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Resonances In a Box

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Abstract. We investigate a numerical method for studying resonances in quantum mechanics. We prove rigorously that this method yields accurate approximations to resonance energies and widths for shape resonances in the semiclassical limit.

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1. Introduction

In this paper we rigorously analyze the validity of a numerical technique for studying resonances in quantum mechanics. The technique is called, "A spherical box approach to resonances," by its inventors, Maier *et al* [8]. We prove that the technique yields correct energies and lifetimes for shape resonances in the semiclassical limit.

The technique is an "L^2 method," in contrast to time–independent scattering theory methods, such as the calculation of phase shifts near energies where a resonance is expected. These L^2 methods are surveyed, *e.g.* , in [6].

The basic physical idea underlying all L^2 methods is that a resonance wavefunction is a state that is concentrated mainly in the interaction region. In contrast, states associated with the rest of the continuous spectrum are not concentrated in any bounded interval. As a consequence, when the system is confined to a box that is large compared to the interaction region and the size of the box is varied, the resonance wavefunction is much less influenced than the states from the rest of the continuous spectrum. This should be visible in the spectrum, and is the basis of the technique we study.

To make this precise, we consider the Schrödinger operator

$$H := D^2 + V\,, \qquad D := \frac{\hbar}{i}\frac{d}{dx} \tag{1}$$

with a resonance producing potential V that is defined on all of $I\!R$. We restrict the system to the interval $(-\ell,\, \ell)$ with Dirichlet boundary conditions at $x = \pm\ell$, and plot the eigenvalues of the resulting operator $H(\ell)$ as a function of ℓ.

Figure 1 presents the results obtained by doing this for the potential V that is depicted in Figure 2.

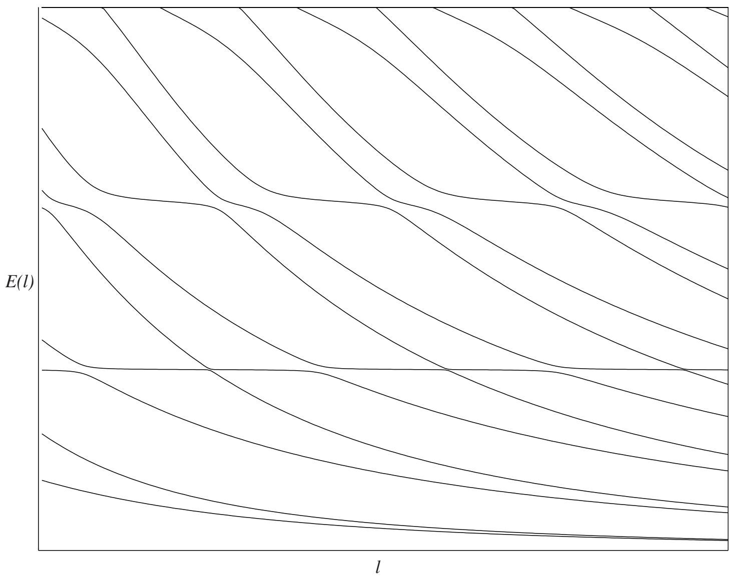

Figure 1. An example of the dependence of the eigenvalues on the box size ℓ.

In this figure, one can clearly distinguish between eigenvalues that depend strongly on ℓ and others that seem to be almost independent of ℓ. Furthermore, there are avoided eigenvalue crossings when a strongly dependent eigenvalue is close to an eigenvalue that is almost independent of ℓ. Note that in our example, eigenvalues are not expected to cross [11], since the potential has no apparent symmetry properties.

In addition to relating the almost constant eigenvalues to resonance energies, Maier *et al* [8] also relate the sizes of the gaps in the avoided crossings to the imaginary part (or width, or inverse lifetime) of the resonance. In [8], spherically symmetric potentials are treated. After the reduction to an angular momentum subspace, the particle can escape to infinity in only one way, by increasing the radial coordinate r. In the model we consider, the particle can escape toward either plus or minus infinity. Since the probablilities for going in the two directions can be different, we observe two different size gaps for each given resonance. This is obviously the case in Figure 1. For our model, the resonance width is related to the larger of the two gaps.

In this paper, we provide rigorous justification of these results in the semiclassical limit. As a first step, we adopt a standard definition of a resonance that is presented in [2, 10]. This definition identifies a resonance with a complex eigenvalue of a suitably constructed analytic family of operators obtained from the original Hamiltonian (1).

In many instances, as in the case of shape resonances, such a complex eigenvalue can be viewed as arising from the perturbation of an eigenvalue embedded in the continuous spectrum. We take this viewpoint and employ the framework of, "The Shape Resonance," [4] by Combes *et al.* We temporarily impose supplementary Dirichlet boundary conditions at points $\omega_\pm$ to decouple the interaction region from the rest of $I\!R$. This yields an unperturbed operator on all of $I\!R$ that has embedded eigenvalues whose eigenfunctions are supported in the interaction region. Removal of these Dirichlet conditions perturbs the embedded eigenvalues to produce the resonances (that are realized as complex eigenvalues of certain non-self-adjoint operators). The perturbation calculations are facilitated by the use of Krein's formula [4].

To relate the resonances of H defined on $L^2(I\!R)$ to the almost ℓ–independent eigenvalues of $H(\ell)$, we show that the techniques of [4] can also be applied in a box to study $H(\ell)$. We then employ the following strategy: For small values of $\hbar$, resonances of H are very close to embedded eigenvalues of H with supplementary Dirichlet conditions at $\omega_\pm$. For $\ell > \max\{|\omega_+|,\, |\omega_-|\}$, these embedded eigenvalues are also eigenvalues of $H(\ell)$ with supplementary Dirichlet conditions at $\omega_\pm$. For large ℓ and small $\hbar$, removal of these supplementary Dirichlet conditions perturbs these eigenvalues only slightly. Thus, the resonances of H are near eigenvalues of $H(\ell)$. These results are made precise in Theorem 2.

This approach also allows us to prove rigorously that the gap in the avoided crossing is on the order of the square root of the resonance width, in accordance with [8]. We accomplish this by relating both the gap and the resonance width to the thickness of the potential barrier as measured by the Agmon distance [1]. The relationship between resonance widths and Agmon distances is already established in [4], so we need only examine the relationship between the Agmon distances and the gaps in the avoided crossings. This is done in Theorem 3.

2. Hypothesis and Results

For simplicity, we assume the potential V to be bounded. We wish to study resonances that are produced by a single well and to avoid asymptotically degenerate eigenvalues with an exponentially small separation in $\hbar$. Furthermore, we want the bottom v_0 of the well to be above the scattering threshold. We force this situation by imposing a hypothesis that can be expressed nicely with the help of the notion of *the classical forbidden region at energy E*. This is defined as

$$J(E) := \{x \in \mathbb{R} : \; V(x) > E\}.$$

Our precise hypothesis is the following:

(H1) $V \in C^1(\mathbb{R})$ is bounded and has a local minimum v_0 at x_0, such that $\overline{J(v_0)}$ is connected, and $\limsup_{|x|\to\infty} V(x) < v_0$.

By translating the origin if necessary, we choose an interior region

$$\Omega_i := (\omega_-, \omega_+), \quad \text{with } \omega_- < 0 \text{ and } \omega_+ > 0, \text{ such that } \quad \overline{\Omega}_i \setminus \{x_0\} \subset J(v_0).$$

We define the exterior region to be $\Omega_e := \mathbb{R} \setminus \overline{\Omega}_i$, and let $\Omega_e^- = (-\infty, \omega_-)$ and $\Omega_e^+ = (\omega_+, \infty)$. We define the decoupled comparison operator H^d as having the same symbol as H, but with supplementary Dirichlet conditions at ω_- and ω_+. This operator decomposes into

$$H^d = H^i \oplus H^e \quad \text{with} \quad \mathcal{D}(H^\alpha) = \mathcal{H}_0^1 \cap \mathcal{H}^2(\Omega_\alpha), \quad \text{where} \quad \alpha \in \{i, e\}.$$

Since we want to focus on shape resonances, we impose a hypothesis that prevents resonances from being produced in the exterior region for energies near v_0. We phrase this hypothesis in terms of a non-trapping condition [3]: We say *the potential V is non-trapping in Ω_e at energy E (abbreviated E is NT)*, if the following condition is satisfied for $\alpha \in \{-, +\}$:

$$\exists S > 0, \; \forall x \in \Omega_e^\alpha \setminus J(E), \quad \frac{x - \omega_\alpha}{x}\big(2(V(x) - E) + xV'(x)\big) < -S. \tag{2}$$

We assume:

(H2) v_0 is NT.

Note that formula (2) is equivalent to the more standard virial condition

$$\exists \tilde{S} > 0, \; \forall x \in \Omega_e \setminus J(E), \quad 2(V(x) - E) + xV'(x) < -\tilde{S}.$$

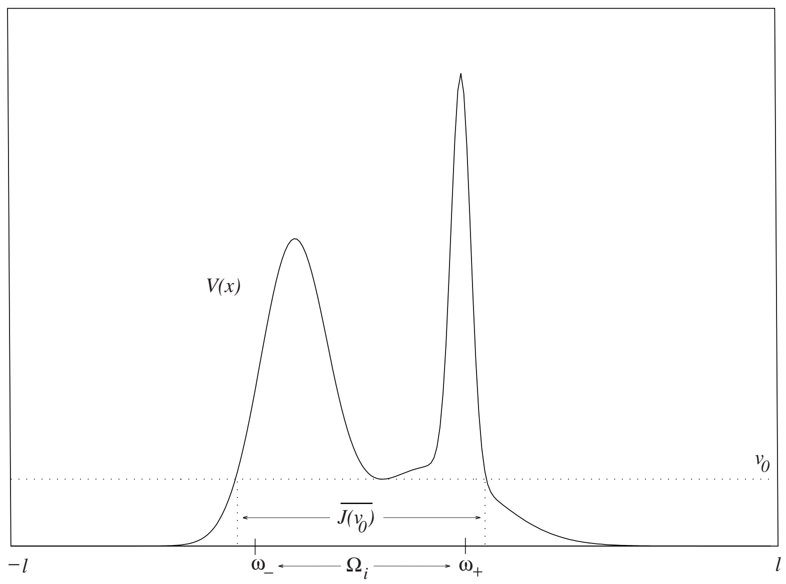

Figure 2. The potential associated to Figure 1 and relevant parameters

Furthermore (2) implies the "exterior" virial condition

$$\exists S > 0,\ \forall x \in \Omega_e^\alpha \setminus J(E), \quad \big(2(V(x) - E) + (x - \omega_\alpha)V'(x)\big) < -S,\ \alpha \in \{-, +\}\,.$$

Our third hypothesis concerns analyticity under exterior dilation. For $\theta \in I\!R$, we define

$U_\theta : L^2(I\!R) \to L^2(I\!R)$ by

$$U_\theta : \phi \mapsto \sqrt{r'_\theta}\,\phi \circ r_\theta \quad \text{where} \quad r_\theta(x) := \begin{cases} \omega_- + e^\theta(x - \omega_-), & x < \omega_- \\ x, & x \in (\omega_-, \omega_+). \\ \omega_+ + e^\theta(x - \omega_+), & x > \omega_+ \end{cases}$$

We then assume:

(H3) $V_\theta := U_\theta V U_\theta^{-1}$ defined initially for $\theta \in I\!R$, has an analytic continuation as a bounded operator to the strip $\{\theta \in C\!\!\!\!I : |\mathrm{Im}\,\theta| < \beta\}$, for some $\beta \in (0, \pi/4)$.

For $\theta \in I\!R$ we also define the operators $H_\theta := U_\theta H U_\theta^{-1}$ and $H_\theta^d := U_\theta H^d U_\theta^{-1}$. It is a straightforward calculation to obtain the associated symbol

$$U_\theta(D^2 + V)U_\theta^{-1} = {r'_\theta}^{-2} D^2 + V \circ r_\theta,$$

where
$$[{r'_\theta}^{-2} D^2 u](x) = \begin{cases} -\hbar^2 u''(x), & x \in (\omega_-, \omega_+) \\ -\hbar^2 e^{-2\theta} u''(x), & x \notin [\omega_-, \omega_+]\,. \end{cases}$$

Since U_θ is a unitary operator on $L^2(I\!R)$ for $\theta \in I\!R$, we easily compute the domains for the operators H_θ^d and H_θ, for $\theta \in I\!R$:

$$\mathcal{D}(H_\theta^d) = \mathcal{D}(H^i) \oplus \mathcal{D}(H^e),$$

$$\mathcal{D}(H_\theta) = \{u_i \oplus u_e \in \mathcal{H}^2(\Omega_i) \oplus \mathcal{H}^2(\Omega_e) : u_e(\omega_\pm) = e^{\frac{\theta}{2}} u_i(\omega_\pm),\ u'_e(\omega_\pm) = e^{\frac{3\theta}{2}} u'_i(\omega_\pm)\}. \quad (3)$$

We define the restrictions of these operators to the box $(-\ell,\,\ell)$ to be

$$\begin{aligned} H_\theta^d(\ell) &:= {r'_\theta}^{-2} D^2 + V\circ r_\theta \quad \text{on} \quad \mathcal{D}(H_\theta^d)\cap \mathcal{H}_0^1((-\ell,\ell)), \quad \text{and} \\ H_\theta(\ell) &:= {r'_\theta}^{-2} D^2 + V\circ r_\theta \quad \text{on} \quad \mathcal{D}(H_\theta)\cap \mathcal{H}_0^1((-\ell,\ell)). \end{aligned} \tag{4}$$

For $\theta=0$, $H_{\theta=0}(\ell)$ is simply the Schrödinger operator $H(\ell)$ described in the introduction that is used to produce plots, such as Figure 1.

The following lemma describes the analytic continuations of these families of operators to complex values of θ:

Lemma 1 *Hypotheses **(H1)–(H3)** imply the following two conclusions:*

(i) $\{H_\theta^d,\ |\mathrm{Im}\theta|<\beta\}$ *and* $\{H_\theta^d(\ell),\ |\mathrm{Im}\theta|<\beta\}$ *are self-adjoint analytic families of Type (A) of m-sectorial operators.*

(ii) $\{H_\theta,\ |\mathrm{Im}\theta|<\beta\}$ *and* $\{H_\theta(\ell),\ |\mathrm{Im}\theta|<\beta\}$ *are self-adjoint analytic families of operators.*

Proof: These conclusions for the families H_θ^d and H_θ are proved in [4]. The same proofs apply for the families $H_\theta^d(\ell)$ and $H_\theta(\ell)$ since the proofs in [4] make no use of the (un)boundedness of Ω_e. ∎

We next recall the Agmon distance [1], that we denote by the symbol d_E. It is the distance associated to the pseudo-metric $ds^2 := \max\{0, V(x)-E\}dx^2$. We introduce the abbreviations

$$d_{v_0}^\alpha := d_{v_0}(x_0,\,\alpha\ell),\quad \alpha\in\{-,\,+\}, \qquad \text{and} \qquad d^\star := \min\{d_{v_0}^-,\,d_{v_0}^+\}.$$

The following theorem gives precise information about the resonance on the line and the "resonance in the box." Its first conclusion follows from [4].

Theorem 2 *Assume **(H1)–(H3)** and that E^d is the n^{th} eigenvalue of H^i.*

(i) For any $\vartheta\in(0,1)$ and sufficiently small $\hbar$, there exists $\beta_0\in(0,\beta)$, such that $H_{i\beta_0}$ has a (complex) eigenvalue E close to E^d that satisfies:

$$E = E^d + \sum_{n\geq 1}\frac{t^n\sigma_n}{n!}, \quad \textit{with} \quad t = o(e^{-2\vartheta d^\star/\hbar}), \quad \textit{where} \quad \sigma_n = o(1),\ \forall n\geq 1.$$

(ii) The same is true for the operator $H_{i\beta_0}(\ell)$. Furthermore its eigenvalue is stable in the sense of Kato [7, Sec. VIII.1.4], as the box size ℓ tends to infinity. As ℓ tends to infinity, this eigenvalue converges to the corresponding eigenvalue of $H_{i\beta_0}$.

(iii) For sufficiently small $\hbar$ and those values of ℓ, for which there exist positive constants c and N, such that $\mathrm{dist}(E^d, \sigma(H^d(\ell))\setminus\{E^d\})\geq c\hbar^N$, there exists a real eigenvalue of $H(\ell)$ close to E^d that satisfies the same type of expansion as above.

Remark: (a) Note that in [4], the theorem is stated with $d^\star$ replaced by $d_{v_0}(x_0, \partial\Omega_i)$. Due to the possible choices of $\omega_\pm$, the difference between the two quantities can be made arbitrarily small and can be absorbed into ϑ. But then, how small $\hbar$ must be chosen, depends on ϑ.

(b) In the third conclusion of this theorem, one cannot expect uniform results in ℓ and $\hbar$. The eigenvalues of the exterior operator $H^e(\ell)$ have different dependence on ℓ and $\hbar$ than the eigenvalues of the interior operator H^i. The condition $\mathrm{dist}(E^d, \sigma(H^d(\ell))\setminus\{E^d\}) \geq c\hbar^N$ is technical; we cannot handle exponentially closely spaced eigenvalues. It is well known that under our hypotheses, the eigenvalues of H^i near the bottom of the well (close to v_0) cannot be spaced more closely than $\mathcal{O}(\hbar^\gamma)$. Here, the constant γ is strictly smaller than 2. Its value depends on how flat the bottom of the well is. In order to prove that eigenvalues from $H^e(\ell)$ do not cause $\mathrm{dist}(E^d, \sigma(H^d(\ell))\setminus\{E^d\}) \geq c\hbar^N$ to be violated for all ℓ, we would need an additional assumption on the decay of the potential. For example, together with dilation analyticity, it would be enough to assume that V tends to a limit at infinity like $|x|^{-\epsilon}$ for any $\epsilon > 0$.

We now turn our attention to the gaps in the avoided crossings that occur in graphs of the eigenvalues of $H(\ell)$. For this part of our analysis, we replace hypotheses **(H2)** and **(H3)** by the following:

(H4) $V \in C^3(I\!R)$. For $x \in \Omega_e \setminus \overline{J(v_0)}$, the potential obeys $V(x) < v_0$ and there exist two constants $v_\pm < v_0$, such that $V - v_\pm = \mathcal{O}(|x|^{-\epsilon})$ as x tends to $\pm\infty$. Furthermore for $n = 1, 2$, we have $V^{(n)} = \mathcal{O}(|x|^{-\epsilon-1})$ as x tends to $\pm\infty$.

This hypothesis allows us to use WKB estimates to analyze the behavior of eigenvalues of $H^e(\ell)$. We note that $H^e(\ell)$ decomposes into the direct sum of $H^e_-(\ell)$ and $H^e_+(\ell)$, where $H^e_-(\ell)$ acts on $L^2((-\ell,\, \omega_-))$ and $H^e_+(\ell)$ acts on $L^2((\omega_+,\, \ell))$.

We have the following result on the gaps:

Theorem 3 *Assume* ***(H1)*** *and* ***(H4)****. Suppose E^d is an eigenvalue of H^i and of $H^e_\alpha(\ell_0)$, but not of $H^e_{-\alpha}(\ell_0)$. Assume it satisfies $\mathrm{dist}(E^d, \sigma(H^e_{-\alpha}(\ell_0))) \geq c\hbar^N$, for some positive constants c and N and $\alpha \in \{-, +\}$. Then we have the following: For fixed values of $\hbar$ that are sufficiently small, there exists a neighborhood $\mathcal{V}(\ell_0)$ of ℓ_0, such that for all ℓ in $\mathcal{V}(\ell_0)$, $H(\ell)$ has two eigenvalues E_+ and E_- that are exponentially close to E^d. These two eigenvalues are separated by a gap that satisfies*

$$\min_{\ell \in \mathcal{V}(\ell_0)} \{|E_+ - E_-|\} = \left| \sum_{n\geq 1} \frac{(t_1+t_2)^n \sigma_n}{n!} \right|, \quad \textit{where} \quad \sigma_n = o(1),\ \forall n \geq 1.$$

In this estimate, t_1 and t_2 satisfy the following for any $\vartheta \in (0,1)$:

$$t_1 = t_2 = o(\exp(-\vartheta d^-_{v_0}/\hbar)) \quad \textit{if} \quad E^d \in \sigma(H^i) \cap \sigma(H^e_-(\ell_0))\,,$$
$$t_1 = t_2 = o(\exp(-\vartheta d^+_{v_0}/\hbar)) \quad \textit{if} \quad E^d \in \sigma(H^i) \cap \sigma(H^e_+(\ell_0))\,.$$

Remark: (a) Here, $\hbar$ does not depend on ϑ.

(b) The width of the resonance is given by the tunneling parameter t according to Theorem 2. We do not know whether the resonance is going to tunnel to the left or right, so we only obtain the estimate $t = o(\exp(-\vartheta 2d^\star/\hbar))$. In Theorem 3 we know to which side the resonance escapes, and the result is more precise. We also obtain estimates for both of the gap sizes that can occur in the avoided crossings for a given resonance. Since $d^\star = \min\{d^-_{v_0}, d^+_{v_0}\}$, Theorem 3 shows that the larger gap is of the same order as the square root of the resonance width. We again note that in [8], a radial symmetric situation is studied, so that there is only one way for the resonance to escape, and hence only one gap size.

(c) The eigenvalues of H^i are obviously independent of ℓ, but not of $\omega_\pm$. Thus, it might seem that the condition of having a double eigenvalue is crucially dependent on the choice of $\omega_\pm$. This is not case: From Theorem 2 (iii) we see that the eigenvalues of H^i vary only by an exponentially small quantity in $\hbar$ when the $\omega_\pm$ are varied. For the eigenvalues of $H^e_\pm(\ell)$, we show in Appendix B, that **(H4)** implies that eigenvalues $E \in \sigma(H^e_\alpha(\ell))$ that belong to an interval $(v_0, v_0 + \delta)$ are related to $\hbar$, ℓ, and a quantum number m by the asymptotic formula

$$E = v_\alpha + \left((m + \frac{3}{4})\frac{\pi\hbar}{\ell}\right)^2 \left(1 + \mathcal{O}(\hbar) + \mathcal{O}(\ell^{-\epsilon})\right), \quad \alpha \in \{-, +\}.$$

We thus have the following consequence: Suppose, for example, that the n-th eigenvalue E^d of H^i coincides with an eigenvalue of $H^e_+(\ell_0)$ for some choice of $\omega_\pm$, and that E^d is at least a distance of $\mathcal{O}(\hbar^N)$ from the spectrum of $H^e_-(\ell_0)$. Then for any other choice of $\omega_\pm$, there exists an ℓ in a neighborhood of ℓ_0, such that E^d is an eigenvalue of $H^e_+(\ell)$, and the distance from E^d to the spectrum of $H^e_-(\ell)$ is still at least $\mathcal{O}(\hbar^N)$.

3. The Proofs

Inspection of the proofs of [4] for Theorem 2 (i) shows that they are valid whether or not Ω_e is bounded. Furthermore, these proofs can be separated into two parts: The first is a formal algebraic part that shows the stability of the eigenvalue of H^i for the whole operator and constructs the asymptotic expansion of the perturbed eigenvalue in powers of the tunneling parameter t. It is quite simple and short. The second part is the justification of these algebraic formulas with the corresponding estimates. This part is more complicated and involves estimation of the operators involved in Krein's formula.

We present the formal algebraic part, which is needed in all of the situations treated in Theorems 2 (ii), 2 (iii), and Theorem 3. We do this in Section 3.1 in the context of Theorem 2 (iii). In Section 3.2, we treat the stability of the resonance eigenvalue of $H_{i\beta_0}(\ell)$ as the box size ℓ tends to infinity. Finally, in Section 3.3 we prove Theorem 3. In the Appendix, we recall Krein's formula and present the more technical estimates, including the WKB estimates.

We omit the estimates required to prove the existence and the series expansion of the eigenvalue of $H_{i\beta_0}(\ell)$ because they are identical to those in [4].

3.1. Stability and Tunneling Expansion for The Box

We view $H(\ell)$ as a perturbation of $H^d(\ell)$. This perturbation involves two Dirichlet conditions. It is most easily approached by way of Krein's formula, that exhibits the difference of the resolvents of $H(\ell)$ and $H^d(\ell)$ as a rank two operator.

The norm of this rank two operator is not small. However, because the Dirichlet conditions are imposed inside the classically forbidden region, its norm does not explode in proportion to the inverse of the distance from the spectrum to the spectral parameter in the resolvents. This allows us to choose the parameters in such a way that the resolvent of the resolvent of $H^d(\ell)$ is small in norm, and we can still use perturbation theory.

The tunneling expansion is based upon a Feshbach type reduction of the eigenvalue equation with respect to the unperturbed eigenprojection. This leads to an implicit equation that we solve by using the Lagrange inversion formula.

3.1.1. Stability To simplify the notation, we suppress the ℓ dependence in many of the formulas. We define

$$R^d(z) := (H^d(\ell) - z)^{-1} \quad \text{and} \quad R(z) := (H(\ell) - z)^{-1} .$$

We choose a contour Γ that lies in the resolvent set of $H^d(\ell)$ and encloses only E^d in $\sigma(H^d(\ell))$. We then choose a point z_0 in the intersection of the resolvent sets of $H(\ell)$ and $H^d(\ell)$, but outside of Γ. By using the identity

$$\left(R^d(z_0) - \frac{1}{z - z_0} \right)^{-1} = -(z - z_0) - (z - z_0)^2 R^d(z), \tag{5}$$

we obtain the following expression for the eigenprojection $P^d \equiv P^d(\ell)$ associated to E^d:

$$P^d = -\frac{1}{2\pi i} \int_\Gamma R^d(z)\, dz = -\frac{1}{2\pi i} \int_{\widetilde{\Gamma}} \left(R^d(z_0) - \widetilde{z} \right)^{-1} d\widetilde{z} \, ,$$

where $\{ \widetilde{\Gamma} := \widetilde{z} \in \mathbb{C} : \widetilde{z} = \frac{1}{z - z_0}, \, z \in \Gamma \}$. By defining

$$\pi(z_0) := (H(\ell) - z_0)^{-1} - (H^d(\ell) - z_0)^{-1} ,$$

we can formally write the eigenprojection $P \equiv P(\ell)$ associated to the perturbed eigenvalue E as

$$P = -\frac{1}{2\pi i} \int_{\widetilde{\Gamma}} \left(R^d(z_0) - \widetilde{z} \right)^{-1} \left(1 + \pi(z_0) \left(R^d(z_0) - \widetilde{z} \right)^{-1} \right)^{-1} d\widetilde{z} \, .$$

If we can choose Γ and z_0, such that $\left\| \pi(z_0) \left(R^d(z_0) - \widetilde{z} \right)^{-1} \right\| < 1$, then the inverse term in the integral for P can be computed by geometric series. Then the eigenprojection is well defined, and by standard arguments, we can deduce the stability of the eigenvalue for $H(\ell)$.

To see that we can do this, fix any $n \in \mathbb{N}$. Let

$$\Delta := \operatorname{dist}(E^d, \sigma(H^d(\ell)) \setminus \{E^d\}), \quad \text{and fix} \quad r \in [\min\{\hbar^n, \frac{1}{2}\Delta\}, \frac{1}{2}\Delta]. \tag{6}$$

Note that by hypothesis, $\Delta \geq c\hbar^N$, for some $N \in \mathbb{N}$, and that we can choose r to be as small as any power of $\hbar$.

We define $\Gamma := \{z \in \mathbb{C} : |z - E^d| = r\}$ and $z_0 = E^d + 2ir$. Then, formula (5) implies $\left(R^d(z_0) - \widetilde{z}\right)^{-1} = \mathcal{O}(r)$. Thus, the stability follows from the following proposition that we prove in Appendix A.1:

Proposition 4 $\pi(z_0) = \mathcal{O}(1)$.

3.1.2. Tunneling expansion Since we have proven the stability of the eigenvalue and constructed $P(\ell)$, we can write the eigenvalue equation as

$$R(z_0)P(\ell) = \frac{1}{E - z_0} P(\ell).$$

We perform a Feshbach type reduction to this equation, with respect to the projections P^d and $Q^d = 1 - P^d$. We define the "reduced" resolvent

$$\widehat{R}(z;\, z_0) := Q^d \left(Q^d (R(z_0) - z) Q^d\right)^{-1} Q^d.$$

It satisfies the following estimate:

Proposition 5 *For any z in the disc delimited by Γ, one has $\widehat{R}(\frac{1}{z-z_0};\, z_0) = \mathcal{O}(r)$.*

Proof: If we replace the $R(z_0)$ by $R^d(z_0)$ in the definition of $\widehat{R}(z;\, z_0)$, we obtain a trivial result. The conclusion to the proposition is obtained by applying perturbation theory to this trivial result. ■

For $(E - z_0)^{-1}$ the reduction yields the implicit equation

$$\left(\frac{1}{E - z_0} - \frac{1}{E^d - z_0}\right) P^d P = P^d \left(\pi(z_0) - \pi(z_0)\, \widehat{R}(\frac{1}{E - z_0};\, z_0)\, \pi(z_0)\right) P^d P.$$

Using properties of the trace and the factorization $\pi(z) = \hbar A^\star(\bar{z}) B(z)$, *c.f.* Appendix A.1, we obtain

$$\frac{1}{E - z_0} - \frac{1}{E^d - z_0} = \hbar \operatorname{Tr} \left(B(z_0) P^d A^\star(z_0) \Big(1 - \hbar B(z_0)\, \widehat{R}(\frac{1}{E - z_0};\, z_0)\, A^\star(\bar{z}_0)\Big)\right),$$

or equivalently

$$\frac{1}{E - z_0} - \frac{1}{E^d - z_0} = t\, s\left(\frac{1}{E - z_0}\right), \tag{7}$$

where (suppressing z_0 in A and B)

$$t := \hbar\, |\operatorname{Tr}(B P^d A^\star)| \quad \text{and} \quad s(z) := \frac{1}{t} \operatorname{Tr}\left(\hbar B P^d A^\star (1 - \hbar B \widehat{R}(z; z_0) A^\star)\right). \tag{8}$$

For any z in the disc delimited by Γ and $\tilde{z} = \frac{1}{z-z_0}$, we have the following estimate on $s(\tilde{z})$:

$$|s(\tilde{z})| \leq \|1 - \hbar B\widehat{R}(\tilde{z}; z_0)A^\star\| = 1 + \mathcal{O}(r).$$

This follows from Proposition 5 and the bound on π, *c.f.* Appendix A.1. If we can establish the estimate $t = o(e^{-2\vartheta d^\star/\hbar})$ of Theorem 2, then equation (7) can be solved with Lagrange's inversion formula [5, p.250]

$$\frac{1}{E-z_0} = \frac{1}{E^d-z_0} + \sum_{n\geq 1} \frac{t^n}{n!}\left[\frac{d^{n-1}}{dz^{n-1}}s^n\right](\frac{1}{E^d-z_0}) =: \frac{1}{E^d-z_0} + \sum_{n\geq 1}\frac{t^n}{n!}\widetilde{\sigma}_n\,.$$

Multiplying by $(E-z_0)(E^d-z_0)$ and rearranging, we obtain

$$E = E^d - (E-z_0)(E^d-z_0)\sum_{n\geq 1}\frac{t^n}{n!}\widetilde{\sigma}_n = E^d - \sum_{k\geq 1}(z_0-E^d)^{k+1}\left(\sum_{n\geq 1}\frac{t^n}{n!}\widetilde{\sigma}_n\right)^k.$$

We estimate the coefficients $\widetilde{\sigma}_n$ by using the Cauchy formula

$$\widetilde{\sigma}_n = \frac{(n-1)!}{2\pi i}\int_{\widetilde{\Gamma}} \frac{s(\widetilde{z})^n}{(\frac{1}{E^d-z_0} - \widetilde{z})^n}\,d\widetilde{z}, \quad \text{and} \quad (\frac{1}{E^d-z_0} - \widetilde{z})^{-1} = \mathcal{O}(r)\,.$$

We define $\sigma_n := (E–z_0)(E^d–z_0)\widetilde{\sigma}_n$ and easily obtain the estimate $\sigma_n = o(1)$ of Theorem 2.

3.1.3. The tunneling parameter The above calculation relies on the estimate $t = o(e^{-2\vartheta d^\star/\hbar})$. To prove this, we note that if ϕ_d denotes the eigenfunction associated to E^d, then using the definitions and estimations of Appendix A.1,

$$\begin{aligned} t &\leq \hbar\,\|B\phi_d\|\,\|A\phi_d\| \leq \hbar^2\,\|TRT^\star\|\,\|B\phi_d\|^2 \\ &= \frac{\hbar^2\,\|TRT^\star\|}{|E^d-z_0|^2}\,\|T^dD\phi_d\|^2 \leq \frac{c\hbar^3}{4r^2}\,(|\phi_d'(\omega_-)|^2 + |\phi_d'(\omega_+)|^2)\,. \end{aligned}$$

For each part of Theorem 2, we can estimate the expression $|\phi_d'(\omega_-)|^2 + |\phi_d'(\omega_+)|^2$ by the well known decay estimates of Agmon [1]. This implies the results of Theorem 2.

3.2. Stability as The Box Size Tends to Infinity

We consider the operator

$$H_\theta^D(\ell) := H_\theta(\ell) \oplus H_\theta^{ee}(\ell)\,, \tag{9}$$

where $H_\theta(\ell)$ is the operator defined in (4), and

$$H_\theta^{ee}(\ell) := e^{-2\theta}D^2 + V\circ r_\theta \quad \text{on} \quad \mathcal{H}_0^1 \cap \mathcal{H}^2(I\!R \setminus [-\ell,\ell])\,.$$

It is easy to see that $H_\theta^{ee}(\ell)$ is an analytic family of Type (A) in θ, and that we have the following resolvent estimate:

Proposition 6 *Assume **(H1)–(H3)** and let S denote the constant in the non-trapping condition **(H2)**. Let $\nu = \{z \in \mathbb{C} : |\mathrm{Re}\, z - v_0| < S/4,\ \mathrm{Im}\, z > -S/4\}$. Then*

$$\forall\, z \in \nu, \qquad \|R^{ee}_{i\beta}(z)\| \leq \frac{4}{|\beta| S}\,(1 + \mathcal{O}(\beta)).$$

Proof: $H^{ee}_{i\beta}(\ell)$ decomposes into a direct sum of operators that act on $L^2((-\infty, -\ell))$ and $L^2((\ell, \infty))$. We consider only the term associated to the interval (ℓ, ∞); analogous formulas hold for the other term. We mimic arguments of [3]. For $u \in \mathcal{H}^1_0 \cap \mathcal{H}^2((\ell, \infty))$ and any $v \in L^2((\ell, \infty))$, we have

$$\|v\|\, \|(H^{ee}_{i\beta}(\ell) - z)u\| \geq \mathrm{Re}\,((H^{ee}_{i\beta}(\ell) - z)u,\, v)\,.$$

For $\beta > 0$ we use this with $v = -ie^{-i2\beta}u$ to obtain

$$\begin{aligned}
\mathrm{Re}\,((H^{ee}_{i\beta}(\ell) - z)u, v) &= -\,\mathrm{Im}\,(e^{2i\beta}(e^{-2i\beta}D^2 + V \circ r_{i\beta} - z)u,\, u) \\
&= -\,\mathrm{Im}\,(e^{2i\beta}(V \circ r_{i\beta} - z)u,\, u) \\
&= -\,((\beta\,(2(V - \mathrm{Re}\, z) + (x - \omega_+)V' - \mathrm{Im}\, z) + \mathcal{O}(\beta^2))u,\, u) \\
&> (\beta\,(S - 2(v_0 - \mathrm{Re}\, z) + \mathrm{Im}\, z) + \mathcal{O}(\beta^2))\, \|u\|^2 \\
&> \left(\frac{\beta\, S}{4} + \mathcal{O}(\beta^2)\right) \|u\|^2\,.
\end{aligned}$$

For negative β we repeat this calculation with $v = ie^{-i2\beta}u$. This proves the proposition.

■

We now fix $\theta = i\beta_0$ as in [4]. With the definitions of z_0 and $\widetilde{\Gamma}$ as in Section 3.1, we define

$$P_{i\beta_0}(\ell) = -\frac{1}{2\pi i} \int_{\widetilde{\Gamma}} \left((H_{i\beta_0}(\ell) - z_0)^{-1} - \widetilde{z}\right)^{-1} \oplus \left((H^{ee}_{i\beta_0}(\ell) - z_0)^{-1} - \widetilde{z}\right)^{-1} d\widetilde{z}\,.$$

Here, $P_{i\beta_0}(\ell)$ projects onto the eigenspace for the eigenvalue $E \in \sigma(H_{i\beta_0}(\ell))$, but does so in the space $L^2(\mathbb{R})$. To prove stability of the eigenvalue in the generalized sense (*c.f.* Kato, [7, Sec. VIII.1.4]), we must show that $P_{i\beta_0}(\ell) \xrightarrow{s} P_{i\beta_0}$ as ℓ tends to ∞, where

$$P_{i\beta_0} = -\frac{1}{2\pi i} \int_{\widetilde{\Gamma}} \left((H_{i\beta_0} - z_0)^{-1} - \widetilde{z}\right)^{-1} d\widetilde{z}\,.$$

It is shown in [4] that for sufficiently small $\hbar$, $((H_{i\beta_0} - z_0)^{-1} - \widetilde{z})^{-1} = \mathcal{O}(r)$, uniformly on $\widetilde{\Gamma}$. The estimates of [4] are also valid for $((H_{i\beta_0}(\ell) - z_0)^{-1} - \widetilde{z})^{-1}$. So, from Proposition 6 and identity (5), we see that,

$$\left((H^D_{i\beta_0}(\ell) - z_0)^{-1} - \widetilde{z}\right)^{-1} = \mathcal{O}(r)\,,$$

uniformly on $\widetilde{\Gamma}$. Thus, we need only show that for any $u \in L^2(\mathbb{R})$,

$$\lim_{\ell \to \infty} \left\| \left((H_{i\beta_0} - z_0)^{-1} - (H^D_{i\beta_0}(\ell) - z_0)^{-1}\right) u \right\| = 0\,,$$

uniformly in $\hbar$. This is shown in Appendix A.2

3.3. Proof of Theorem 3

In the degenerate case, we must solve for two eigenvalues. So, we cannot *a priori* use the Lagrange inversion formula to solve equation (7) in the disc delimited by Γ.

However, we could use the formula if one of the solutions were known to be $\frac{1}{E^d - z_0}$. This would happen if π were a rank one operator. In that case, the spectra of H^d and H would intertwine, and as a consequence, at the crossing of two eigenvalues of H^d there would have to be an eigenvalue of H.

In our situation such a scenario can be realized by lifting the two Dirichlet conditions one after the other.

It suffices to consider the case where $E^d \in \sigma(H^i) \cap \sigma(H^e_+(\ell_0))$. In the first step, we consider the operators

$$H^d_-(\ell) := H^e_-(\ell) \oplus H^i \quad \text{and} \quad H_-(\ell) := D^2 + V \quad \text{on} \quad L^2((-\ell, \omega_+)).$$

By hypothesis, $\hbar$ is small and fixed, and H^i has the eigenvalue E^d, which for $\ell = \ell_0$ is a distance of $\mathcal{O}(\hbar^N)$ from the rest of the spectrum of $H^d_-(\ell_0)$, *i.e.* E^d is a simple, conveniently isolated eigenvalue of $H^d_-(\ell_0)$. Thus, the analog Theorem 2 (iii) is valid:

Lemma 7 *Assume the hypotheses of Theorem 3 with $E^d \in \sigma(H^i) \cap \sigma(H^e_+(\ell_0))$. Then there exists a neighborhood of $\mathcal{V}(\ell_0)$, of size $c\hbar^N$, such that for each $\ell \in \mathcal{V}(\ell_0)$, the operator $H_-(\ell)$ has an eigenvalue E_- close to E^d that satisfies the following for any $\vartheta \in (0,1)$*

$$E_- = E^d + \sum_{n\geq 1} \frac{t^n \sigma_n}{n!} \quad \textit{with} \quad t = o(e^{-2\vartheta d_{v_0}(\omega_-, x_0)/\hbar}) \quad \textit{and} \quad \sigma_n = o(1), \, \forall n \geq 1.$$

Proof: We first note that as we vary ℓ, with the restriction that $|\ell - \ell_0| \leq c\hbar^N$, E^d remains isolated from the rest of the spectrum by a distance of size $c\hbar^N$. Thus, we can prove the lemma by mimicking the proof of Theorem 2 (iii). ∎

For the second step, we note that due to the behavior of $E^e_+(\ell)$ there exists an $\ell_1 \in \mathcal{V}(\ell_0)$, such that

$$E_- = E^e_+(\ell_1).$$

We now use the intertwining of the spectra of $H_-(\ell_1) \oplus H^e_+(\ell_1)$ and $H(\ell_1)$. We obtain the following lemma by using the techniques we used for Lemma 7 and noting that the eigenfunction ϕ_d associated to E_- has the form $\phi_d = \phi_- \oplus \phi_+$, where $H_-(\ell_1)\phi_- = E_-\phi_-$ and $H^e_+(\ell_1)\phi_+ = E_-\phi_+$:

Lemma 8 *Assume **H(1)** and **(H4)** and that E_- is a double eigenvalue of $H_-(\ell_1) \oplus H^e_+(\ell_1)$ as constructed above. Then the operator $H(\ell_1)$ has two eigenvalues E_- and E_+ that satisfy*

$$E_+ = E_- + \sum_{n\geq 1} \frac{(t_1 + t_2)^n \sigma_n}{n!} \quad \textit{with} \quad \sigma_n = o(1), \ \forall n \geq 1,$$

where, for any $\vartheta \in (0,1)$,

$$t_1 = o(e^{-2\vartheta d_{v_0}(x_0,\omega_+)/\hbar}) \qquad \textit{and} \qquad t_2 = o(e^{-2\vartheta d_{v_0}(\omega_+,\ell_1)/\hbar}).$$

The last step in the proof of Theorem 3 is to note that the first two steps can be done for any admissible ω_+. The n-th eigenvalue E^d of H^i changes by only an exponentially small amount in $\hbar$ when ω_+ is varied, so it remains properly isolated from $\sigma(H^e_-(\ell_0))$. Furthermore, by the behavior of the exterior eigenvalues, there exists an ℓ_2 in a neighborhood of ℓ_0, such that the new E_- is also an eigenvalue of $H^e_+(\ell_2)$. The optimal estimate is obtained when $t_1 = t_2$, in which case we have $t_1 = t_2 = o(e^{-\vartheta d^+_{v_0}/\hbar})$.

Appendix A. Krein's Formula

Since we need Krein's formula for one and two supplementary Dirichlet boundary conditions, taken at different points depending on the situation, we wish to present the formula in a general setting. On the other hand, for simplicity, we leave out the exterior dilation. We deal with this only when necessary.

Suppose $n \geq 2$, and $-\infty \leq x_0 < x_1 < \ldots < x_n \leq \infty$ are specified. Let $\Omega := (x_0, x_n)$ and $\Omega_k := (x_{k-1}, x_k)$ for $k = 1, \ldots, n$. Let $H := D^2 + V$ be a Schrödinger operator on Ω, with self-adjoint boundary conditions at x_0 and x_n, and let H^d be the corresponding decoupled operator with supplementary Dirichlet conditions at $x_1, x_2, \ldots, x_{n-1}$. Denote their resolvents by R and R^d, respectively.

Let $z \in \rho(H) \cap \rho(H^d)$ and $u, v \in L^2(I\!R)$. Define $\hat{u} := R^d(z)u$ and $\hat{v} := R(z)^\star v$. Clearly, $\hat{u} \in \mathcal{D}(H^d)$, and thus, $\hat{u} = \oplus_{k=1}^n \hat{u}_k$ with $\hat{u}(x_k) = 0$, $k = 1, \ldots, n-1$. We have

$$\begin{aligned}
\big((R(z) - R^d(z))u, v\big) &= (u, \hat{v}) - (\hat{u}, v) \\
&= \sum_{k=1}^n (D^2\hat{u}_k, \hat{v})_{\Omega_k} - (\hat{u}_k, D^2\hat{v})_{\Omega_k} \\
&= -\hbar^2 \sum_{k=1}^n \hat{u}_k' \,\overline{\hat{v}}\Big|_{\partial\Omega_k} \\
&= \hbar^2 \sum_{k=1}^{n-1} \left(\hat{u}_{k+1}' - \hat{u}_k'\right) \overline{\hat{v}}\Big|_{x_k}.
\end{aligned}$$

We use standard Sobolev space notation and define functionals $T^j_{x_k}$ by the following relations, where $f \in \oplus_{k=1}^n \mathcal{H}^1(\Omega_k)$:

$$T^j_{x_k} : \mathcal{H}^1(\Omega_j) \longrightarrow \mathbb{C}, \quad T^j_{x_k} f := \lim_{y\to x,\, y\in\Omega_j} f(y), \quad \text{for} \quad j = k,\, k+1, \quad k = 1, \ldots, n-1.$$

If $T^k_{x_k} f = T^{k+1}_{x_k} f$ for all f, we simply write T_{x_k}. It is well known that $T^j_{x_k}$ is compact, and consequently, $(T^j_{x_k})^\star : \mathbb{C}^2 \to \mathcal{H}^{-1}(\Omega_j)$ is continuous. Furthermore, Lemma 4 of Section III of [4] shows that whenever $\chi \in C_0^\infty(I\!R)$ satisfies $\chi(x_k) = 1$ for $k = 1, \ldots, n-1$,

$$\left\|T^j_{x_k} u\right\|^2 \leq 2\hbar^{-1} \|\chi u_j\| \, \|D\chi u_j\| \leq c\hbar^{-1} \|\chi u_j\|_{\mathcal{H}^1}, \quad \text{for} \quad j = k,\, k+1. \tag{A.1}$$

Finally, we define

$$T^- := \begin{pmatrix} T^1_{x_1} \\ \vdots \\ T^{n-1}_{x_{n-1}} \end{pmatrix}, \quad T^+ := \begin{pmatrix} T^2_{x_1} \\ \vdots \\ T^n_{x_{n-1}} \end{pmatrix}, \quad T^d := -T^- \oplus T^+ \quad \text{and} \quad T := \begin{pmatrix} T_{x_1} \\ \vdots \\ T_{x_{n-1}} \end{pmatrix}.$$

With these definitions, we have the following formula,

$$\left((R(z) - R^d(z))u,\, v\right) \;=\; \hbar\left(R(z)T^\star iT^dDR^d(z)u,\, v\right),$$

where all the multiplications are understood to be matrix multiplications.

Appendix A.1. Applying Krein's Formula for Theorem 2 (iii)

In the proof of Theorem 2 (iii), we have $x_0 = -\ell$, $x_1 = -\omega_-$, $x_2 = \omega_+$, $x_3 = \ell$,

$$R^d(z) = (H^d(\ell) - z)^{-1}, \quad \text{and} \quad R(z) = (H(\ell) - z)^{-1}.$$

Following [4], we define

$$B(z) := iT^dDR^d(z) \quad \text{and} \quad A(z) := TR(z).$$

Since H is self-adjoint, we can write

$$\pi(z) = R(z) - R^d(z) = \hbar\, A^\star(\overline{z})B(z).$$

Furthermore, since $TR^d(z) = 0$, we have

$$T\pi(z) = TR(z) = A(z) = \hbar\, TR(z)T^\star B(z).$$

We combine the two formulas to obtain

$$\pi(z) = \hbar^2 B^\star(\overline{z})\, TR(z)T^\star\, B(z).$$

Proposition 4 now follows from

Proposition 9 *Let $z_0 = E^d + 2ir$. Fix any $N \in \mathbb{N}$. Then for sufficiently small $\hbar$ and any $r \in [\min\{\hbar^N, \frac{1}{2}\Delta\}, \frac{1}{2}\Delta]$,*

$$B(z_0) = \mathcal{O}(\hbar^{-1/2}) \qquad \text{and} \qquad TR(z_0)T^\star = \mathcal{O}(\hbar^{-1}).$$

Proof: The assertion on $TR(z_0)T^\star$ is proved in step 5 of the proof of Theorem III.3 of [4]. As for $B(z_0)$ we have

$$\|B(z_0)\|^2 = \|T^1_{\omega_-}DR^e(z_0)\|^2 + \|T^2_{\omega_-}DR^i(z_0)\|^2 + \|T^2_{\omega_+}DR^i(z_0)\|^2 + \|T^3_{\omega_-}DR^e(z_0)\|^2,$$

where $R^i(z_0) := (H^i - z_0)^{-1}$ and $R^e(z_0) := (H^e(\ell) - z_0)^{-1}$. Let χ be a C_0^∞ function supported around $\omega_\pm$ such that $\chi(\omega_\pm) = 1$. Using the estimate (A.1), it suffices to find a uniform bound on the expressions

$$\chi DR^i(z_0), \quad D\chi DR^i(z_0), \qquad \text{and} \qquad \chi DR^e(z_0), \quad D\chi DR^e(z_0).$$

We choose χ, such that $V(x) - v_0 \geq \varepsilon > 0$ for $x \in \operatorname{supp}\chi$. Then steps 1 and 2 of the proof of Theorem III.3 of [4] show that all theses terms are uniformly bounded. ∎

Appendix A.2. Applying Krein's Formula for Theorem 2 (ii)

Here we consider the difference of the resolvents of the operators $H_{i\beta_0}$ defined by formula (3) of the introduction and $H^D_{i\beta_0}(\ell)$ defined by formula (9). In this case, $n = 3$, $x_0 = -\infty$, $x_1 = -\ell$, $x_2 = \ell$, and $x_3 = \infty$. The difference of the resolvents is

$$R_{i\beta_0}(z_0) - R^d_{i\beta_0}(z_0) = \hbar R_{i\beta_0}(z_0) T^\star i e^{-2i\beta_0} T^d D R^d_{i\beta_0}(z_0)\,.$$

Let χ be a C_0^∞ function supported around $\pm\ell$, with $\chi(\pm\ell) = 1$. To show that $T^d D R^D_{i\beta_0}(z_0)$ and $T R_{-i\beta}(\overline{z}_0)$ are uniformly bounded operators we use the estimate (A.1). Thus, it suffices to show that $\chi D R^D_{i\beta_0}(z_0)$ and $\chi R_{-i\beta}(\overline{z}_0)$ are uniformly bounded operators from L^2 to $\mathcal{H}^1$. If that is true, then for $u \in L^2(I\!R)$, we have

$$\begin{aligned}\left\| \left(R_{i\beta_0}(z_0) - R^d_{i\beta_0}(z_0)\right) u \right\| &\le \|T R_{-i\beta}(\overline{z}_0)\| \left(|\hat{u}(-\ell)| + |\hat{u}(\ell)|\right)\\ &\le c(|\hat{u}(-\ell)| + |\hat{u}(\ell)|) \overset{\ell\to\infty}{\longrightarrow} 0\,,\end{aligned}$$

uniformly in $\hbar$, since $\hat{u} = \chi D R^D_{i\beta_0}(z_0) u \in \mathcal{H}^1(I\!R)$.

We now address the required uniform bounds. Commuting χ and D, we need only consider $\chi D R^D_{i\beta_0}(z_0)$ and $\chi D^2 R^D_{i\beta_0}(z_0)$. The expressions for $T R_{-i\beta}(\overline{z}_0)$ are analogous and can be treated the same way. The formula

$$\|\chi D R^D_{i\beta_0}(z_0)\|^2 = \mathrm{Re}\, R^D_{i\beta_0}(z_0)^\star \chi^2 \left(D^2 - 2\hbar^2 (\chi^2)''\right) R^D_{i\beta_0}(z_0)$$

shows that it is sufficient to bound $\chi D^2 R^D_{i\beta_0}(z_0)$ and $\chi R^D_{i\beta_0}(z_0)$. We have

$$\begin{aligned}\chi D^2 R^D_{i\beta_0}(z_0) &= e^{2i\beta} \chi \left(H^D_{i\beta_0} - z_0 - (V \circ r_{i\beta_0} - z_0)\right) R^D_{i\beta_0}(z_0)\\ &= e^{2i\beta}\left(1 - (V \circ r_{i\beta_0} - z_0) \chi R^D_{i\beta_0}(z_0)\right)\end{aligned}$$

For $\chi R^D_{i\beta_0}(z_0)$, we set $\pi_{i\beta_0}(z_0) := (H_{i\beta_0}(\ell) - z)^{-1} - (H^d_{i\beta_0}(\ell) - z)^{-1}$, and then write

$$\begin{aligned}\chi R^D_{i\beta_0}(z_0) &= \chi\left(R^i(z_0) \oplus (H^e_{i\beta_0}(\ell) - z_0)^{-1} + \pi_{i\beta_0}(z_0)\right) \oplus R^{ee}_{i\beta_0}(z_0)\\ &= \chi\left((H^e_{i\beta_0}(\ell) - z_0)^{-1} + \pi_{i\beta_0}(z_0)\right) \oplus R^{ee}_{i\beta_0}(z_0)\,.\end{aligned}$$

The right hand side is uniformly bounded in $\hbar$ and ℓ by Propostion 6 and Lemma II.3 and Theorem III.3 of [4], which are also valid for $(H^e_{i\beta_0}(\ell) - z_0)^{-1}$ and $\pi_{i\beta_0}(z_0)$, respectively.

Appendix B. WKB Estimates

For these estimates, we follow Olver [9, Ch. 11]. The goal is to find approximate solutions to the differential equation

$$-\hbar^2 w'' + (V - E) w = 0 \tag{B.1}$$

in Ω_e with $v_0 + \delta > E > v_0$ for some positive δ. Due to either the non-trapping condition or the explicit assumption **(H4)**, there is at most one turning point in each of the intervals (ω_+, ∞) and $(-\infty, \omega_-)$. There is exactly one, if δ is sufficiently small. We assume δ has been chosen so that this is the case.

It suffices to consider the interval (ω_+, ∞), and we denote the turning point by x_t. We define a new independent variable $\xi := s(x)$ by

$$s(x)\, s'(x)^2 = E - V(x)\,, \quad s(x_t) = 0\,, \quad s'(x_t) > 0\,.$$

By integration, we obtain

$$\xi = \operatorname{sgn}(x - x_t)\left(\frac{3}{2}\mathcal{S}(x)\right)^{2/3} \quad \text{where} \quad \mathcal{S}(x) := \int_{\min\{x,x_t\}}^{\max\{x,x_t\}} \sqrt{|V(t) - E|}\, dt\,.$$

Note that $\operatorname{sgn}(V(x) - E) = \operatorname{sgn}(x_t - x)$. It is easy to check that under our conditions, Theorem 3.1 of [9, Ch. 11] shows that equation (B.1) has two C^2 solutions w_1 and w_2 in (ω_+, ∞), such that

$$\begin{aligned} w_1(x;\hbar) &= s'(x)^{-1/2}\left(\mathrm{Bi}(-\xi/\hbar^{2/3}) + \mathcal{O}(\hbar\, \mathrm{Bi}(-\xi/\hbar^{2/3}))\right), \\ w_2(x;\hbar) &= s'(x)^{-1/2}\left(\mathrm{Ai}(-\xi/\hbar^{2/3}) + \mathcal{O}(\hbar\, \mathrm{Ai}(-\xi/\hbar^{2/3}))\right). \end{aligned} \tag{B.2}$$

Higher order approximations are also known, *c.f.* [9, Sec. 11.7].

The Dirichlet boundary conditions imply the quantization condition

$$w_1(\omega^+;\hbar) w_2(\ell;\hbar) - w_2(\omega^+;\hbar) w_1(\ell;\hbar) = 0\,.$$

Factoring the error in (B.2) in the classically forbidden region, using the asymptotic expansions of the Airy functions [9, p.392/3], and substituting all this into the quantization condition yields

$$e^{\mathcal{S}(\omega^+)/\hbar}\left(\cos(\frac{\mathcal{S}(\ell)}{\hbar} - \frac{\pi}{4}) + \mathcal{O}(\hbar)\right) + \frac{1}{2} e^{-\mathcal{S}(\omega^+)/\hbar}\left(\sin(\frac{\mathcal{S}(\ell)}{\hbar} - \frac{\pi}{4}) + \mathcal{O}(\hbar)\right) = 0\,.$$

If this equation is satisfied, then necessarily, $\cos(\frac{\mathcal{S}(\ell)}{\hbar} - \frac{\pi}{4}) = \mathcal{O}(\hbar)$. This implies $\frac{\mathcal{S}(\ell)}{\hbar} - \frac{\pi}{4} = \frac{2n+1}{2}\pi + \mathcal{O}(\hbar)$, or equivalently

$$\int_{x_t}^{\ell} \sqrt{E - V(t)}\, dt = (n + \frac{3}{4})\pi\hbar + \mathcal{O}(\hbar^2)\,.$$

Now using **(H4)**, we have

$$\begin{aligned} \int_{x_t}^{\ell} \sqrt{E - V(t)}\, dt &= \int_{x_t}^{\ell} \sqrt{E - v_+}\, dt + \int_{x_t}^{\ell} (\sqrt{E - V(t)} - \sqrt{E - v_+})\, dt \\ &= \sqrt{E - v_+}\,(\ell - x_t) + \int_{x_t}^{\ell} \frac{v_+ - V(t)}{\sqrt{E - V(t)} + \sqrt{E - v_+}}\, dt \\ &= \ell\, \sqrt{E - v_+}\,(1 + \mathcal{O}(\ell^{-\epsilon})) \end{aligned}$$

From this, it follows that

$$E = v_+ + \left(\frac{(n + 3/4)\,\pi\hbar}{\ell}\right)^2 \left(1 + \mathcal{O}(\hbar) + \mathcal{O}(\ell^{-\epsilon})\right)\,.$$

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