimate we will need for the matrix elements $|\langle V\phi_k, \phi_{k'} \rangle|$. This estimate is valid in a parabolic region around the diagonal $k = k'$; the width of this region is governed by the quantity

$$\gamma := \min_{\mathbf{a} \in \Lambda'} |\mathbf{a}|_{\alpha},$$

which is positive since Λ' is discrete and doesn't contain $\mathbf{0}$. Although not required in this paper, we remark that for a general parabolic region around the diagonal one is restricted to estimates of the form $|\langle V\phi_k, \phi_{k'} \rangle| \leq C(V)(k' + k + 1)^{-1/6}$.

Proposition 2.7. *Suppose V satisfies condition (5) and set*

$$\kappa = \min\{1/3, \gamma/(2\sqrt{3})\}. \quad (18)$$

If $n \in \mathbb{N}$ and $k, k' \in \mathbb{N}_0$ satisfy $|k - n|, |k' - n| \leq \kappa n^{1/2}$ then

$$|\langle V\phi_k, \phi_{k'} \rangle| \leq C(V)n^{-1/4}. \quad (19)$$

Proof. We have $|\langle V\phi_k, \phi_{k'} \rangle| \leq \|V\|$ for any $k, k' \in \mathbb{N}_0$ so we can increase $C(V)$ if necessary to ensure that (19) is satisfied for $n = 1, 2$. Furthermore V is self-adjoint so $|\langle V\phi_{k'}, \phi_k \rangle| = |\langle V\phi_k, \phi_{k'} \rangle|$. It thus suffices to prove the result assuming $n \geq 3$ and $k', k \in \mathbb{N}_0$ satisfy $k' \geq k$ and $|k - n|, |k' - n| \leq \kappa n^{1/2}$. Then $k', k \geq n - \frac{1}{3}n^{1/2} \geq \frac{2}{3}n$ so $k' \geq 2$,

$$k' + k + 1 \geq \frac{4}{3}n \quad (20)$$

and

$$0 \leq k' - k \leq 2\kappa n^{1/2} \leq \frac{\gamma}{2}(k' + k + 1)^{1/2}. \quad (21)$$

Now set $K = (k' + k + 1)^{1/6}$. Using (2), (7) and (8) we have

$$|\langle V\phi_k, \phi_{k'} \rangle| \leq \sum_{\mathbf{a} \in \Lambda'} |U_{\mathbf{a}}^{k,k'}| |V_{\mathbf{a}}| \leq \sum_{\substack{\mathbf{a} \in \Lambda' \\ |\mathbf{a}|_{\alpha} \leq K}} |U_{\mathbf{a}}^{k,k'}| |V_{\mathbf{a}}| + \sum_{\substack{\mathbf{a} \in \Lambda' \\ |\mathbf{a}|_{\alpha} > K}} |V_{\mathbf{a}}|. \quad (22)$$

Since $1 < K^{-3/2} |\mathbf{a}|_{\alpha}^{3/2}$ whenever $|\mathbf{a}|_{\alpha} > K$, (5) and (20) give us

$$\sum_{\substack{\mathbf{a} \in \Lambda' \\ |\mathbf{a}|_{\alpha} > K}} |V_{\mathbf{a}}| \leq K^{-3/2} \sum_{\mathbf{a} \in \Lambda'} |\mathbf{a}|_{\alpha}^{3/2} |V_{\mathbf{a}}| \leq C(V) n^{-1/4}.$$

Now let $\mathbf{a} \in \Lambda'$. Since $|\mathbf{a}|_{\alpha} = 2\rho$ (see (10)) the definition of γ implies $\gamma/2 \leq \rho$ and thus $k' - k \leq \rho K^3$ by (21). Lemma 2.6, (5) and (20) then give

$$\sum_{\substack{\mathbf{a} \in \Lambda' \\ |\mathbf{a}|_{\alpha} \leq K}} |U_{\mathbf{a}}^{k,k'}| |V_{\mathbf{a}}| \leq K^{-3/2} \sum_{\mathbf{a} \in \Lambda'} (4|\mathbf{a}|_{\alpha}^{-1/2} + \frac{1}{2}|\mathbf{a}|_{\alpha}^2) |V_{\mathbf{a}}| \leq C(V) n^{-1/4}.$$

The result follows. ■

First order term

The next result is used to obtain the explicit form for the first order correction term in the asymptotics for $\lambda_n(H + V)$.

Proposition 2.8. *Suppose V satisfies condition (5). Then*

$$\langle V\phi_n, \phi_n \rangle = W(\sqrt{n}) n^{-1/4} + O(n^{-1/2})$$

as $n \rightarrow +\infty$, where W is defined by (6).

Proof. Let $\mathbf{a} \in T^*\mathbb{R} \setminus \{\mathbf{0}\}$ and set $\rho = |\mathbf{a}|_{\alpha}/2$. Using (13) and the fact that $F_{n,n} = 1$ we get

$$U_{\mathbf{a}}^{n,n} = \sum_{j=0}^{\infty} A_j \frac{\rho^j}{(2n+1)^{j/2}} J_j(2\rho\sqrt{2n+1}).$$

Now suppose $2\rho \leq N$ where $N := (2n+1)^{1/6}$. Using (11), (17) and Lemma 2.2 we have

$$\begin{aligned} |U_{\mathbf{a}}^{n,n} - J_0(2\rho\sqrt{2n+1})| &\leq \frac{1}{2}\rho^2(2n+1)^{-1} + \sum_{j \geq 3}^{\infty} \rho^j (2n+1)^{-j/6} \\ &\leq \frac{1}{8}|\mathbf{a}|_{\alpha}^2(2n+1)^{-1} + \frac{1}{4}|\mathbf{a}|_{\alpha}^3(2n+1)^{-1/2}. \end{aligned}$$

Standard asymptotic forms for Bessel functions (see 9.2.1 in [AS]) give us

$$J_0(z) = \sqrt{\frac{2}{\pi z}} \cos\left(z - \frac{\pi}{4}\right) + O(z^{-3/2})$$

while

$$\left| \frac{d}{dz} \left(\frac{1}{\sqrt{z}} \cos\left(z - \frac{\pi}{4}\right) \right) \right| \leq z^{-1/2} + \frac{1}{2} z^{-3/2}$$

and $2\rho\sqrt{2n+1} - 2\rho\sqrt{2n} \leq 2^{-1/2}\rho n^{-1/2}$. It follows that

$$\begin{aligned} & \left| J_0(2\rho\sqrt{2n+1}) - \sqrt{\frac{2}{\pi}} (2\rho)^{-1/2} (2n)^{-1/4} \cos\left(2\rho\sqrt{2n} - \frac{\pi}{4}\right) \right| \\ & \leq C(2\rho)^{-3/2} (2n+1)^{-3/4} \\ & \quad + \sqrt{\frac{2}{\pi}} \left((2\rho)^{-1/2} (2n)^{-1/4} + \frac{1}{2} (2\rho)^{-3/2} (2n)^{-3/4} \right) 2^{-1/2} \rho n^{-1/2} \\ & \leq C((2\rho)^{-3/2} + (2\rho)^{1/2}) n^{-3/4}. \end{aligned}$$

Combining the above estimates we thus obtain

$$\left| U_{\mathbf{a}}^{n,n} - \frac{2^{1/4}}{\sqrt{\pi}} |\mathbf{a}|_{\alpha}^{-1/2} n^{-1/4} \cos\left(|\mathbf{a}|_{\alpha} \sqrt{2n} - \frac{\pi}{4}\right) \right| \leq C(|\mathbf{a}|_{\alpha}^{-3/2} + |\mathbf{a}|_{\alpha}^3) n^{-1/2}$$

whenever $|\mathbf{a}|_{\alpha} \leq N$. Using (2), (6), (7) and (8) we thus have

$$\begin{aligned} & |\langle V\phi_n, \phi_n \rangle - W(\sqrt{n}) n^{-1/4}| \\ & \leq Cn^{-1/2} \sum_{\substack{\mathbf{a} \in \Lambda' \\ |\mathbf{a}|_{\alpha} \leq N}} (|\mathbf{a}|_{\alpha}^{-3/2} + |\mathbf{a}|_{\alpha}^3) |V_{\mathbf{a}}| + \sum_{\substack{\mathbf{a} \in \Lambda' \\ |\mathbf{a}|_{\alpha} > N}} (1 + |\mathbf{a}|_{\alpha}^{-1/2}) |V_{\mathbf{a}}|. \end{aligned}$$

Since $1 < N^{-3} |\mathbf{a}|_{\alpha}^3 < n^{-1/2} |\mathbf{a}|_{\alpha}^3$ whenever $|\mathbf{a}|_{\alpha} > N$ the term inside the last sum can be replaced with $n^{-1/2} (|\mathbf{a}|_{\alpha}^3 + |\mathbf{a}|_{\alpha}^{5/2}) |V_{\mathbf{a}}|$. Using (5) we then get

$$|\langle V\phi_n, \phi_n \rangle - W(\sqrt{n}) n^{-1/4}| \leq Cn^{-1/2} \sum_{\mathbf{a} \in \Lambda'} (|\mathbf{a}|_{\alpha}^{-3/2} + |\mathbf{a}|_{\alpha}^3) |V_{\mathbf{a}}| \leq C(V) n^{-1/2},$$

completing the result. ■

3 Resolvent Estimates

For any $\lambda \in \mathbb{C} \setminus \sigma(H)$ let $R(\lambda) = (H - \lambda)^{-1}$ denote the resolvent of the operator H ; we will also write R for $R(\lambda)$ where this should not cause confusion.

Let κ denote the constant defined in (18). For a given $n \in \mathbb{N}$ we will make repeated use of the partition of \mathbb{N}_0 defined by

$$I = \{k \in \mathbb{N}_0 \mid |k - n| \leq \kappa n^{1/2}\} \quad \text{and} \quad J = \mathbb{N}_0 \setminus I. \quad (23)$$

For any $\varepsilon \in (0, \alpha)$ and $n \in \mathbb{N}_0$, let $\Gamma_{\varepsilon, n}$ be the anti-clockwise circular contour in \mathbb{C} centred at $\lambda_n = \lambda_n(H) = \alpha(2n + 1)$. If $\lambda \in \Gamma_{\varepsilon, n}$ then $\lambda = \alpha(2n + 1) + \varepsilon e^{i\theta}$ for some $\theta \in [0, 2\pi)$. It follows that $|\lambda - \lambda_k| = |2\alpha(n - k) + \varepsilon e^{i\theta}|$ for any $k \in \mathbb{N}_0$. Straightforward arguments then lead to the following estimates;

$$\sum_{k \in I} |\lambda - \lambda_k|^{-1} \leq C(\varepsilon) \ln(n), \quad (24)$$

$$\sum_{k \in \mathbb{N}_0} |\lambda - \lambda_k|^{-2} \leq C(\varepsilon), \quad (25)$$

$$\sum_{k \in J} |\lambda - \lambda_k|^{-2} \leq C n^{-1/2} \quad (26)$$

and

$$|\lambda - \lambda_k| \geq C n^{1/2} \quad \text{for any } k \in J. \quad (27)$$

The first two results in this section relate to the operator $R(\lambda)VR(\lambda)$, which is clearly bounded whenever λ is in the resolvent set of H . We show that it is in fact trace class while its operator norm decreases as $n^{-1/4}$ for $\lambda \in \Gamma_{\varepsilon, n}$.

Lemma 3.1. *For any $n \in \mathbb{N}$ and $\lambda \in \Gamma_{\varepsilon, n}$ we have*

$$\|R(\lambda)VR(\lambda)\| \leq \|R(\lambda)VR(\lambda)\|_2 \leq C(V, \varepsilon) n^{-1/4}.$$

We remark that since $\{\phi_k \mid k \in \mathbb{N}_0\}$ is an orthonormal basis of $L^2(\mathbb{R})$

$$\sum_{k' \in \mathbb{N}_0} |\langle V\phi_k, \phi_{k'} \rangle|^2 = \|V\phi_k\|^2 \leq \|V\|^2. \quad (28)$$

Proof. Using the orthonormal basis $\{\phi_k \mid k \in \mathbb{N}_0\}$ we have

$$\|RVR\|_2^2 = \sum_{k, k' \in \mathbb{N}_0} |\langle RVR\phi_k, \phi_{k'} \rangle|^2 = \sum_{k, k' \in \mathbb{N}_0} \frac{|\langle V\phi_k, \phi_{k'} \rangle|^2}{|\lambda_k - \lambda|^2 |\lambda_{k'} - \lambda|^2}. \quad (29)$$

We will split this sum using the partition (23). Firstly Proposition 2.7 and (25) imply

$$\sum_{k, k' \in I} \frac{|\langle V\phi_k, \phi_{k'} \rangle|^2}{|\lambda_k - \lambda|^2 |\lambda_{k'} - \lambda|^2} \leq C(V) n^{-1/2} \left(\sum_{k \in I} \frac{1}{|\lambda_k - \lambda|^2} \right)^2 \leq C(V, \varepsilon) n^{-1/2}.$$

Now using (27), (28) and (25) we get

$$\begin{aligned} \sum_{\substack{k \in \mathbb{N}_0 \\ k' \in J}} \frac{|\langle V\phi_k, \phi_{k'} \rangle|^2}{|\lambda_k - \lambda|^2 |\lambda_{k'} - \lambda|^2} &\leq Cn^{-1} \sum_{k \in \mathbb{N}_0} \frac{1}{|\lambda_k - \lambda|^2} \sum_{k' \in J} |\langle V\phi_k, \phi_{k'} \rangle|^2 \\ &\leq C(V, \varepsilon)n^{-1}. \end{aligned}$$

The remaining part of the sum on the right hand side of (29) involves $k \in J$ and $k' \in I \subset \mathbb{N}_0$; thus we can estimate this part using an argument similar to the last one with k and k' swapped. \blacksquare

Lemma 3.2. *For any $n \in \mathbb{N}_0$ and $\lambda \in \Gamma_{\varepsilon, n}$ the operator $R(\lambda)VR(\lambda)$ is trace class. Furthermore $\|R(\lambda)VR(\lambda)\|_1$ is uniformly bounded (in n and $\lambda \in \Gamma_{\varepsilon, n}$).*

Proof. The set $\{\phi_k \mid k \in \mathbb{N}_0\}$ is an orthonormal eigenbasis for R with corresponding eigenvalues $(\lambda_k - \lambda)^{-1}$, $k \in \mathbb{N}_0$ so (25) implies

$$\|R\|_2^2 = \sum_{k \in \mathbb{N}_0} |\lambda_k - \lambda|^{-2} \leq C(\varepsilon).$$

Thus $\|RVR\|_1 = \|VR^2\|_1 \leq \|V\| \|R^2\|_1 \leq \|V\| \|R\|_2^2 \leq C(\varepsilon) \|V\|$. \blacksquare

Suppose $n \in \mathbb{N}_0$ and $j \in \mathbb{N}$. From the previous result we know that $R(\lambda)VR(\lambda)$ is trace class for any $\lambda \in \Gamma_{\varepsilon, n}$. On the other hand $R(\lambda)V$ is bounded (in fact $\|R(\lambda)V\| \leq \varepsilon^{-1}\|V\|$). It follows that

$$(R(\lambda)V)^j R(\lambda) = (R(\lambda)V)^{j-1} R(\lambda)VR(\lambda)$$

is also trace class with trace norm uniformly bounded for $\lambda \in \Gamma_{\varepsilon, n}$. The work in the remainder of this section leads to Proposition 3.5 where we obtain an estimate for the trace of an integral of such operators.

Lemma 3.3. *Let $n \geq 2$, $\lambda \in \Gamma_{\varepsilon, n}$ and suppose $f : \mathbb{N}_0 \rightarrow \mathbb{C}$ satisfies*

$$\sum_{k \in \mathbb{N}_0} |f(k)|^2 \leq C_1^2 \quad \text{and} \quad |f(k)| \leq C_1 n^{-1/4} \quad \text{when } k \in I \quad (30)$$

for some constant C_1 . For each $k \in \mathbb{N}_0$ set

$$g(k) = \sum_{k' \in \mathbb{N}_0} \frac{f(k') \langle V\phi_{k'}, \phi_k \rangle}{\lambda - \lambda_{k'}}.$$

Then there exists a constant $K = K(V, \varepsilon)$ such that

$$\sum_{k \in \mathbb{N}_0} |g(k)|^2 \leq C_1^2 K^2 n^{-1/2} \ln^2(n) \quad \text{and} \quad |g(k)| \leq C_1 K n^{-1/2} \ln(n) \quad \text{when } k \in I.$$

Proof. Since

$$\sum_{k \in \mathbb{N}_0} |g(k)|^2 = \sum_{k, k', k'' \in \mathbb{N}_0} \frac{f(k') \overline{f(k'')} \langle V \phi_{k'}, \phi_k \rangle \langle \phi_k, V \phi_{k''} \rangle}{(\lambda - \lambda_{k'}) (\lambda - \lambda_{k''})}$$

and

$$\left| \sum_{k \in \mathbb{N}_0} \langle V \phi_{k'}, \phi_k \rangle \langle \phi_k, V \phi_{k''} \rangle \right| = |\langle V \phi_{k'}, V \phi_{k''} \rangle| \leq \|V\|^2$$

it follows that

$$\sum_{k \in \mathbb{N}_0} |g(k)|^2 \leq \|V\|^2 \left(\sum_{k \in I} \frac{|f(k)|}{|\lambda - \lambda_k|} + \sum_{k \in J} \frac{|f(k)|}{|\lambda - \lambda_k|} \right)^2.$$

Using the second part of (30) and (24) we get

$$\sum_{k \in I} \frac{|f(k)|}{|\lambda - \lambda_k|} \leq C_1 n^{-1/4} \sum_{k \in I} |\lambda - \lambda_k|^{-1} \leq C_1 C_2(\varepsilon) n^{-1/4} \ln(n).$$

On the other hand the first part of (30) and (26) give

$$\begin{aligned} \sum_{k \in J} \frac{|f(k)|}{|\lambda - \lambda_k|} &\leq \left(\sum_{k \in J} |f(k)|^2 \right)^{1/2} \left(\sum_{k \in J} |\lambda - \lambda_k|^{-2} \right)^{1/2} \\ &\leq C_1 C_3 n^{-1/4} \leq 2C_1 C_3 n^{-1/4} \ln(n). \end{aligned}$$

Putting these estimates together now leads to

$$\sum_{k \in \mathbb{N}_0} |g(k)|^2 \leq C_1^2 K_1^2 n^{-1/2} \ln^2(n),$$

with $K_1 = \|V\| (C_2(\varepsilon) + 2C_3)$. Now suppose $k \in I$ and write $g(k) = g_I(k) + g_J(k)$ where

$$g_I(k) = \sum_{k' \in I} \frac{f(k') \langle V \phi_{k'}, \phi_k \rangle}{\lambda - \lambda_{k'}} \quad \text{and} \quad g_J(k) = \sum_{k' \in J} \frac{f(k') \langle V \phi_{k'}, \phi_k \rangle}{\lambda - \lambda_{k'}}.$$

From Proposition 2.7, the second part of (30) and (24) we get

$$|g_I(k)| \leq C_1 C(V) n^{-1/2} \sum_{k' \in I} |\lambda - \lambda_{k'}|^{-1} \leq C_1 C_4(V, \varepsilon) n^{-1/2} \ln(n).$$

On the other hand (27), the first part of (30) and (28) give us

$$\begin{aligned} |g_J(k)| &\leq C(\varepsilon) n^{-1/2} \left(\sum_{k' \in J} |f(k')|^2 \right)^{1/2} \left(\sum_{k' \in J} |\langle V \phi_{k'}, \phi_k \rangle|^2 \right)^{1/2} \\ &\leq C_1 C_5(\varepsilon) \|V\| n^{-1/2} \leq 2C_1 C_5(\varepsilon) \|V\| n^{-1/2} \ln(n). \end{aligned}$$

Putting these estimates together now leads to $|g(k)| \leq C_1 K_2 n^{-1/2} \ln(n)$ with $K_2 = C_4(V, \varepsilon) + 2C_5(\varepsilon) \|V\|$. Taking $K = \max\{K_1, K_2\}$, completes the result. \blacksquare

Taking $f(k) = \langle V\phi_n, \phi_k \rangle$ we can use (28) and Proposition 2.7 to check that (30) is satisfied. The next result then follows from Lemma 3.3 by use of induction; we can take $K = \max\{\|V\|, C(V), K'\}$ where $C(V)$ and K' are the constants coming from Proposition 2.7 and Lemma 3.3 respectively.

Lemma 3.4. *Suppose $n \geq 2$ and $j \in \mathbb{N}_0$. Then there exists a constant $K = K(V, \varepsilon)$ such that for all $\lambda \in \Gamma_{\varepsilon, n}$ we have*

$$\left| \sum_{k_1, \dots, k_j \in \mathbb{N}_0} \frac{\langle V\phi_n, \phi_{k_1} \rangle \langle V\phi_{k_1}, \phi_{k_2} \rangle \dots \langle V\phi_{k_j}, \phi_n \rangle}{(\lambda - \lambda_{k_1}) \dots (\lambda - \lambda_{k_j})} \right| \leq K^{j+1} n^{-(j+1)/4} \ln^j(n).$$

Proposition 3.5. *Suppose $n \geq 2$ and $j \in \mathbb{N}$. Then*

$$\left| \operatorname{Tr} \frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon, n}} \lambda R(\lambda) (VR(\lambda))^j d\lambda \right| \leq K^j n^{-j/4} \ln^{j-1}(n),$$

where K is the constant from Lemma 3.4.

Proof. Since $\{\phi_{k'} \mid k' \in \mathbb{N}_0\}$ is an orthonormal basis of $L^2(\mathbb{R})$ we have

$$(VR)\phi_k = \sum_{k' \in \mathbb{N}_0} \langle VR\phi_k, \phi_{k'} \rangle \phi_{k'} = \sum_{k' \in \mathbb{N}_0} \frac{\langle V\phi_k, \phi_{k'} \rangle}{\lambda_k - \lambda} \phi_{k'}.$$

Continuing by induction we get

$$(VR)^j \phi_k = \sum_{k_1, \dots, k_j \in \mathbb{N}_0} \frac{\langle V\phi_k, \phi_{k_1} \rangle \langle V\phi_{k_1}, \phi_{k_2} \rangle \dots \langle V\phi_{k_{j-1}}, \phi_{k_j} \rangle}{(\lambda_k - \lambda)(\lambda_{k_1} - \lambda) \dots (\lambda_{k_{j-1}} - \lambda)} \phi_{k_j}.$$

Together with the fact that $\langle R\phi_{k_j}, \phi_{k_0} \rangle = \delta_{k_j, k_0} (\lambda_{k_0} - \lambda)^{-1}$ we now get

$$\begin{aligned} \operatorname{Tr}(R(VR)^j) &= \sum_{k_0 \in \mathbb{N}_0} \langle R(VR)^j \phi_{k_0}, \phi_{k_0} \rangle \\ &= \sum_{k_0, \dots, k_j \in \mathbb{N}_0} \frac{\langle V\phi_{k_0}, \phi_{k_1} \rangle \langle V\phi_{k_1}, \phi_{k_2} \rangle \dots \langle V\phi_{k_{j-1}}, \phi_{k_j} \rangle}{(\lambda_{k_0} - \lambda)(\lambda_{k_1} - \lambda) \dots (\lambda_{k_{j-1}} - \lambda)} \langle R\phi_{k_j}, \phi_{k_0} \rangle \\ &= \sum_{k_0, \dots, k_{j-1} \in \mathbb{N}_0} \frac{\langle V\phi_{k_0}, \phi_{k_1} \rangle \langle V\phi_{k_1}, \phi_{k_2} \rangle \dots \langle V\phi_{k_{j-1}}, \phi_{k_0} \rangle}{(\lambda_{k_0} - \lambda)^2 (\lambda_{k_1} - \lambda) \dots (\lambda_{k_{j-1}} - \lambda)} = \sum_{l=0}^{j-1} \frac{1}{\lambda_{k_l} - \lambda} A(\lambda), \end{aligned}$$

where $A(\lambda)$ is the meromorphic function

$$A(\lambda) = \frac{1}{j} \sum_{k_0, \dots, k_{j-1} \in \mathbb{N}_0} \frac{\langle V\phi_{k_0}, \phi_{k_1} \rangle \langle V\phi_{k_1}, \phi_{k_2} \rangle \dots \langle V\phi_{k_{j-1}}, \phi_{k_0} \rangle}{(\lambda_{k_0} - \lambda)(\lambda_{k_1} - \lambda) \dots (\lambda_{k_{j-1}} - \lambda)}. \quad (31)$$

Since

$$\frac{d}{d\lambda} \lambda \left(\prod_{i=0}^{j-1} \frac{1}{\lambda_{k_i} - \lambda} \right) = \prod_{i=0}^{j-1} \frac{1}{\lambda_{k_i} - \lambda} + \lambda \sum_{l=0}^{j-1} \frac{1}{\lambda_{k_l} - \lambda} \left(\prod_{i=0}^{j-1} \frac{1}{\lambda_{k_i} - \lambda} \right)$$

for any $k_0, \dots, k_{j-1} \in \mathbb{N}_0$, we can rewrite the above equation as

$$\text{Tr } \lambda R(VR)^j = \frac{d}{d\lambda} (\lambda A(\lambda)) - A(\lambda).$$

Integrating around the contour $\Gamma_{\varepsilon, n}$ it follows that

$$\text{Tr } \frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon, n}} \lambda R(VR)^j d\lambda = -\frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon, n}} A(\lambda) d\lambda. \quad (32)$$

The poles of the meromorphic function $A(\lambda)$ occur at the points $\lambda = \lambda_k$ for $k \in \mathbb{N}_0$. Since the only such point enclosed by the contour $\Gamma_{\varepsilon, n}$ is $\lambda = \lambda_n$, it follows that the only terms in the series (31) which contribute to the right hand side of (32) are those with at least one of k_0, \dots, k_{j-1} equal to n . With the help of symmetry we then obtain the identity

$$\begin{aligned} & \text{Tr } \frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon, n}} \lambda R(VR)^j d\lambda \\ &= -\frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon, n}} \frac{1}{\lambda_n - \lambda} \sum_{k_1, \dots, k_{j-1} \in \mathbb{N}_0} \frac{\langle V\phi_n, \phi_{k_1} \rangle \langle V\phi_{k_1}, \phi_{k_2} \rangle \dots \langle V\phi_{k_{j-1}}, \phi_n \rangle}{(\lambda_{k_1} - \lambda) \dots (\lambda_{k_{j-1}} - \lambda)} d\lambda. \end{aligned} \quad (33)$$

For any $\lambda \in \Gamma_{\varepsilon, n}$ we have $|\lambda_n - \lambda| = \varepsilon$ while

$$\left| \sum_{k_1, \dots, k_{j-1} \in \mathbb{N}_0} \frac{\langle V\phi_n, \phi_{k_1} \rangle \langle V\phi_{k_1}, \phi_{k_2} \rangle \dots \langle V\phi_{k_{j-1}}, \phi_n \rangle}{(\lambda_{k_1} - \lambda) \dots (\lambda_{k_{j-1}} - \lambda)} \right| \leq K^j n^{-j/4} \ln^{j-1}(n)$$

by Lemma 3.4. Since the length of $\Gamma_{\varepsilon, n}$ is $2\pi\varepsilon$ we finally get

$$\left| \text{Tr } \frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon, n}} \lambda R(VR)^j d\lambda \right| \leq \frac{1}{2\pi} \oint_{\Gamma_{\varepsilon, n}} \frac{1}{\varepsilon} K^j n^{-j/4} \ln^{j-1}(n) d\lambda = K^j n^{-j/4} \ln^{j-1}(n),$$

completing the result. ■

Taking $j = 1$ in (33) leads to the formula

$$\begin{aligned} & \text{Tr } \frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon, n}} \lambda R(\lambda) V R(\lambda) d\lambda \\ &= -\frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon, n}} \frac{1}{\lambda_n - \lambda} \langle V\phi_n, \phi_n \rangle d\lambda = \langle V\phi_n, \phi_n \rangle. \end{aligned} \quad (34)$$

This is needed to obtain the first order correction term in Theorem 1.1.

4 Proof of Theorem 1.1

Lemmas 3.1 and 3.2 give us $\|R(\lambda)VR(\lambda)\| \leq C_1 n^{-1/4}$ and $\|R(\lambda)VR(\lambda)\|_1 \leq C_2$ for all $n \in \mathbb{N}$ and $\lambda \in \Gamma_{\varepsilon, n}$. In particular $\|(VR(\lambda))^2\| \leq \|V\|C_1 n^{-1/4}$. We also note that $\|R(\lambda)\| = \varepsilon^{-1}$. It follows that for any $j \in \mathbb{N}_0$ we get

$$\|(VR(\lambda))^{2j}\| \leq \|(VR(\lambda))^2\|^j \leq (\|V\|C_1 n^{-1/4})^j$$

and

$$\|(VR(\lambda))^{2j+1}\| \leq \|V\| \|R(\lambda)\| \|(VR(\lambda))^{2j}\| \leq \|V\| \varepsilon^{-1} (\|V\|C_1 n^{-1/4})^j.$$

Choose $N' \in \mathbb{N}$ so that $\|V\|C_1 N'^{-1/4} \leq 1/2$. It follows that for any $n \geq N'$ and $\lambda \in \Gamma_{\varepsilon, n}$ the series

$$(I + VR(\lambda))^{-1} = \sum_{j=0}^{\infty} (-VR(\lambda))^j \quad (35)$$

is absolutely convergent and has norm bounded by $2(1 + \|V\|\varepsilon^{-1})$. In particular, $I + VR(\lambda)$ is invertible with a uniformly bounded inverse for all $n \geq N'$ and $\lambda \in \Gamma_{\varepsilon, n}$. On the other hand, the series

$$T(\lambda) := \sum_{j=1}^{\infty} R(\lambda)(-VR(\lambda))^j = -R(\lambda)VR(\lambda) \sum_{j=0}^{\infty} (-VR(\lambda))^j$$

is convergent in trace class with

$$\|T(\lambda)\|_1 \leq \|R(\lambda)VR(\lambda)\|_1 \|(I + VR(\lambda))^{-1}\| \leq 2C_2(1 + \|V\|\varepsilon^{-1})$$

for $n \geq N'$ and $\lambda \in \Gamma_{\varepsilon, n}$. Setting

$$T_n = -\frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon, n}} \lambda T(\lambda) d\lambda$$

it follows that we have an absolutely convergent expansion

$$\text{Tr } T_n = -\sum_{j=1}^{\infty} \text{Tr} \frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon, n}} \lambda R(\lambda)(-VR(\lambda))^j d\lambda$$

whenever $n \geq N'$.

Now choose $N \geq N'$ so that $KN^{-1/4} \ln(N) \leq 1/2$ where K is the constant given by Proposition 3.5. Using this Proposition and the above results it follows that

$$\left| \sum_{j=2}^{\infty} \text{Tr} \frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon, n}} \lambda R(\lambda)(-VR(\lambda))^j d\lambda \right| \leq 2K^2 n^{-1/2} \ln(n)$$

for all $n \geq N$. Therefore

$$\begin{aligned}\mathrm{Tr} T_n &= \mathrm{Tr} \frac{1}{2\pi i} \oint_{\Gamma_{\varepsilon,n}} \lambda R(\lambda) V R(\lambda) d\lambda + O(n^{-1/2} \ln(n)) \\ &= \langle V \phi_n, \phi_n \rangle + O(n^{-1/2} \ln(n))\end{aligned}$$

for all $n \geq N$, where we have used (34).

The argument can be tied together using a standard resolvent expansion. Set $R_V(\lambda) = (H + V - \lambda)^{-1}$ and let $n \geq N$. Then

$$R_V(\lambda) = R(\lambda)(1 + VR(\lambda))^{-1} = R(\lambda) \sum_{j=0}^{\infty} (-VR(\lambda))^j.$$

The right hand side of (35) will still converge if V is replaced with gV for some $g \in [0, 1]$. Hence $\sigma(H + gV) \cap \Gamma_{\varepsilon,n} = \emptyset$. Since the eigenvalues of $H + gV$ depend continuously on g , it follows that $\Gamma_{\varepsilon,n}$ must enclose $\lambda_n(H + V)$ but no other points of $\sigma(H + V)$. Thus we can write

$$\begin{aligned}\lambda_n(H + V) - \lambda_n(H) &= -\frac{1}{2\pi i} \mathrm{Tr} \oint_{\Gamma_{\varepsilon,n}} \lambda (R_V(\lambda) - R(\lambda)) d\lambda \\ &= -\frac{1}{2\pi i} \mathrm{Tr} \oint_{\Gamma_{\varepsilon,n}} \lambda \sum_{j=1}^{\infty} R(\lambda) (-VR(\lambda))^j d\lambda \\ &= \mathrm{Tr} T_n = \langle V \phi_n, \phi_n \rangle + O(n^{-1/2} \ln(n)).\end{aligned}$$

Theorem 1.1 now follows from Proposition 2.8.

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