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Quasiclassical eigenvalues

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Abstract. The quasiclassical approximation to the eigenvalues at the bottom of a one-dimensional potential well are obtained by applying the 'twisting trick' of Simon and Davies to reduce the problem to an ordinary Rayleigh–Schrödinger problem. The key is that the twist occurs on a scale intermediate between the two scales of the problem.

Introduction

The asymptotics of the eigenvalues at the bottom of a potential well are well known [3, 7]. Here we shall derive these results by a somewhat different method which was employed by McDonnell and the author [4] to discuss the asymptotics of Stark effect resonance widths. This method of *'twisting at intermediate scales'* relies on the notion that in a problem with multiple length scales, phenomena which take place on different scales frequently act as though they are in orthogonal subspaces. A precise version of this notion can sometimes be arranged by use of the 'twisting trick' [1, 2, 6].

We shall consider the Hamiltonian

$$\epsilon^4 p^2 + v(x)$$

on $L_2(-\infty, +\infty)$, where $p = -\mathrm{i}\,\mathrm{d}/\mathrm{d}x$ and $v(x)$ is a C^∞ function having a *unique* global minimum $v(0) = 0$ at the origin. More complicated cases have been considered (higher dimensions, several minima, degeneracies, other forms of dependence on the parameter ϵ, etc) but our purpose is to illustrate a method, not to achieve maximum generality, so we shall stick to the simplest case.

The relevant length scales are as follows. The potential $v(x)$ changes on a scale of order 1. The eigenfunctions at the bottom of the well are asymptotically of the form $\phi_n(x/\epsilon)$, where ϕ_n is a Hermite function, and so decay exponentially on a scale of order ϵ. We shall therefore cut out a region with length of order ϵ^α, $0 < \alpha < 1$ about the origin. This region is very small on a scale of order 1 and very large on a scale of order ϵ. The behaviour in the two regions is separated approximately by twisting, and the result is then obtained by ordinary perturbation theory.

1. Main theorem

To be precise, we shall make the following assumptions about $v(x)$.

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Hypothesis 1. Let $v(x)$ be a C^∞ function on $-\infty < x < \infty$, and assume that $v(x)$ has a unique global minimum $v(0) = 0$ at $x = 0$, which is non-degenerate in the sense that $v''(0) > 0$. For normalization, we shall take $v''(0) = 2$. Assume further that

$$\liminf_{|x|\to\infty} v(x) > 0. \tag{1.1}$$

Rather than dealing directly with

$$\epsilon^4 p^2 + v(x) \tag{1.2}$$

we shall scale $x \to \epsilon x$ to obtain

$$\epsilon^2[p^2 + \epsilon^{-2} v(\epsilon x)] \tag{1.3}$$

and will work with

$$h_\epsilon = p^2 + \epsilon^{-2} v(\epsilon x). \tag{1.4}$$

(Note that the scales ϵ and 1 become 1 and $1/\epsilon$ here, so that the twist will come on a scale of order $\epsilon^{-\alpha}$, $0 < \alpha < 1$.)

Theorem 1. If $v(x)$ satisfies hypothesis 1, then for each N, the lowest N eigenvalues of h_ϵ are given asymptotically by

$$E_n = (2n+1) + c_1(n)\epsilon + \cdots c_k(n)\epsilon^k + \cdots \tag{1.5}$$

for $0 \leqslant n < N$, where the coefficients $c_k(n)$ are obtained from the formal Rayleigh–Schrödinger perturbation series for the problem

$$p^2 + x^2 + a_1 x^3 + \cdots + a_k \epsilon^k x^{k+2} + \cdots \tag{1.6}$$

where

$$a_k = \frac{v^{(k+2)}(0)}{(k+2)!}.$$

2. Twisting

Fix $0 < \alpha < \frac{1}{3}$. Define a function $w_\epsilon(x)$ by

$$w_\epsilon(x) = \begin{cases} x^2 & |x| \geqslant 2\epsilon^{-\alpha} \\ \epsilon^{-2\alpha} & |x| \leqslant \epsilon^{-\alpha}. \end{cases} \tag{2.1}$$

Consider the matrix operator

$$\tilde{H}_\epsilon = \begin{pmatrix} h_\epsilon & 0 \\ 0 & p^2 + w_\epsilon(x) \end{pmatrix} = P^2 + \begin{pmatrix} \epsilon^{-2} v(\epsilon x) & 0 \\ 0 & w_\epsilon(x) \end{pmatrix} \tag{2.2}$$

on $L_2(-\infty, +\infty) \otimes \mathbb{C}^2$ where $P^2 = p^2 \otimes I$, and note that H_ϵ has the same low-lying eigenvalues as h_ϵ, since $p^2 + w_\epsilon(x) \geqslant \epsilon^{-2\alpha}$.

Let $U(x)$ be a real orthogonal 2×2 matrix, C^∞ in x, with

$$U(x) = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \text{for } |x| \leqslant 1$$

and

$$U(x) = J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \qquad \text{for } |x| \geqslant 2$$

(see, e.g., [1]). Transforming $\tilde{H}_\epsilon$ by $U(\epsilon^\alpha x)$, we find that $\tilde{H}_\epsilon$ is unitarily equivalent to

$$H_\epsilon = U^*(\epsilon^\alpha x)\tilde{H}_\epsilon U(\epsilon^\alpha x). \tag{2.3}$$

This operator is described by the following lemma.

Lemma 1. For $0 < \alpha < \frac{1}{3}$, $\tilde{H}_\epsilon$ is unitarily equivalent to an operator

$$H_\epsilon = \begin{pmatrix} h_0 + v_\epsilon & d_\epsilon \\ d_\epsilon^* & k_\epsilon \end{pmatrix} \tag{2.4}$$

where (a) $h_0 = p^2 + x^2$ is the harmonic oscillator, and

$$v_\epsilon = v_\epsilon(x) = \mathcal{O}(\epsilon^\gamma) \tag{2.5}$$

where $\gamma = 1 - 3\alpha > 0$; (b) $k_\epsilon = p^2 + \tilde{w}_\epsilon(x)$, where

$$\tilde{w}_\epsilon(x) \geqslant \tfrac{1}{2}\epsilon^{-2\alpha}$$

and (c) $d_\epsilon = a_\epsilon(x)p + b_\epsilon(x)$, with

$$a_\epsilon(x) = \mathcal{O}(\epsilon^\alpha) \qquad \text{and} \qquad b_\epsilon(x) = \mathcal{O}(\epsilon^\beta) \tag{2.6}$$

where $\beta = \min(\gamma, 2\alpha)$. Moreover, $v_\epsilon(x)$ is supported in $|x| \leqslant 2\epsilon^{-\alpha}$, while $a_\epsilon(x)$ and $b_\epsilon(x)$ are supported in $\epsilon^{-\alpha} \leqslant |x| \leqslant 2\epsilon^{-\alpha}$.

Note. By commuting $a_\epsilon(x)$ with p, one can also write

$$d_\epsilon = p\tilde{a}_\epsilon(x) + \tilde{b}_\epsilon(x)$$

where $\tilde{a}_\epsilon$ and $\tilde{b}_\epsilon$ have the same properties as a_ϵ and b_ϵ.

Proof. By Taylor's theorem

$$\tilde{v}_\epsilon(x) = \epsilon^{-2}v(\epsilon x) = x^2 + R_2(x, \epsilon) \tag{2.7}$$

where

$$R_2(x, \epsilon) = \tfrac{1}{6}v'''(\xi)\epsilon x^3$$

with $|\xi| < |\epsilon x|$. For $|x| \leqslant 2\epsilon^{-\alpha}$, we have

$$|R_2(x, \epsilon)| \leqslant M\epsilon\epsilon^{-3\alpha} = \mathcal{O}(\epsilon^{\gamma)} \tag{2.8}$$

where $M = \frac{4}{3}\sup\{|v'''(\xi)| : |\xi| \leqslant 1\}$, and $\gamma = 1 - 3\alpha > 0$.

Let

$$U = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix}$$

and consider the term

$$W(x, \epsilon) \equiv U(\epsilon^\alpha x)^* \begin{pmatrix} \tilde{v}_\epsilon & 0 \\ 0 & w_\epsilon \end{pmatrix} U(\epsilon^\alpha x).$$

We compute

$$w_{11} = u_{11}^2\tilde{\gamma}_\epsilon + u_{12}^2 w_\epsilon.$$

Since u_{11}^2 is supported in $|x| \leqslant 2\epsilon^{-\alpha}$ and u_{12}^2 in $|x| \geqslant \epsilon^{-\alpha}$, we find from equations (2.8) and (2.9) that

$$u_{11}^2\tilde{v}_\epsilon = u_{11}^2 x^2 + \mathcal{O}(\epsilon^\gamma)$$

while from equation (2.1)

$$u_{12}^2 w_\epsilon = x^2$$

exactly, so that, adding,

$$w_{11} = x^2 + \mathcal{O}(\epsilon^\gamma). \tag{2.9}$$

Similarly

$$w_{12} = w_{21} = u_{11}u_{12}\tilde{v}_\epsilon + u_{21}u_{22}w_\epsilon.$$

This vanishes except in the range $\epsilon^{-\alpha} \leqslant |x| \leqslant 2\epsilon^{-\alpha}$. In that range, $\tilde{v}_\epsilon = x^2 + \mathcal{O}(\epsilon^\gamma)$, while $w_\epsilon = x^2$ exactly. Thus

$$w_{12} = (u_{11}u_{12} + u_{21}u_{22})x^2 + \mathcal{O}(\epsilon^\gamma).$$

But the coefficient of x^2 is zero, since $U^*U = I$, so that

$$w_{12} = \mathcal{O}(\epsilon^\gamma). \tag{2.10}$$

Finally, since $x = 0$ is the *unique* minimum of $v(x)$, and since $v(x)$ is bounded away from zero at infinity, the global minimum of $v(x)$ on $|x| \geqslant \epsilon^{1-\alpha}$ is its minimum on $\epsilon^{1-\alpha} \leqslant |x| \leqslant 2\epsilon^{1-\alpha}$ so that

$$\tilde{v}_\epsilon(x) \geqslant \epsilon^{-2\alpha} + \mathcal{O}(\epsilon^\gamma)$$

on $|x| \geqslant \epsilon^{-\alpha}$.

Using equation (2.9), we obtain

$$w_{22} = u_{22}^2 w_\epsilon + u_{21}^2 \tilde{v}_\epsilon \geqslant \tfrac{1}{2}\epsilon^{-2\alpha}. \tag{2.11}$$

These terms are therefore consistent with the claims of lemma 1.

The remaining terms are P^2 and the commutator

$$U(\epsilon^\alpha x)^*[P^2, U(\epsilon^\alpha x)] = A(x,\epsilon)p + pA(x,\epsilon) \tag{2.12}$$

where

$$A(x,\epsilon) = \mathrm{i}\epsilon^\alpha U(\epsilon^\alpha x)^* U'(\epsilon^\alpha x) = A(x,\epsilon)^*$$

vanishes except on $\epsilon^{-\alpha} \leqslant |x| \leqslant 2\epsilon^{-\alpha}$. Since $U(x)$ is orthogonal, $U^*(x)U'(x)$ is skew symmetric, and hence the *diagonal terms* of the matrix $A(x,\epsilon)$ *are zero*. Clearly

$$A(x,\epsilon) = \mathcal{O}(\epsilon^\alpha). \tag{2.13}$$

Moreover

$$pA(x,\epsilon) = A(x,\epsilon)p - \mathrm{i}A'(x,\epsilon) \tag{2.14}$$

where

$$A'(x,\epsilon) = \mathcal{O}(\epsilon^{2\alpha}). \tag{2.15}$$

Combining this with the preceding yields the lemma. □

3. Perturbation theory

We shall write equation (2.4) as

$$H_\epsilon = H_\epsilon^0 + V_\epsilon + D_\epsilon \tag{3.1}$$

where

$$H_\epsilon^0 = \begin{pmatrix} h_0 & 0 \\ 0 & k_\epsilon \end{pmatrix} \tag{3.2}$$

$$V_\epsilon = \begin{pmatrix} v_\epsilon & 0 \\ 0 & 0 \end{pmatrix} \tag{3.3}$$

and

$$D_\epsilon = \begin{pmatrix} 0 & d_\epsilon \\ d_\epsilon^* & 0 \end{pmatrix} \tag{3.4}$$

and will regard $V_\epsilon + D_\epsilon$ as a perturbation of H_ϵ^0.

Define $r_0(z) = (h_0 - z)^{-1}$, $g_\epsilon(z) = (k_\epsilon - z)^{-1}$, $R_\epsilon(z) = (H_\epsilon - z)^{-1}$ and $R_\epsilon^0(z) = (H_\epsilon^0 - z)^{-1}$.

Lemma 2. Let $B_\epsilon = pg_\epsilon(z)$. Then for any $a > 0$

$$\|B_\epsilon\| = \mathcal{O}(\epsilon^\alpha)$$

uniformly for $\operatorname{Re} z \leqslant a$.

Proof. Let $z = t + \mathrm{i}s$. Then, since $w_\epsilon \geqslant 0$,

$$B_\epsilon^* B_\epsilon = g_\epsilon(z)^* p^2 g_\epsilon(z) \leqslant g_\epsilon(z)^*(p^2 + w_\epsilon) g_\epsilon^*(z) \tag{3.5}$$

$$= (k_\epsilon - t + \mathrm{i}s)^{-1} k_\epsilon (k_\epsilon - t - is)^{-1} \tag{3.6}$$

$$= \frac{k_\epsilon}{(k_\epsilon - t)^2 + s^2} \leqslant \frac{k_\epsilon}{(k_\epsilon - a)^2}. \tag{3.7}$$

The norm of this is the minimum of $\lambda(\lambda + a)^{-2}$ over the spectrum of k_ϵ, which is contained in $\left[\epsilon^{-2\alpha}/2, \infty\right)$. If $\epsilon^{-2\alpha} > 2a$, this will not exceed

$$2\epsilon^{-2\alpha}(\epsilon^{-2\alpha} + 2a)^{-2} = \mathcal{O}(\epsilon^{2\alpha}).$$

Consider the non-degenerate eigenvalue $\lambda_0 = 2n + 1$ of h_0, and hence also of H_ϵ^0 (for small ϵ). Let Γ be the circle with centre λ_0 and radius 1. We shall compute the perturbed eigenvalue of

$$H_\epsilon = H_\epsilon^0 + T_\epsilon. \tag{3.8}$$

As in [5, p 79], this can be done if the series

$$R_\epsilon(z) = \sum_{k=0}^{\infty} R_\epsilon^0(z)[T_\epsilon R_\epsilon^0(z)]^k \tag{3.9}$$

converges uniformly on Γ. But

$$T_\epsilon R_\epsilon^0(z) = \begin{pmatrix} v_\epsilon r_0(z) & d_\epsilon g_\epsilon(z) \\ d_\epsilon^* r_0(z) & 0 \end{pmatrix}.$$

Using lemmas 1 and 2, and the fact that $pr_0(z)$ is bounded on Γ, we find that

$$\|T_\epsilon R_\epsilon^0(z)\| = \mathcal{O}(\epsilon^{\gamma'}) \tag{3.10}$$

uniformly on Γ where $\gamma' = \min(\gamma, \alpha)$. This ensures the existence of a unique eigenvalue of H_ϵ inside Γ.

4. Asymptotic series

It remains for us to identify the terms of the series for $E_n(\epsilon)$ to all orders in ϵ. Let

$$s = \lim_{\lambda\to\lambda_0} \left[r_0(\lambda) - (\lambda-\lambda_0)^{-1}|\phi_0\rangle\langle\phi_0|\right]$$

be the reduced resolvent for $h_0 = p^2 + x^2$ at $\lambda_0 = 2n+1$, where ϕ_0 is the normalized eigenfunction. The reduced resolvent for H_ϵ^0 is then

$$S_\epsilon = \begin{pmatrix} s & 0 \\ 0 & g_\epsilon(\lambda_0) \end{pmatrix}. \tag{4.1}$$

Let $\langle x\rangle = (1+x^2)^{\frac{1}{2}}$.

Lemma 3. For every $N > 0$, $\langle x\rangle^N S\langle x\rangle^{-N}$ is bounded.

Proof. By a standard result [7], $\langle x\rangle^N r_0(z)\langle x\rangle^{-N}$ is bounded for $z \notin \sigma(h_0)$. Subtracting $\langle x\rangle^N|\phi_0\rangle\langle\phi_0|\langle x\rangle^{-N}(\lambda_0 - z)^{-1}$ gives an operator which is analytic in a neighbourhood of λ_0, with no singularity, so we may pass to the limit $z \to \lambda_0$. □

Expand the resolvent in powers of the perturbation $V_\epsilon + D_\epsilon \equiv G_\epsilon$. Then [5, p 79, equation (2.31)]

$$E_n(\epsilon) = \sum_{k=0}^{\infty} \frac{(-1)^r}{k} \sum_{\substack{k_1+\cdots+k_n=r-1\\ k_h\geqslant 0}} \operatorname{tr}\left(G_\epsilon S^{(k_1)} G_\epsilon S^{(k_2)}\cdots G_\epsilon S^{(k_r)}\right) \tag{4.2}$$

where $S^{(1)} = S$ and $S^{(0)} = -|\phi_0\rangle\langle\phi_0| = -P_0$. By equation (3.9), the rth term is $\mathcal{O}(\epsilon^{r\gamma'})$ so to $\mathcal{O}(\epsilon^N)$ for any fixed N only a finite number of terms contribute to $E_n(\epsilon)$. Furthermore, each term of (4.2) is a sum of products of factors of the form

$$\langle\phi_0|G_\epsilon S G_\epsilon S\cdots SG_\epsilon|\phi_0\rangle. \tag{4.3}$$

Putting $G_\epsilon = V_\epsilon + D_\epsilon$ and expanding, we have further a sum of products of factors

$$T = \langle\phi_0|G_\epsilon^{(1)} S X_\epsilon^{(2)} S\cdots S X_\epsilon^{(\ell)}|\phi_0\rangle \tag{4.4}$$

where $X_\epsilon^{(j)}$ is either V_ϵ or D_ϵ.

Lemma 4. If at least one $X_\epsilon^{(j)} = D_\epsilon$, then

$$T = \mathcal{O}(\epsilon^N) \tag{4.5}$$

for every N.

Proof. Let m be the first index with $X_\epsilon^{(m)} = D_\epsilon$. Then

$$T = \langle\psi_\epsilon^{(1)}|\psi_\epsilon\rangle \tag{4.6}$$

where

$$\psi_\epsilon = [SV_\epsilon]^{m-1}\phi_0 = \begin{pmatrix} (SV_\epsilon)^{m-1}\phi_0 \\ 0 \end{pmatrix} \tag{4.7}$$

and

$$\psi_\epsilon^{(1)} = D_\epsilon S X_\epsilon^{(m+1)}\cdots X_\epsilon^{(r)}\phi_0. \tag{4.8}$$

Let $\chi_\epsilon(x)$ be the characteristic function of $[\epsilon^{-\alpha}, 2\epsilon^{-\alpha}]$. Since $\chi_a\psi_\epsilon^{(1)} = \psi_\epsilon^{(1)}$, we have

$$T = \langle\chi_\epsilon\psi_\epsilon^{(1)}|\psi_\epsilon\rangle = \langle\psi_\epsilon^{(1)}|\chi_\epsilon\psi_\epsilon\rangle. \tag{4.9}$$

By the estimates above, $\psi_\epsilon^{(1)} = \mathcal{O}(\epsilon^p)$ for some p, so it suffices to prove that $\chi_\epsilon\psi_\epsilon$ tends rapidly to zero.

Let N be arbitrary and write

$$\chi_\epsilon \psi_\epsilon = \left(\chi_\epsilon \langle x\rangle^{-N}\right) \left[\langle x\rangle^N s \langle x\rangle^{-N} v_\epsilon\right]^{m-1} (\langle x\rangle^N \phi_0). \tag{4.10}$$

The first factor is $\mathcal{O}(\epsilon^{N\alpha})$, while the rest is $\mathcal{O}(\epsilon^p)$ for some p. Since N is arbitrary, this completes the proof. □

This means that to all orders of ϵ, $E_n(\epsilon)$ is given by the perturbation problem

$$h_\epsilon = h_0 + v_\epsilon. \tag{4.11}$$

Now, by construction,

$$\begin{aligned} v_\epsilon(x) &= Y_\epsilon(x)[\epsilon^{-2} v(\epsilon x) - x^2] \\ &= Y_\epsilon(x)[\epsilon a_1 x^3 + \cdots + \epsilon^N a_N x^{N+2} + R_N(x,\epsilon)] \end{aligned} \tag{4.12}$$

where $Y_\epsilon(x) = Y(\epsilon^\alpha x) = u_{11}^2(\epsilon^\alpha x)$ is unity for $|x| \leqslant \epsilon^{-\alpha}$ and vanishes for $|x| \geqslant 2\epsilon^{-\alpha}$. By equation (2.9)

$$R_N(x,\epsilon) = \mathcal{O}\left(\epsilon^{N+1-\alpha(N+3)}\right). \tag{4.13}$$

If we choose, as we may, α small, depending on N, then

$$R_N(x,\epsilon) = \mathcal{O}(\epsilon^N)$$

so that it may be dropped to order N.

Use equation (4.2) again, this time for the problem (4.11). Expand and collect terms, treating $Y_\epsilon(x)$ formally as 1, to obtain a sum of products of factors like

$$T = \langle \phi_0 | x_\epsilon^{p_1} s x_\epsilon^{p_2} s \cdots x_\epsilon^{p_r} | \phi_0 \rangle \tag{4.14}$$

where $x_\epsilon^p = Y_\epsilon(x) x^p$. If x_ϵ^p is replaced by x^p, these are exactly the coefficients for the formal problem (1.5), so it remains for us to show that this replacement in T yields a term which differs from T to arbitrarily high order.

Another way to say this is that if Y_ϵ is replaced by $\tilde{Y}_\epsilon = 1 - Y_\epsilon$ in T, the result is $\mathcal{O}(\epsilon^N)$.

Let $S_k = \langle x\rangle^k S \langle x\rangle^{-k}$. Suppose $x^{p_\ell} Y_\epsilon$ is replaced by $x^{p_\ell}\tilde{Y}_\epsilon$ in T to give $\tilde{T}$. We have

$$\tilde{T} = \langle \tilde{\phi}_\epsilon | \psi_\epsilon \rangle \tag{4.15}$$

where

$$\tilde{\psi}_\epsilon = \tilde{x}^{p_\ell} \tilde{Y}_\epsilon x_\epsilon^{p_{\ell-1}} \cdots x_\epsilon^{p_1} \phi_0 \tag{4.16}$$

and

$$\psi_\epsilon = S x^{p_{\ell+1}} S \cdots x^{p_r} \phi_0. \tag{4.17}$$

Write

$$\begin{aligned} \tilde{\psi}_\epsilon = {} & \left(\tilde{Y}_\epsilon \langle x\rangle^{-N}\right) \left(x_\epsilon^{p_\ell} \langle x\rangle^{-p_\ell}\right) S_{N+p_\ell} \left(x_\epsilon^{p_{\ell-1}} \langle x\rangle^{-p_{\ell-1}}\right) S_{N+p_\ell+p_{\ell-1}} \cdots x_\epsilon^{p_r} \langle x\rangle^{-p_r} \\ & \cdots \langle x\rangle^{N+p_1+\cdots+p_r} \phi_0. \end{aligned} \tag{4.18}$$

Now $\tilde{Y}_\epsilon \langle x\rangle^{-N} = \mathcal{O}(\epsilon^{\alpha N})$, while the remaining factors are bounded. A similar argument shows that ψ_ϵ is bounded. Thus

$$\tilde{T} = \mathcal{O}(\epsilon^{\alpha N}).$$

Since N is arbitrary, this proves the result, since the same argument works if some of the x_ϵ's are replaced by x's. □

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