

RESONANCES OF A POTENTIAL WELL WITH A THICK BARRIER

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Abstract. This work is motivated by the desire to develop a method that allows for easy and accurate calculation of complex resonances of a one-dimensional Schrödinger's equation whose potential is a low-energy well surrounded by a thick barrier. The resonance is calculated as a perturbation of the bound state associated with a barrier of infinite thickness. We show that the corrector to the bound state energy is exponentially small in the barrier thickness. A simple computational strategy that exploits this smallness is devised and numerically verified to be very accurate. We also provide a study of high-frequency resonances and show how they can be approximated. Numerical examples are given to illustrate the main ideas in this work.

Key words. Resonances for Schrödinger's equation, asymptotic analysis of resonances, approximate methods for calculating resonances

AMS subject classifications. 35Pxx, 24L16, 65L15

1. Introduction. Resonances are important in the study of transient phenomena associated with the wave equation. In particular, long-time behavior of the solution of the wave equation is well described using resonances when radiation losses are small, as in the case of a potential well surrounded by a thick barrier (Fig. 1.1).

Consider the wave equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} - V(x)u, \quad (1.1)$$

$$u(x, 0) = u_0(x), \quad \frac{\partial u}{\partial t}(x, 0) = u_1(x). \quad (1.2)$$

Here $V(x)$ is a low-energy potential surrounded by a barrier, and supported in $[-L, L]$. We assume that $u_0 \in H^1([-R, R])$ and $u_1 \in L^2([-R, R])$, where $R > 0$. To solve (1.1)-(1.2), we first determine *resonances* and *quasi-modes* which are solutions to the nonlinear eigenvalue problem

$$-\psi'' + V(x)\psi = k^2\psi, \quad (1.3)$$

$$\psi' + ik\psi = 0, \quad \text{for } x = L, \quad (1.4)$$

$$\psi' - ik\psi = 0, \quad \text{for } x = -L. \quad (1.5)$$

There will be an infinity of resonances k_n and their associated quasi-modes $\psi_n(x)$. We note that $\text{Im}k_n < 0$ and assuming that the resonances are simple. Furthermore, for any $A > 0$, we can write [13]

$$u(x, t) = \sum_{\text{Im}k_n > -A} c_j e^{-ik_j t} \psi_j(x) + r_A(x, t). \quad (1.6)$$

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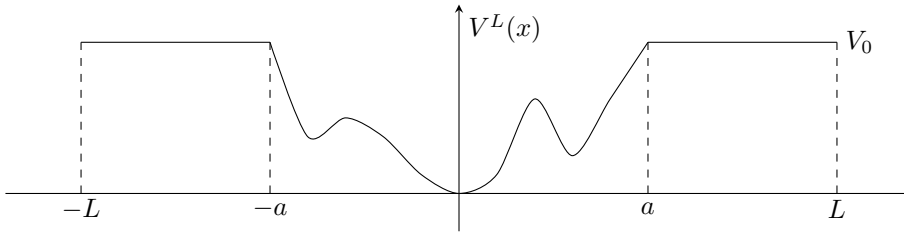


FIG. 1.1. A one-dimensional potential with a well of width a and height V_0 surrounded by a wall of thickness $(L - a)$. The potential vanishes for $|x| > L$.

The remainder, r_A , decays in a local energy sense, *i.e.* for any $K > 0$

$$\|r_A(t, \cdot)\|_{H^1([-K, K])} \leq C(R, K)e^{-At}(\|u_0\|_{H^1} + \|u_1\|_{L^2}).$$

The importance in the representation (1.6) is that for large t , the solution is well described by

$$u(x, t) \sim c_{j_0} e^{-ik_{j_0} t} \psi_{j_0}(x),$$

where j_0 is the index for which k_j has the smallest negative imaginary part, *i.e.* k_{j_0} is closest to the real axis. As we shall see below, the size of the negative imaginary part is exponentially small in the barrier thickness $L - a$ (Fig. 1.1).

We refer the reader to Bindel and Zworski [1, 13] for a discussion of theoretical, intuitive, and computational aspects of resonances with ample references to the literature. For computational approaches, there are several in literature. Wei, Majda, and Strauss [11] report an algorithm for computing acoustic resonances for a bounded scatterer by relating time samples at a point in space to a quasi-normal mode expansion and using Prony's method to extract the resonant exponents. The method of complex scaling of the spatial variable of Aguilar, Balslev, Combes and Simon [8] can be used to convert resonances into eigenvalues of a modified non-self-adjoint operator—see also Datchev and Zworski [3, 13]. An introduction to this method and its relation to method of perfectly matched layers (PML) can be found in [3]. The potential we consider in this paper can be thought of as a well in an island potential similar to that of Sec. 11 of [5], except that we send the width of the island to infinity.

In this work, we look specifically at computing resonances in certain asymptotic regimes: (1) a potential wall surrounding a well becomes infinitely thick ($L \rightarrow \infty$ with a fixed), keeping k bounded, and (2) L fixed and $\Re k \rightarrow \infty$, high frequencies. As a prototypical example, consider the one-dimensional Schrödinger equation whose potential, $V^L(x)$ shown in Figure 1.1. We will assume that $V^L(x) \geq 0$ consists of a low-energy well surrounded by a barrier of finite thickness, in this case a wall of height V_0 and width $(L - a)$. Denote by $V^\infty(x)$, the limiting potential well ($L = \infty$), for which $V^\infty(x) = V_0$ for $|x| > a$. Introduce

$$H_L = -\partial_x^2 + V^L(x) \quad \text{and} \quad H_\infty = -\partial_x^2 + V^\infty(x).$$

For finite L , H_L has no bound states. We give a short proof in Appendix A. If $a < L < \infty$, the spectrum of H_L is continuous and occupies the nonnegative real line: $\sigma(H_L) = [0, \infty)$. As explained above, a solution with spatially localized initial conditions will decay in the local energy sense as time advances. We are particularly interested in the case where the wall thickness is large and the leakage of energy is

slow. We shall quantify this leakage rate by relating it to the scattering resonance eigenvalue problem for $V^L(x)$.

As L becomes large, two classes of resonances of H_L emerge:

- (a) A finite number of low-frequency resonances, $E_{\text{res},i}(L)$, $i = 1, \dots, M$, whose real parts lie in the interval $(0, V_0) \subset \sigma(H_L)$ and which converge, as $L \uparrow$, exponentially fast to the real eigenvalues, $E_{\infty,i}$, $i = 1, \dots, M$, of H_∞ located in the real interval $(0, V_0)$, below the continuous spectrum $[V_0, \infty)$ of H_∞ . Within the wall in $[-L, L]$, these resonant modes resemble the bound states of H_∞ , being concentrated in the well in $[-a, a]$; outside of the wall, they grow at a slow exponential rate.
- (b) An infinite family of discrete scattering resonances, $E_{\text{c-res},m}(L)$, $m \geq 1$, which for each fixed $L < \infty$, lies along an unbounded curve in the lower half plane, emanating from the real point V_0 , with $\text{Re}\sqrt{E_{\text{c-res},m}} \sim \pi \frac{m}{L}$ and $\text{Im}\sqrt{E_{\text{c-res},m}} \sim -\frac{1}{L} \log\left(\frac{m}{L}\right)$, $m \gg 1$. These discrete points become increasingly clustered along this curve which approaches the continuous spectrum $[V_0, \infty)$, of the limit operator H_∞ . As L increases, these resonances become increasingly insensitive to the well in $[-a, a]$. See Regge [7], Zworski [12] and Sjöstrand-Zworski [10].

Our main results are as follows:

1. Theorem 2.2 states that for sufficiently large but finite wall thickness L , there is in a neighborhood of every discrete eigenvalue of H_∞ , a nearby scattering resonance in the lower half plane for H_L . These resonances converge to the eigenvalues of H_∞ exponentially fast as $L \rightarrow \infty$. The scattering resonances are fixed points of a complex-valued function whose iterates converge and provide a numerical scheme for computing the resonances.
2. A second approach to the construction and computation of near bound-state scattering resonances is discussed in Section 3. In this approach, the resonances are obtained by viewing H_∞ as the unperturbed operator and H_L as the perturbed operator. Such a perturbative approach is nontrivial, since $V^L(x) - V^\infty(x) = -V_0 \mathbf{1}_{[L,\infty)}(x)$ is a non-compact perturbation of V^∞ ; while the eigenvalues of $V^\infty(x)$ are real with L^2 eigenfunctions, those for H_L are complex non- L^2 (only L_{loc}^2) eigenstates. We numerically implement this perturbative approach and demonstrate, for L large, that it gives excellent agreement with very accurate direct numerical calculations of the resonances of H_L .
3. For computing high-frequency resonances, we offer in Section 4 an approximate iterative numerical scheme based on leading terms of the high- E asymptotics of solutions of the ODE. The scheme excludes terms that depend on the particular form of the well. In two simple cases, $V(x) = V_0$ (no well) and $V(x) = 0$ (square well) in $|x| < a$, we are able to compare the results of the scheme with the exact values of the resonances. In the latter case and for small L , there is appreciable imprecision in the imaginary part of the computed resonances. This error vanishes as L increases, indicating that the shape of the well has a negligible effect as, L , the width of the wall increases.

2. Near bound-state resonances. Assuming $E > 0$, let us put $E = k^2$, with $\text{Re}k > 0$. For simplicity, we consider a symmetric potential $V(-x) = V(x)$. In this case all quasi-normal modes are even or odd. We restrict our attention to even quasi-normal modes (scattering resonances) for which the pair $(\psi(x), k)$ satisfies the

eigenvalue problem:

$$H_L \psi := -\psi'' + V^L(x)\psi = k^2\psi, \quad 0 < x < \infty, \quad (2.1)$$

$$\psi(0) = 1, \quad \psi'(0) = 0, \quad (2.2)$$

$$\psi'(L) - ik\psi(L) = 0, \quad (2.3)$$

in which the prime indicates differentiation with respect to x . The potential is of the type illustrated in Figure 1.1:

$$V^L(x) = \begin{cases} v(x) & \text{for } 0 \leq x < a \\ V_0 & \text{for } a \leq x < L \\ 0 & \text{for } x \geq L \end{cases}, \quad (2.4)$$

where $0 \leq v(x) \leq V_0$. The initial conditions (2.2) imply that $\psi(x)$ can be continued to a symmetric function on \mathbb{R} satisfying outgoing radiation conditions at $\pm\infty$. Condition (2.3) is the outgoing radiation condition. Due to the boundary condition at $x = L$, the boundary-value problem (2.1)-(2.3) is non-self-adjoint. Thus, its eigenvalues can be expected to be complex and, in fact, form a discrete subset of the open lower half plane; see Appendix B.

2.1. The resonance condition. We next derive a characterization of scattering resonance energies, k , as zeros of a function defined on a subset of \mathbb{C} . Denote by $\psi(x, k)$ the unique solution of the initial value problem (2.1)-(2.2). For $V(x) \equiv V_0$, for $a \leq x \leq L$, we will also be able to make use the explicit form of the solution in this region,

$$\psi(x) = Ae^{i\sqrt{k^2 - V_0}(x-a)} + Be^{-i\sqrt{k^2 - V_0}(x-a)}, \quad (2.5)$$

where A, B are unknown constants. For $x > L$, $V(x) = 0$, and applying the radiation boundary condition (2.3), we obtain

$$\psi(x) = Ce^{ik(x-L)}, \quad x > L, \quad (2.6)$$

where C is also unknown.

We first briefly deal with the case $L = \infty$. The condition for H_∞ that is consistent with the outgoing condition in the case $L < \infty$, is that $\psi'(a) - i\sqrt{k^2 - V_0}\psi(a) = 0$, or

$$\psi(x) = Ae^{i\sqrt{k^2 - V_0}(x-a)}, \quad x > a.$$

For $k^2 < V_0$, this condition implies decay of the solution. Since $\psi(a, k) \neq 0$ the condition for a bound state can be written as

$$\sqrt{k^2 - V_0} - \frac{\psi'(a, k)}{i\psi(a, k)} = 0. \quad (2.7)$$

Equation (2.7) has a finite number of solutions (a proof is given in Appendix C) giving rise to eigenvalues of H_∞ :

$$E_{\infty, i} = k_{\infty, i}^2 \in (0, V_0), \quad i = 1, \dots, M. \quad (2.8)$$

These eigenvalues are simple, corresponding to the zeros, k_B , of the expression in (2.7) being simple. We present a proof of this in Appendix D. For the remainder we will denote by k_B a generic bound state frequency satisfying (2.7).

For L finite, we now derive the extension of (2.7) to resonances. Continuity of ψ and ψ' at $x = a$ and (2.5) imply

$$\psi(a) = A + B, \quad \text{and} \quad \psi'(a) = i\sqrt{k^2 - V_0}(A - B).$$

Continuity of ψ and ψ' at $x = L$ implies

$$\begin{aligned} Ae^{i\sqrt{k^2 - V_0}(L-a)} + Be^{-i\sqrt{k^2 - V_0}(L-a)} &= C, \\ i\sqrt{k^2 - V_0} \left(Ae^{i\sqrt{k^2 - V_0}(L-a)} - Be^{-i\sqrt{k^2 - V_0}(L-a)} \right) &= ikC. \end{aligned}$$

Eliminating A , B , and C , we arrive at an equation for the resonance energies $E = k^2$:

$$\begin{aligned} &\left(\psi(a, k) + \frac{\psi'(a, k)}{i\sqrt{k^2 - V_0}} \right) \left(1 - \frac{\sqrt{k^2 - V_0}}{k} \right) e^{i\sqrt{k^2 - V_0}(L-a)} \\ &+ \left(\psi(a, k) - \frac{\psi'(a, k)}{i\sqrt{k^2 - V_0}} \right) \left(1 + \frac{\sqrt{k^2 - V_0}}{k} \right) e^{-i\sqrt{k^2 - V_0}(L-a)} = 0. \end{aligned} \quad (2.9)$$

Multiplication of (2.9) by

$$\frac{(k\sqrt{k^2 - V_0})e^{i\sqrt{k^2 - V_0}(L-a)}}{\psi(a, k)(k + \sqrt{k^2 - V_0})}$$

yields the equivalent equation

$$F_B(k) + g(k)e^{2i\sqrt{k^2 - V_0}(L-a)} = 0, \quad (\text{resonance condition}) \quad (2.10)$$

where

$$F_B(k) \equiv \sqrt{k^2 - V_0} - \frac{\psi'(a, k)}{i\psi(a, k)}, \quad (2.11)$$

$$g(k) \equiv \left(\sqrt{k^2 - V_0} + \frac{\psi'(a, k)}{i\psi(a, k)} \right) \frac{k - \sqrt{k^2 - V_0}}{k(k + \sqrt{k^2 - V_0})}. \quad (2.12)$$

By (2.7), the bound state energies k_B^2 of H_∞ are characterized by $F_B(k_B) = 0$, and $0 < k_B^2 < V_0$. The scattering resonance energies are solutions of the perturbed equation (2.10).

Remark 2.1 Equation (2.10) for the scattering resonance energies is equivalent to

$$\mathcal{W}(k; L) \equiv \phi_1(x, k)\partial_x\phi_2(x; k) - \phi_2(x; k)\partial_x\phi_1(x; k) = 0,$$

where $\mathcal{W}(k; L)$ is the Wronskian of the two solutions $\phi_j(x, k)$, $j = 1, 2$, satisfying $H_L\phi = k^2\phi$ with ϕ_1 satisfying the boundary condition (2.2), and ϕ_2 satisfying the boundary condition (2.3) and $\phi_2(L; k) = 1$. The Green function for $-\partial_x^2 + V - k^2$ explicitly given by variation of constants, has poles (scattering resonances) in $\text{Im}k < 0$, at the zeros of $\mathcal{W}(k; L)$.

2.2. Resonances converging to eigenvalues as $L \rightarrow \infty$. We now construct the complex scattering resonances for H_L and prove that they converge exponentially to the discrete eigenvalues $\{k_B\}$ of H_∞ as $L \rightarrow \infty$.

Write $k = k_B + \kappa$, recalling that k_B is real, and anticipate that κ is complex. From (2.10) we have

$$F_B(k_B + \kappa) + g(k_B + \kappa) \exp\{-2\sqrt{V_0 - (k_B + \kappa)^2}(L - a)\} = 0. \quad (2.13)$$

We shall seek solutions to (2.13) in the complex κ plane. These turn out to lie in the lower half plane and, for L large, exponentially close to the real zeros of $F_B(k)$.

Since $F_B(k_B) = 0$, and k_B is a simple zero of F_B , we have

$$F_B(k_B + \kappa) = \kappa \int_0^1 F'_B(k_B + \theta\kappa) d\theta \equiv \kappa f_1(k_B + \kappa). \quad (2.14)$$

$F'_B(k_B) \neq 0$ and $f_1(k_B + \kappa)$ is non-vanishing for $|\kappa|$ sufficiently small. Thus (2.13), may be rewritten as

$$\kappa = G(\kappa) := -\frac{g(k_B + \kappa)}{f_1(k_B + \kappa)} \exp\{-2\sqrt{V_0 - (k_B + \kappa)^2}(L - a)\}. \quad (2.15)$$

Theorem 2.2 *Let k_B be such that $F_B(k_B) = 0$, and thus $0 < k_B^2 < V_0$ is a bound state energy of H_∞ .*

1. *There are positive constants C , α , and L' such that, if $L > L'$, then the scattering resonance eigenvalue problem (2.1–2.3) has a solution with scattering resonance eigenvalue $k = k_B + \kappa$ and*

$$|\kappa| \leq C e^{-2\alpha(L-a)}.$$

2. *$\text{Im}\kappa < 0$ and*

$$\kappa \sim K e^{-2\sqrt{V_0 - k_B^2}L} \quad (L \rightarrow \infty) \quad (2.16)$$

with $K = -g(k_B)f_1(k_B)^{-1} \exp(2a\sqrt{V_0 - k_B^2})$, in the sense that the ratio of the two sides of the expression tends to 1.

Proof. To prove the theorem we use the following claim, proved below:

Claim: $f_1(k_B + \kappa)$ and $g(k_B + \kappa)$ are analytic in a neighborhood of $\kappa = 0$ and there exist positive constants C , α , and r such that

$$\left| \frac{g(k_B + \kappa)}{f_1(k_B + \kappa)} \right| \leq C \quad \text{and} \quad \text{Re} \sqrt{V_0 - (k_B + \kappa)^2} \geq \alpha, \quad \text{for } |\kappa| < r. \quad (2.17)$$

The theorem then is proved as follows. Let L' be such that, for $L \geq L'$,

$$C e^{-2\alpha(L-a)} < r \quad \text{and} \quad \left| \frac{dG(\kappa)}{d\kappa} \right| \leq 0.99, \quad \text{for } |\kappa| < r.$$

The bound on $\partial G/\partial \kappa$ comes from the analyticity of g/f_1 and the exponential factor in (2.15). It follows that for $|\kappa| < r$, we have

$$|G(\kappa)| \leq C e^{-2\alpha(L-a)} < r. \quad (2.18)$$

Thus G maps the disk $\{|\kappa| < r\}$ into itself. Furthermore, G is a contraction on this disk because $|G'(\kappa)| < 1$ for $|\kappa| < r$. It follows that (2.15) has a unique solution in $\{|\kappa| < r\}$, which satisfies the bound (2.18). Therefore, to complete the proof, we need only verify the above claim.

To verify the claim it suffices to show that $f_1(k_B + \kappa)$ does not vanish in some neighborhood k_B . The expression for f_1 in (2.14) suggests calculation of $F'_B(k_B)$, using that $F(k_B) = 0$. We obtain

$$\begin{aligned} \left. \frac{d}{dk} F_B(k) \right|_{k=k_B} &= \frac{d}{dk} (k + \sqrt{k^2 - V_0}) \cdot \left(\sqrt{k^2 - V_0} - \frac{\psi'(a, k)}{i\psi(a, k)} \right) \Big|_{k=k_B} \\ &\quad + (k_B + \sqrt{k_B^2 - V_0}) \cdot \frac{d}{dk} \left(\sqrt{k^2 - V_0} - \frac{\psi'(a, k)}{i\psi(a, k)} \right) \Big|_{k=k_B} \\ &= (k_B + \sqrt{k_B^2 - V_0}) \cdot \frac{d}{dk} \left(\sqrt{k^2 - V_0} - \frac{\psi'(a, k)}{i\psi(a, k)} \right) \Big|_{k=k_B} \end{aligned} \quad (2.19)$$

We now observe that $F'_B(k_B) \neq 0$. Indeed, the second factor in (2.19), is the derivative at $k = k_B$ of the function detecting bound states of H_∞ , which is non-zero (Appendix D). Thus, $F'_B(k_B) \neq 0$ and by analyticity of $F_B(k)$ near k_B and the expression for f_1 in (2.14), there exists $r > 0$, such that

$$|f_1(k_B + \kappa)| > 0 \quad \text{for } |\kappa| < r.$$

Finally, let $\kappa = \kappa_1 + i\kappa_2$ and consider

$$V_0 - (k_B + \kappa)^2 = (V_0 - k_B^2 - 2k_B\kappa_2 - \kappa_1^2 + \kappa_2^2) - 2i(k_B\kappa_2 + \kappa_1\kappa_2).$$

Since $V_0 > k_B^2$, there by perhaps taking r smaller, but still positive, we have that for $|\kappa| < r$, the real part of $(V_0 - (k_B + \kappa)^2) > 0$, and hence

$$\operatorname{Re} \sqrt{V_0 - (k_B + \kappa)^2} \geq \alpha > 0,$$

for some α . This completes the proof of the claim and therewith Part 1 of Theorem 2.2. Part 2 comes from (2.15), the fact that $\kappa \rightarrow 0$ exponentially as $L \rightarrow \infty$, and the fact that $g(k_B)$ and $f_1(k_B)$ are nonzero. That $\operatorname{Im}\kappa < 0$ is standard; see Appendix B. \square

Remark 2.3 *This result shows that for a resonance k near a bound state k_B , $k - k_B$ is exponentially small in $(L - a)$, or the thickness of the wall. The equation (2.15) suggests that for $L - a \gg 1$*

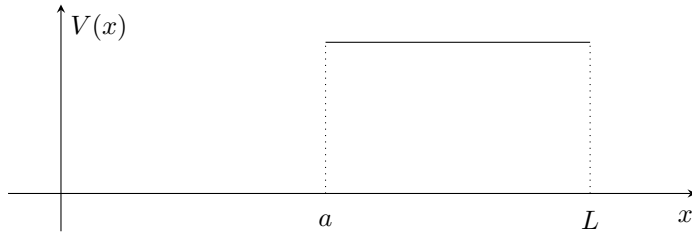
$$\kappa \approx \kappa_1 = -\frac{g(k_B)}{F'_B(k_B)} \exp\{-2\sqrt{V_0 - (k_B)^2} (L - a)\}. \quad (2.20)$$

2.3. A numerical illustration. To illustrate the conclusions of Theorem 2.2 we consider the simple example of a piecewise constant potential:

$$V_L(x) = \begin{cases} 0 & \text{for } 0 \leq x < a \\ V_0 & \text{for } a \leq x < L \\ 0 & \text{for } x \geq L \end{cases} .$$

For this case,

$$\psi(x, k) = \cos kx, \quad \text{for } 0 \leq x < a.$$

FIG. 2.1. *The potential used in the example in §3.*

The equation for the bound states (2.7) simplifies to

$$-k \tan ka = i\sqrt{k^2 - V_0},$$

which has solution(s) for $k < \sqrt{V_0}$. We denote the bound state k by k_B . The equation for resonances (2.9) becomes

$$\begin{aligned} & \left(\cos ka - \frac{k \sin ka}{i\sqrt{k^2 - V_0}} \right) \left(1 - \frac{\sqrt{k^2 - V_0}}{k} \right) e^{i\sqrt{k^2 - V_0}(L-a)} \\ & + \left(\cos ka + \frac{k \sin ka}{i\sqrt{k^2 - V_0}} \right) \left(1 + \frac{\sqrt{k^2 - V_0}}{k} \right) e^{-i\sqrt{k^2 - V_0}(L-a)} = 0. \end{aligned}$$

Let us denote the resonances by $k = k_B + \kappa$, which are complex numbers with negative imaginary parts.

As an example, we set $V_0 = 4$ and $a = 1$. We then use Newton's method to solve for k_B and k for different barrier widths L . There are a finite number of solutions k_B of $F_B(k) = 0$. The lowest energy bound state is $k_B = 1.02986652932226$. The table below shows the dependence of the resonance k , which is a perturbation of k_B , approaching k_B as $L \uparrow \infty$ by Theorem 2.2. Note the exponential decay of κ in L .

L	k
3	1.02959049042796 - 0.00051708051625i
4	1.02985760250922 - 0.00001677632024i
5	1.02986623992970 - 0.00000054394364i
6	1.02986651993964 - 0.00000001763573i

TABLE 2.1

The dependence of a resonance on the barrier thickness L . The barrier height is $V_0 = 4$ and the defect thickness is $a = 1$.

Table 2.2 shows the real and imaginary parts of $\kappa = k - k_B$. It is clear from the table that κ decays exponentially as a function of $(L - a)$. These results illustrate the estimate in Theorem 2.2. They also illustrate that, even for barriers that are not so thick ($L = 3$), the estimate of k_B is very good—the exponential decay of κ provides very quick convergence.

3. Direct perturbation for near bound-state resonances. We now take a direct approach to the construction of near-bound states as perturbations of true bound states. This leads to a computational method, explored in sections 3.2–3.3. We remark that parts of this approach may be applicable to problems in higher dimensions.

$L - a$	$\text{Re } \kappa$	$\text{Im } \kappa$
2	$-2.76038894295727 \times 10^{-4}$	$-5.17080516251752 \times 10^{-4}$
3	$-8.92681303588105 \times 10^{-6}$	$-1.67763202402731 \times 10^{-5}$
4	$-2.89392557917267 \times 10^{-7}$	$-5.43943636731303 \times 10^{-7}$
5	$-9.38261446314925 \times 10^{-9}$	$-1.76357251517556 \times 10^{-9}$

TABLE 2.2

The real and imaginary parts of κ for different L . Note the negative exponential dependence on $(L - a)$. Here, $V_0 = 4$ and $a = 1$.

3.1. Direct perturbation of bound states. For a compactly supported potential V^L , it is possible to reduce the scattering resonance problem (2.1)–(2.3) to a nonlocal (boundary integral) equation at $x = L$. We seek solutions of (2.1)–(2.3) in the form

$$\psi(x; k) = \psi_B(x) + \xi(x), \quad k = k_B + \kappa,$$

where

$$H_\infty \psi_B = k_B^2 \psi_B, \quad \psi_B \in L^2(\mathbb{R}), \quad 0 < k_B^2 < V_0. \quad (3.1)$$

Substitution of (3.1) into (2.1)–(2.3) yields the following system for $\xi(x)$ and κ :

$$-\xi'' + V^\infty(x)\xi - (k_B + \kappa)^2 \xi = (2k_B \kappa + \kappa^2) \psi_B, \quad 0 < x < L, \quad (3.2)$$

$$\xi(0) = 0, \quad \xi'(0) = 0, \quad (3.3)$$

$$\xi' - i(k_B + \kappa)\xi = -\psi_B' + i(k_B + \kappa)\psi_B, \quad x = L. \quad (3.4)$$

In obtaining (3.2) we used that $V^L(x) = V^\infty(x)$ for $0 \leq x \leq L$. One must determine κ such that (3.4) is satisfied.

Introduce $f \mapsto S_k f$ the solution operator of the inhomogeneous initial value problem:

$$\begin{aligned} -u'' + V^\infty(x)u - k^2 u &= f, \quad 0 < x < L, \\ u(0) &= 0, \quad u'(0) = 0. \end{aligned}$$

Note that for each fixed $f \in C^0([0, L])$, the mapping $k \mapsto S[k]f$ varies smoothly with k . Equation (3.2)–(3.3) can now be solved in terms of the operator $S_{k_B + \kappa}$:

$$\xi = (2k_B \kappa + \kappa^2) S_{k_B + \kappa} \psi_B. \quad (3.5)$$

Substitution of (3.5) into the outgoing radiation condition (3.4) yields a nonlocal equation for $\kappa = \kappa(L)$, the correction to k_B , due to finite barrier width. Anticipating that κ will be small, we organize the terms of this equation in ascending order in κ :

$$\begin{aligned} &\psi_B' - ik_B \psi_B + \kappa q_B(L) + \\ &+ \kappa [2k_B(\partial - ik_B) \{S_{k_B + \kappa} - S_{k_B}\} \psi_B] \\ &+ \kappa^2 [\partial S_{k_B + \kappa} \psi_B - i(3k_B + \kappa) S_{k_B + \kappa} \psi_B] = 0, \end{aligned} \quad (3.6)$$

in which

$$q_B(L) \equiv [2k_B(\partial - ik_B) S_{k_B} \psi_B - i\psi_B]. \quad (3.7)$$

In (3.6), we have used the following conventions: $\partial S_k f = \partial_x (S_k f)|_{x=L}$ and all evaluations of ψ_B , $S_{k_B} \psi_B$, and $\partial S_{k_B} \psi_B$ are at $x = L$ and $k = k_B$. By smoothness of $k \mapsto S_k f$, the terms on the second and third lines of (3.6) can be expressed, for κ in a neighborhood of zero, in the form $-\kappa \Lambda(\kappa, L)$, where Λ is smooth in κ .

Thus we can re-express (3.6) as

$$q_B(L)\kappa = ik_B \psi_B(L) - \psi_B'(L) - \kappa \Lambda(\kappa, L),$$

or

$$\kappa = \frac{ik_B \psi_B(L) - \psi_B'(L)}{q_B(L)} - \kappa \frac{\Lambda(\kappa, L)}{q_B(L)}, \quad (3.8)$$

where

$$\begin{aligned} \Lambda(\kappa, L) = & [2k_B(\partial - ik_B)(S_{k_B+\kappa} \psi_B - S_{k_B} \psi_B)] \\ & + \kappa [\partial S_{k_B+\kappa} \psi_B - i(3k_B - \kappa)S_{k_B+\kappa} \psi_B] \end{aligned} \quad (3.9)$$

We will show that (3.8) admits a solution and that it is exponentially small in L .

Notice that $V^L(x) = V_0$ for $x > a$. Therefore, from (3.1) we have

$$\psi_B(x) = \psi_B(a)e^{-\sigma_B(x-a)}, \quad x > a,$$

where $\sigma_B = \sqrt{V_0 - k_B^2} > 0$. To study the properties of $q_B(L)$, consider $u_B(x)$ satisfying

$$-u_B'' + \sigma_B^2 u_B = \psi_B(a)e^{-\sigma_B(x-a)}, \quad x > a.$$

This can be solved explicitly to give

$$u_B(x) = C_1 e^{\sigma_B(x-a)} + C_2 e^{-\sigma_B(x-a)} + \frac{\psi_B(a)}{2\sigma_B} x e^{-\sigma_B(x-a)}, \quad x > a.$$

Observe that for $x > a$, $u_B(x) = S_{k_B} \psi_B$ for some choice of C_1 and C_2 . From (3.7), it is clear that $q_B(L)$ is dominated by the positive exponential terms in $u_B(x)$ as long as $C_1 \neq 0$. Therefore, we argue that, for some $L_0 > 0$ and $C > 0$,

$$|q_B(L)| \geq C e^{\sigma_B L}, \quad (3.10)$$

for all $L > L_0$. We show that $C_1 \neq 0$ in Appendix D.

Theorem 3.1 *For some $r > 0$ (3.8) admits a solution κ with $|\kappa| < r$. Moreover, κ is exponentially small in L for sufficiently large L .*

Proof. We examine the iterative approach to solve (3.8). We write

$$\kappa_0 = \frac{ik_B \psi_B(L) - \psi_B'(L)}{q_B(L)}, \quad (3.11)$$

$$\kappa_{n+1} = \kappa_0 - \kappa_n \frac{\Lambda(\kappa_n, L)}{q_B(L)}. \quad (3.12)$$

Our aim is to show that

$$|\kappa_{n+1} - \kappa_n| \leq C_0 |\kappa_n - \kappa_{n-1}|,$$

for some $C_0 < 1$, and that the iterates remain within some small ball centered at the origin.

Since $L > a$, we can use (3.1) to obtain

$$\kappa_0 = \frac{(ik_B - \sigma_B)\psi_B(a)e^{-\sigma_B(L-a)}}{q_B(L)}.$$

This, together with (3.10) leads to

$$|\kappa_0| \leq C_0 e^{-2\sigma_B L},$$

for some C_0 independent of L . From (3.12), we have

$$|\kappa_{n+1}| \leq |\kappa_0| + |\kappa_n| \frac{|\Lambda(\kappa_n, L)|}{|q_B(L)|}.$$

Suppose

$$|\kappa_n| \leq 2C_0 e^{-2\sigma_B L}, \quad (3.13)$$

then

$$|\kappa_{n+1}| \leq C_0 e^{-2\sigma_B L} \left(1 + 2 \frac{|\Lambda(\kappa_n, L)|}{|q_B(L)|} \right), \quad (3.14)$$

and we must show that $|\Lambda(\kappa_n, L)|/|q_B(L)| < 1/2$ for sufficiently large L .

In the definition of $\Lambda(\kappa, L)$ (3.9), there are two terms. To obtain a bound for the second term, we need to consider $S_{\kappa_B + \kappa}\psi_B$. Let $u(x)$ satisfy

$$-u'' + \sigma^2 u = \psi_B(a)e^{-\sigma_B(x-a)}, \quad x > a, \quad (3.15)$$

where $\sigma = \sqrt{V_0 - k^2}$ and $k = k_B + \kappa_n$. Then $u(x) = S_k\psi_B$ and is given by

$$u(x) = C_1 e^{\sigma(x-a)} + C_2 e^{-\sigma(x-a)} + \frac{\psi_B(a)e^{-\sigma_B(x-a)}}{\sigma^2 - \sigma_B^2}, \quad x > a.$$

One can evaluate C_1 and C_2 using boundary conditions $u(a)$ and $u'(a)$. In doing so, one can see that the expression approaches $[S_{\kappa_B}\psi_B](x)$ as $\sigma \rightarrow \sigma_B$.

For $k = k_B + \kappa$, we have

$$\sigma = \sqrt{V_0 - (k_B + \kappa)^2} = \sigma_B \sqrt{1 - \frac{2k_B\kappa - \kappa^2}{\sigma_B^2}}.$$

Suppose $|\kappa| \leq 2C_0 e^{-2\sigma L}$ as in (3.13), then we can conclude that

$$\operatorname{Re} \sigma > 0, \quad \text{and} \quad |\sigma| \leq \sigma_B(1 + s|\kappa|) \quad \text{for} \quad |\kappa| < r, \quad (3.16)$$

for some $s > 0$. It is clear then that $u(x)$ is dominated by the positive exponential term for large x and therefore

$$|[S_{\kappa_B + \kappa}\psi_B](L)| = |u(L)| \leq C_3 e^{\sigma_B L} e^{s|\kappa|L}.$$

Similarly, we argue that

$$|[S_{\kappa_B + \kappa}\psi_B](L)| = |u'(L)| \leq C_4 e^{\sigma_B L} e^{s|\kappa|L}.$$

To study the first term of $\Lambda(\kappa, L)$, we need to consider $S_{k_B+\kappa}\psi_B - S_{k_B}\psi_B$. Since $S_k\psi_B$ is a smooth function of k , we can use the fundamental theorem of calculus and write

$$S_{k_B+\kappa}\psi_B - S_{k_B}\psi_B = \int_0^1 \kappa \partial_k S_{k_B+\tau\kappa}\psi_B d\tau.$$

Let $\dot{u}(x)$ satisfy the k -differentiated version of (3.15), i.e.,

$$-\dot{u}'' + \sigma^2 \dot{u} = 2k\dot{u}, \quad x > a.$$

Then $\dot{u}(x) = \partial_k S_k \psi_B$, and is given by

$$\begin{aligned} \dot{u}(x) &= D_1 e^{\sigma(x-a)} + D_2 e^{-\sigma(x-a)} \\ &- \frac{kx}{\sigma} C_1 e^{\sigma(x-a)} + \frac{kx}{\sigma} C_2 e^{-\sigma(x-a)} + \frac{2k\psi_B(a)e^{-\sigma_B(x-a)}}{\sigma^2 - \sigma_B^2}. \end{aligned}$$

One concludes that if C_1 does not vanish,

$$|\dot{u}(L)| \leq C_5 e^{\sigma_B L} e^{s|\kappa|L}.$$

The estimates for $u(L)$, $u'(L)$, and $\dot{u}(L)$ lead to the following estimate for $\Lambda(\kappa, L)$

$$|\Lambda(\kappa, L)| \leq \kappa C_6 e^{\sigma L} e^{s|\kappa|L}.$$

Considering the bound in (3.14) and using (3.10), we arrive at

$$\frac{|\Lambda(\kappa_n, L)|}{|q_B(L)|} \leq C \exp[-L(2\sigma_B + 2sC_0 e^{-2\sigma_B L})]. \quad (3.17)$$

It is apparent that we can choose L sufficiently large so that the expression above is less than $1/2$. Therefore, the iterates (3.12) starts and stays in an exponentially small (in L) ball.

To show that the iterates converge, we rewrite

$$\begin{aligned} \kappa_{n+1} - \kappa_n &= -\kappa_n \frac{\Lambda(\kappa_n, L)}{q_B(L)} + \kappa_{n-1} \frac{\Lambda(\kappa_{n-1}, L)}{q_B(L)} \\ &= -(\kappa_n - \kappa_{n-1}) \frac{\Lambda(\kappa_n, L)}{q_B(L)} - \kappa_{n-1} \frac{\Lambda(\kappa_n, L) - \Lambda(\kappa_{n-1}, L)}{q_B(L)}. \end{aligned}$$

From the above bound on $|\Lambda(\kappa_n, L)/|q_B(L)||$, we obtain

$$|\kappa_{n+1} - \kappa_n| \leq |\kappa_n - \kappa_{n-1}| \left(\frac{1}{2} + 2C_0 e^{-2\sigma_B L} \frac{|\Lambda(\kappa_n, L) - \Lambda(\kappa_{n-1}, L)|}{q_B(L)|\kappa_n - \kappa_{n-1}|} \right).$$

Convergence is guaranteed as long as $|\Lambda(\kappa_n, L) - \Lambda(\kappa_{n-1}, L)|/(|q_B(L)||\kappa_n - \kappa_{n-1}|)$ is bounded.

We omit the demonstration of such a bound since the method is very similar to that used to establish the (3.17), namely, the explicit use of the solution of the constant coefficient differential equation for $x > a$. This completes the proof. \square

3.2. A computational framework for near bound-state resonances. The perturbative approach of section 3 suggests a computational approach to near bound state resonances, based on the (3.8) and the method of successive approximations.

Step 1. Solve for a bound state eigenpair $(\psi_B, E_B = k_B^2)$ of H^∞ in (3.1), corresponding to the limiting potential.

Step 2. Solve the initial value problem

$$\begin{aligned} -u_B'' + V^\infty(x)u_B - k_B^2 u_B &= \psi_B(x), \quad 0 < x < L \\ u_B(0) &= 1, \quad u_B'(0) = 0 \end{aligned}$$

for the unique solution, and denote it by $S_{k_B}\psi_B(x)$.

Step 3: Define the correction κ_0 , based on the leading order term in (3.8) by:

$$\kappa_0 \equiv \frac{(ik_B\psi_B(L) - \psi_B'(L))}{2k_B(\partial - ik_B)S_{k_B}\psi_B|_{x=L} - i\psi_B(L)}. \quad (3.18)$$

Step 4. Approximate the resonance eigenpair with energy k near k_B by

$$k_{\text{approx}} = k_B + \kappa_0, \quad (3.19)$$

$$\psi_{\text{approx}}(x) = \psi_B(x) + 2k_B\kappa_0 S_{k_B}\psi_B. \quad (3.20)$$

In the next section, we implement this approximation scheme for a specific example.

3.3. An example perturbation calculation. We will use again the piecewise constant potential $V(x)$ in Figure 2.1 as an example. Recall that the bound state eigenfunction is given by

$$\psi_B(x) = \begin{cases} \cos(k_B x) & \text{for } 0 \leq x < a, \\ \cos(k_B a) e^{-\sqrt{V_0 - k_B^2}(x-a)} & \text{for } x > a. \end{cases}$$

To obtain κ_0 in Step 3, we solve for $\phi := 2k_B S[k_B]\psi_B$. There are two sections to the potential $V(x)$, and therefore

$$\begin{aligned} -u_B'' - k_B^2 u_B &= \cos(k_B x), \quad \text{for } 0 < x < a, \\ -u_B'' + \sigma_B^2 u_B &= \cos(k_B a) e^{-\sqrt{V_0 - k_B^2}(x-a)}, \quad \text{for } a < x < L. \end{aligned}$$

Hence, we have

$$u_B(x) = -\frac{x \sin(k_B x)}{2k_B}, \quad \text{for } 0 \leq x < a.$$

Letting $A = -a \sin(k_B a)/(2k_B)$, and $B = -(\sin k_B a + a k_B \cos(k_B a))/(2k_B)$, we have, for $a < x < L$

$$u_B(x) = u_{Bh}(x) + u_{Bp}(x),$$

where $u_{Bh}(x)$ and $u_{Bp}(x)$ are the homogeneous and particular solutions, given by

$$u_{Bh}(x) = \frac{1}{2\sigma_B} e^{-\sigma_B(x-a)}(A\sigma_B - B) + \frac{1}{2\sigma_B} e^{\sigma_B(x-a)}(A\sigma_B + B),$$

and

$$u_{Bp}(x) = -\left[\left(\frac{1}{4\sigma_B^2} + \frac{(x-a)}{2\sigma_B} \right) e^{-\sigma_B(x-a)} - \frac{1}{4\sigma_B^2} e^{\sigma_B(x-a)} \right] \cos(k_B a).$$

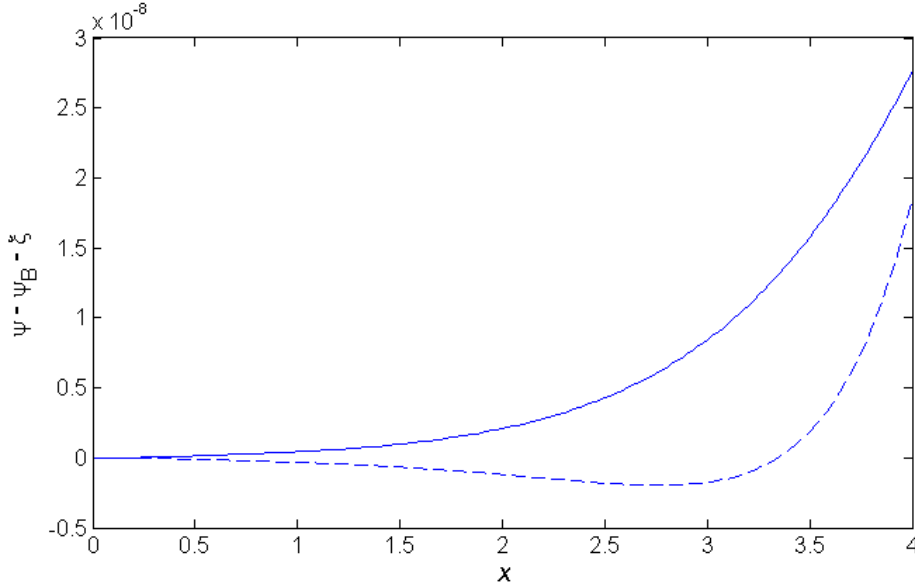


FIG. 3.1. The graph of the approximation error $\psi(x, k) - \psi_{\text{approx}}(x)$ when $L = 4$. The solid and dashed curves correspond to the real and imaginary parts of the expression.

To obtain the approximation κ_0 , one puts $u_B = S_{k_B} \psi_B$ into (3.18):

$$\kappa_0 = \frac{(ik_B + \sigma_B) \cos(k_B a) e^{-\sigma_B(L-a)}}{2k_B(u'_B(L) - ik_B u_B(L)) - i \cos(k_B a) e^{-\sigma_B(L-a)}}. \quad (3.21)$$

We compare in Table 3.1 the true resonances k with the values $k_B + \kappa$ computed by the perturbative approach for different values of L . The agreement between the resonance value and the approximated value via the perturbation approach is excellent; the approximation becomes more accurate as L increases.

L	k	$k_B + \kappa_0$
4	1.029857602509223 - 0.000016776320240i	1.029857602963758 - 0.000016776618066i
5	1.029866239929701 - 0.000000543943637i	1.029866239930306 - 0.000000543944139i
6	1.029866519939643 - 0.000000017635724i	1.029866519939644 - 0.000000017635725i

TABLE 3.1

Comparison of the true resonance values k and the approximate value obtained by perturbing the bound-state values k_B . Note that accuracy increases with barrier thickness L .

We assess the accuracy of the approximation to the quasi-normal mode. The agreement between the exact solution $\psi(x, k)$ and $\psi_{\text{approx}}(x)$ for $L = 4$ is so good that we cannot visually discern between them. As a result, we plot the real and imaginary parts of $\psi(x, \kappa) - \psi_{\text{approx}}(x)$, which we show in Figure 3.1.

4. High-frequency resonances. Having studied the properties of resonances that are near to bound states, we now turn our attention to the case where the resonance k has a large real part. The energies k^2 are far away from the bound state energies and lie in the lower half complex plane.

We will observe that, for large k and L , the solution of equations (2.1-2.3) depends negligibly on the function $v(x)$ describing the defect in the interval $[0, a]$. First, let us consider the simplest case in which $V(x) \equiv V_0$ in $[0, L]$, a potential barrier of width L without the well. In this case, the solution is $\psi(x) = \cos \sqrt{k^2 - V_0} x$, and the radiation condition $\psi'(L) - ik\psi(L) = 0$ yields

$$e^{2iL\sqrt{k^2 - V_0}} = -\frac{4k^2}{V_0} \left(1 - \frac{V_0}{2k(k + \sqrt{k^2 - V_0})}\right)^2. \quad (4.1)$$

by direct computation or by putting $\psi(x) = \cos \sqrt{k^2 - V_0} x$ into equation (2.9). Thus

$$iL\sqrt{k^2 - V_0} = \pi i(m + 1/2) + \log(k) + \log(2\sqrt{V_0}) + \log\left(1 - \frac{V_0}{2k(k + \sqrt{k^2 - V_0})}\right),$$

in which m is an integer. Using the identity $\sqrt{k^2 - V_0} = k - V_0/(k + \sqrt{k^2 - V_0})$ and setting

$$c = -\frac{1}{\pi} \log(2/\sqrt{V_0}),$$

we obtain

$$\begin{aligned} k &= \frac{\pi(m + 1/2 + ic)}{L} - \frac{i}{L} \log(k) + \frac{V_0}{k + \sqrt{k^2 - V_0}} - \frac{i}{L} \log\left(1 - \frac{V_0}{2k(k + \sqrt{k^2 - V_0})}\right) \\ &= \frac{\pi(m + 1/2 + ic)}{L} - \frac{i}{L} \log(k) + \mathcal{O}(|k|^{-1}) \quad (m \gg 1). \end{aligned} \quad (4.2)$$

It seems natural to drop the $\mathcal{O}(|k|^{-1})$ term and use the remaining terms as an approximation for an iterative method for computing the resonances,

$$k \approx \frac{\pi(m + 1/2 + ic)}{L} - \frac{i}{L} \log k. \quad (4.3)$$

Then setting

$$k = \frac{\pi(m + 1/2 + ic)}{L} (1 + \kappa) \quad (4.4)$$

leads to

$$\kappa = f_{\text{ap}}(\kappa) := \frac{-i}{\pi(m + 1/2 + ic)} \left(\log\left(\frac{\pi(m + 1/2 + ic)}{L}\right) + \log(1 + \kappa) \right) \quad (4.5)$$

and hence to the iterative scheme with initial approximation $\kappa_0 = 0$ and recursion rule

$$\kappa_{n+1} = f_{\text{ap}}(\kappa_n). \quad (4.6)$$

Observe that f_{ap} does not depend on the defect in the interval $[0, a]$. Numerical calculations with $v(x) = V_0$ show that fixed points of f_{ap} are altered only negligibly if the full formula in (4.2) is used, as demonstrated in Table 4.3.

If we put $v(x) = 0$ in $[0, a]$, $a < L$, corresponding to a square well, the resonance equation becomes

$$\begin{aligned}
e^{2i\sqrt{k^2-V_0}(L-a)} &= -\frac{1 + \frac{\sqrt{k^2-V_0}}{k} \cos ka - i\frac{k}{\sqrt{k^2-V_0}} \sin ka}{1 - \frac{\sqrt{k^2-V_0}}{k} \cos ka + i\frac{k}{\sqrt{k^2-V_0}} \sin ka} \\
&= -\frac{k^2}{V_0} \left(1 + \frac{\sqrt{k^2-V_0}}{k}\right)^2 \frac{\cos ka - i\frac{k}{\sqrt{k^2-V_0}} \sin ka}{\cos ka + i\frac{k}{\sqrt{k^2-V_0}} \sin ka} \\
&= -\frac{4k^2}{V_0} \left(1 - \frac{V_0}{2k(k + \sqrt{k^2-V_0})}\right)^2 \frac{e^{-ika} - \frac{iV_0}{k^2-V_0+k\sqrt{k^2-V_0}} \sin ka}{e^{ika} + \frac{iV_0}{k^2-V_0+k\sqrt{k^2-V_0}} \sin ka}.
\end{aligned} \tag{4.7}$$

Comparing this equation to (4.1), we see that for $\text{Im } k < 0$, which is the case for the resonances we seek, there is an additional factor on the left decaying like $e^{-2|\text{Im } k|a}$. This factor is not obviously compensated on the right because of the exponentially increasing behavior of $\sin ka$. When L is not too big, numerical computations show that the approximation (4.3) produces k -values whose imaginary parts do in fact deviate appreciably from those of the true resonances. We calculate the exact resonances by a recursion rule $\kappa_{n+1} = f_{\text{ex}}(\kappa_n)$ obtained from (4.7) without making any approximations. As L increases, the approximate results become very good, as demonstrated in Table 4.3. Thus we see that, for small L , the imaginary parts of the resonances are sensitive to the form of the well. The error in the imaginary part in that table for $L = 4$ even for large k is likely due at least in part to the discontinuity of the square-well potential. A full analysis of the accuracy of the iteration (4.6) is evidently subtle and delicate, and it is not our intention to carry this analysis out here.

Remark 4.1 *It is tempting to examine the WKB solution of (2.1)-(2.2) with a general potential $v(x)$ for $0 < x < a$. We found that such an approach needs to be treated with caution because of the subtlety related to an exponential factor $e^{|\text{Im } k|}$ appearing in the WKB expression. See Appendix F for more details.*

Tables 4.1 and 4.2 compare the approximation of k given by (4.4) with $\kappa = 0$ to the value obtained by setting κ equal to the limit of the sequence κ_n defined by the iteration (4.6). When $V_0 = 4$, we have $c = 0$, and the initial approximation of k is real; this is shown in Table 4.1. The term $1/2 + ic$ in f_{ap} is evidently not unimportant; it turns out that it contributes to a shift in the real parts of the computed resonances that is on the order of the spacing between the resonances k_m .

Figure 4.1 shows the computed value of k for $V_0 = 4$ and for various values of m and L . One observes that the density of resonances increases linearly with the width L of the potential wall, in accordance with theoretical results [10, 4, 9], and that the resonances lie on a curve in the lower complex half-plane that tends to the real line as $L \rightarrow \infty$, a phenomenon that is also known to occur within the spectral bands of a one-dimensional layered medium as the number of layers increases [6].

m	k	$\pi(m + 1/2 + ic)/L$	$ \kappa $	$ \kappa $ bound
55	43.5842 - 0.943732 i	43.5896	0.0216508	0.0432995
56	44.3697 - 0.948196 i	44.3750	0.0213681	0.0427344
57	45.1551 - 0.952582 i	45.1604	0.0210936	0.0421854
58	45.9406 - 0.956891 i	45.9458	0.0208268	0.0416519
59	46.7260 - 0.961128 i	46.7312	0.0205675	0.0411333
60	47.5115 - 0.965295 i	47.5166	0.0203152	0.0406287
61	48.2970 - 0.969393 i	48.3020	0.0200697	0.0401378
62	49.0824 - 0.973424 i	49.0874	0.0198307	0.0396599
63	49.8679 - 0.977392 i	49.8728	0.0195980	0.0391945
64	50.6533 - 0.981298 i	50.6582	0.0193712	0.0387410
65	51.4388 - 0.985144 i	51.4436	0.0191502	0.0382991

TABLE 4.1

The values of the quantities in equation (4.4) for barrier width $L = 4$ and height $V_0 = 4$, for which $c = 0$. The last column is the radius of D in Proposition 4.2.

m	k	$\pi(m + 1/2 + ic)/L$	$ \kappa $	$ \kappa $ bound
55	29.0569 - 0.485209 i	29.0597 + 0.0763576 i	0.0193247	0.0386485
56	29.5806 - 0.488185 i	29.5833 + 0.0763576 i	0.0190833	0.0381657
57	30.1042 - 0.491109 i	30.1069 + 0.0763576 i	0.0188485	0.0376962
58	30.6278 - 0.493982 i	30.6305 + 0.0763576 i	0.0186201	0.0372394
59	31.1515 - 0.496807 i	31.1541 + 0.0763576 i	0.0183979	0.0367949
60	31.6751 - 0.499585 i	31.6777 + 0.0763576 i	0.0181814	0.0363621
61	32.1987 - 0.502317 i	32.2013 + 0.0763576 i	0.0179707	0.0359406
62	32.7224 - 0.505005 i	32.7249 + 0.0763576 i	0.0177653	0.0355298
63	33.2460 - 0.507651 i	33.2485 + 0.0763576 i	0.0175651	0.0351294
64	33.7696 - 0.510255 i	33.7721 + 0.0763576 i	0.0173698	0.0347390
65	34.2932 - 0.512819 i	34.2957 + 0.0763576 i	0.0171794	0.0343582

TABLE 4.2

The values of the quantities in equation (4.4) for barrier width $L = 4$ and height $V_0 = 10$, for which $c \neq 0$. The last column is the radius of D in Proposition 4.2.

Proposition 4.2 establishes the convergence of the iteration (4.6) for large enough integers m . The following simple estimate is needed in the proof. Let z_1 and z_2 be complex numbers. Then

$$|\log(1 + z_1) - \log(1 + z_2)| \leq 4|z_1 - z_2|, \quad \text{for all } z_1, z_2 \in \{|z| \leq \frac{1}{2}\}. \quad (4.8)$$

Proposition 4.2 *If*

$$\frac{8}{\pi|m + 1/2 + ic|} < 1 \quad \text{and} \quad \frac{4}{\pi|m + 1/2 + ic|} \left| \log \frac{\pi(m + 1/2 + ic)}{L} \right| < 1,$$

then f_{ap} is a contraction of the disk

$$D = \left\{ \kappa : |\kappa| < \frac{2}{\pi|m + 1/2 + ic|} \left| \log \frac{\pi(m + 1/2 + ic)}{L} \right| \right\}$$

into itself and therefore D contains a unique solution κ to (4.5).

m	$\pi(m + 1/2 + ic)/L$	k_{approx}	$k_{\text{exact}}, v(x) = V_0$	$k_{\text{exact}}, v(x) = 0$
$L = 4$				
55	$43.590 + 0.0279 i$	$43.585 - 0.8600 i$	$43.674 - 0.8585 i$	$43.594 - 0.7153 i$
120	$94.641 + 0.0279 i$	$94.638 - 1.1096 i$	$94.664 - 1.1094 i$	$94.581 - 0.8873 i$
185	$145.70 + 0.0279 i$	$145.69 - 1.2175 i$	$145.71 - 1.2174 i$	$145.47 - 0.9736 i$
250	$196.74 + 0.0279 i$	$196.74 - 1.2926 i$	$196.75 - 1.2925 i$	$196.99 - 1.0343 i$
315	$247.79 + 0.0279 i$	$247.79 - 1.3503 i$	$247.80 - 1.3502 i$	$247.88 - 1.0802 i$
380	$298.84 + 0.0279 i$	$298.84 - 1.3971 i$	$298.85 - 1.3971 i$	$298.77 - 1.1176 i$
$L = 50$				
600	$37.731 + 0.0022 i$	$37.731 - 0.0704 i$	$37.797 - 0.0703 i$	$37.794 - 0.0689 i$
1500	$94.279 + 0.0022 i$	$94.279 - 0.0887 i$	$94.306 - 0.0887 i$	$94.304 - 0.0869 i$
2400	$150.83 + 0.0022 i$	$150.83 - 0.0981 i$	$150.84 - 0.0981 i$	$150.84 - 0.0962 i$
3300	$207.38 + 0.0022 i$	$207.38 - 0.1045 i$	$207.39 - 0.1045 i$	$207.39 - 0.1024 i$
4200	$263.93 + 0.0022 i$	$263.93 - 0.1093 i$	$263.94 - 0.1093 i$	$263.93 - 0.1071 i$
5100	$320.47 + 0.0022 i$	$320.47 - 0.1132 i$	$320.48 - 0.1132 i$	$320.48 - 0.1109 i$
$L = 200$				
2700	$42.419 + 0.0006 i$	$42.419 - 0.0251 i$	$42.423 - 0.0251 i$	$42.423 - 0.0246 i$
6200	$97.397 + 0.0006 i$	$97.397 - 0.0223 i$	$97.423 - 0.0223 i$	$97.423 - 0.0222 i$
9700	$152.38 + 0.0006 i$	$152.38 - 0.0246 i$	$152.39 - 0.0246 i$	$152.40 - 0.0244 i$
13,200	$207.35 + 0.0006 i$	$207.35 - 0.0261 i$	$207.37 - 0.0261 i$	$207.37 - 0.0260 i$
16,700	$262.33 + 0.0006 i$	$262.33 - 0.0273 i$	$262.34 - 0.0273 i$	$262.35 - 0.0272 i$
20,200	$317.31 + 0.0006 i$	$317.31 - 0.0282 i$	$317.32 - 0.0282 i$	$317.32 - 0.0281 i$

TABLE 4.3

A comparison of computations of resonances k_m . The first two values are $k_m = (\pi(m + 1/2 + ic)/L)(1 + \kappa)$, with $\kappa = 0$ and $\kappa = \kappa_*$, where $\kappa_* = f_{\text{ap}}(\kappa_*)$. The exact resonances k_{exact} are calculated by a recursion $\kappa_{n+1} = f_{\text{ex}}(\kappa_n)$ obtained from the resonance equations (4.1) for $v(x) = V_0$ and (4.7) for $v(x) = 0$ without making any approximations. Observe the deviation between the imaginary parts of k_{approx} and k_{exact} for $v(x) = 0$ for various values of L (barrier width) over comparable ranges of $\text{Re} k$. This deviation is significant for small L but diminishes as L increases. The values $a = 1$ (well width) and $V_0 = 5$ (barrier height) are used throughout.

Consequently, there is a unique value of k solving (4.3) exactly such that

$$\left| k - \frac{\pi(m + 1/2 + ic)}{L} \right| < \frac{2}{L} \left| \log \frac{\pi(m + 1/2 + ic)}{L} \right|.$$

Proof. . To see that f_{ap} maps D into itself, assume $\kappa \in D$ and use (4.8) and the hypotheses of the theorem to obtain

$$\begin{aligned} |f_{\text{ap}}(\kappa)| &\leq \frac{1}{\pi|m + 1/2 + ic|} \left(\left| \log \frac{\pi(m + 1/2 + ic)}{L} \right| + |\log(1 + \kappa)| \right) \\ &\leq \frac{1}{\pi|m + 1/2 + ic|} \left(\left| \log \frac{\pi(m + 1/2 + ic)}{L} \right| + 4|\kappa| \right) \\ &\leq \frac{2}{\pi|m + 1/2 + ic|} \left| \log \frac{\pi(m + 1/2 + ic)}{L} \right|, \end{aligned}$$

so that $f_{\text{ap}}(\kappa) \in D$.

To see that f_{ap} is a contraction in D , let κ_1 and κ_2 be in D and use (4.8) to

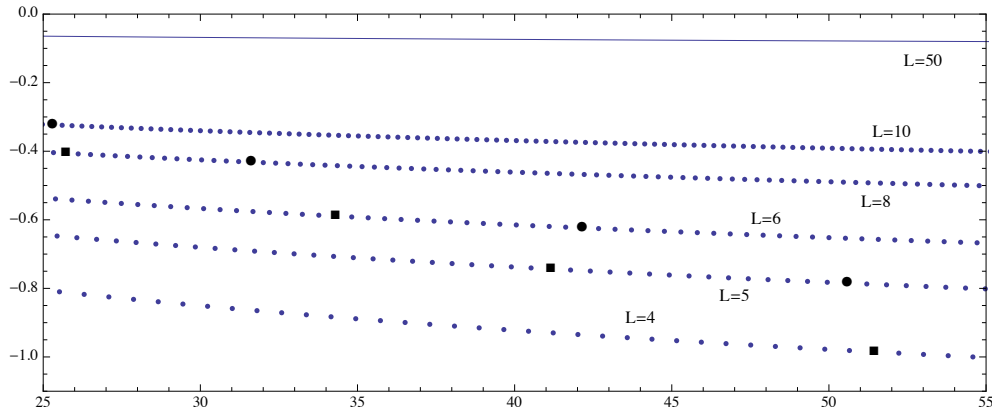


FIG. 4.1. Resonances k_m (plotted in the complex plane) computed by the approximate iterative algorithm (4.4,4.5) with barrier height $V_0 = 4$ and for various values of barrier width L . The squares show k_m for $m = 65$, and the circles for $m = 80$.

obtain

$$\begin{aligned} |f_{\text{ap}}(\kappa_1) - f_{\text{ap}}(\kappa_2)| &= \frac{1}{\pi|m + 1/2 + ic|} |\log(1 + \kappa_1) - \log(1 + \kappa_2)| \\ &\leq \frac{4}{\pi|m + 1/2 + ic|} |\kappa_1 - \kappa_2| \leq \frac{1}{2} |\kappa_1 - \kappa_2|. \end{aligned}$$

Since the solutions to (4.5), or $f(\kappa) = \kappa$, correspond to the solutions k of the resonance equation (4.3) through the relation (4.4), the unique solution of $f(\kappa) = \kappa$ in D yields a unique resonant value k satisfying the inequality claimed in the last statement of the theorem. \square

5. Discussions. Motivated by the desire to devise a computational method for fast and accurate calculation of resonances, we studied the properties of the resonances of a Schrödinger's equation with a potential well that has thick barriers. We showed that the resonances associated with such a potential are close to the defect mode eigen-frequencies of the limiting potential in which the barrier thickness goes to infinity. We established that the difference between the eigen-frequencies and the nearby resonances is exponentially small in the barrier thickness. Inspired by this finding, we developed a perturbational method for approximating resonances that are simple to implement and accurate. To complete our study, we explored the high-frequency resonances of potentials with thick barriers and obtained a picture of their behavior as the barrier thickness becomes large.

The method developed here takes advantage of the one-dimensional nature of the problem. It relies on the theory of ordinary differential equations—the structure of solutions, the role of the Wronskian, existence and uniqueness of the initial-value problem, exact solutions in the barrier, and an exact description of the outgoing condition. We expect the techniques to be applicable to higher-dimensional problems with radial symmetry. It is not clear how this work can be extended to treat general higher-dimensional problems.

A natural extension of the present work is to the study of resonances of a one-dimensional finite (truncated) periodic structure with a defect and to compare them to localized defect modes of its infinite periodic counterpart. One simply replaces

the uniform barrier with a periodic one. By the Floquet theory, the solutions of the time-independent Schrödinger equation in the barrier are periodically distorted exponential functions. Thus, if one takes the end L of the barrier to tend to infinity through a sequence $L = nd$, where d is the period and n is an integer, the calculations in this paper remain essentially unchanged. Now, instead of having bound states only below the bottom of the continuous spectrum of the infinite-barrier problem, there may be defect modes within the gaps of the spectrum created by the periodicity of the potential. Preliminary results for the case of a piecewise constant medium show that the difference between the frequencies of the defect mode of the infinite periodic medium and the resonances of its finite counterpart is exponentially small in the number of periodic layers.

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Appendix A. H_L has no bound states.

If ψ satisfies $-\psi'' + V(x)\psi = k^2\psi$ and ψ decays to 0 as $x \rightarrow \infty$, then $k^2 = -\eta^2$ for some $\eta > 0$. Multiplying the differential equation by $\bar{\psi}$ and integrating over the interval $[a, b]$ yields

$$\int_a^b (V(x) + \eta^2)|\psi|^2 = \int_a^b \psi''\bar{\psi} = - \int_a^b |\psi'|^2 + \psi'(b)\bar{\psi}(b) - \psi'(a)\bar{\psi}(a).$$

Under the assumption that $V(x) \geq 0$, taking $a \rightarrow \infty$ and $b \rightarrow -\infty$ (full-line problem) or $a \rightarrow \infty$ and $b = 0$ (half-line problem) causes the terms of evaluation at a and b to vanish, leaving $\psi(x) \equiv 0$.

Appendix B. Resonances are in the lower half plane.

Let ψ satisfy equations (2.1–2.3), with $\operatorname{Re}k > 0$. Multiplying the ODE by the complex conjugate $\bar{\psi}(x)$ and integrating by parts from 0 to x yields

$$\int_0^x |\psi'(y)|^2 dy - \psi'(x)\bar{\psi}(x) + \int_0^x V(y)|\psi(y)|^2 dy - k^2 \int_0^x |\psi(y)|^2 dy = 0.$$

Using $\psi(x) = Ce^{ikx}$ for $x > L$ from the outgoing condition (2.3), the imaginary part of the later equation is

$$\operatorname{Re}k |C|^2 e^{-2\operatorname{Im}(k)x} + \operatorname{Im}(k^2) \int_0^x |\psi|^2 = 0.$$

Recalling that $\operatorname{Re}k > 0$, we see that $k = 0 \implies C = 0 \implies \psi = 0$. If $\operatorname{Im}k > 0$, then the left-hand term tends to zero as $x \rightarrow \infty$, which implies that $\int_0^\infty |\psi|^2 = 0$, so that $\psi = 0$. We conclude that $\operatorname{Im}k < 0$.

Appendix C. Point spectrum is finite.

We give a proof of the well-known fact that the point spectrum for $H_\infty(x)$ is finite. The proof is adapted from [2, Thm. 3.3] and quantifies the number of bound states as the number of Neumann eigenvalues of the well that are less than V_0 .

The self-adjoint operator $-\partial_x^2 + V(x)$ on $(0, a)$ with homogeneous boundary conditions $\psi'(0) = 0$ and $\psi'(a) + \sqrt{V_0 - k^2}\psi(a) = 0$ has form domain equal to $H^1(a, b)$ on which its associated positive form is given by

$$A_k(\psi, \phi) := \int_0^a (\psi' \bar{\phi}' + V(x)\psi \bar{\phi}) dx + \sqrt{V_0 - k^2} \psi(a) \bar{\phi}(a).$$

A bound-state pair (k_B, ψ_B) is characterized by the equation

$$A_{k_B}(\psi_B, \phi) = k_B^2 \int_0^a \psi_B \bar{\phi} dx \quad \forall \phi \in H^1(0, a). \quad (\text{C.1})$$

The form A_k admits a sequence of eigenfunctions $\psi_j(k; x)$ associated with eigenvalues $\{\lambda_j(k)\}_{j=1}^\infty$ that tends to infinity, defined by

$$A_k(\psi_j(k), \phi) = \lambda_j(k) \int_0^a \psi_j \bar{\phi} dx \quad \forall \phi \in H^1(0, a).$$

One shows that each function $\psi_j(k; x)$ is a decreasing continuous function of k by examining its characterization by means of the Rayleigh quotient,

$$\lambda_j(k) = \min_{X_j \in S_j(H^1)} \max_{\substack{\psi \in X_j \\ \psi \neq 0}} \frac{A_k(\psi, \psi)}{\int_0^a \psi^2 dx},$$

in which $S_j(H^1)$ denotes the set of j -dimensional subspaces of H^1 . Now, each bound-state value k_B satisfies, for some j ,

$$k_B^2 = \lambda_j(k_B).$$

Since the $\lambda_j(k)$ are decreasing and continuous, the number of such relations for $k < \sqrt{V_0}$ is equal to the number of eigenvalues of $A_{\sqrt{V_0}}$ that are less than V_0 . Since the boundary term in $A_{\sqrt{V_0}}$ vanishes, this form is the Neumann one. Thus the number of bound states of $V(x)$ is equal to the number of Neumann eigenvalues of $-\partial_x^2 + V(x)$ on $(0, a)$ that are less than V_0 , and this is finite.

Appendix D. Eigenvalues of H_∞ , zeros of $F_B(k)$, are simple.

We differentiate the expression $iF_B(z)$, which is real for $k^2 < V_0$:

$$\frac{d}{dk}(iF_B(k)) = -\frac{d}{dk} \left[\sqrt{V_0 - k^2} + \left(\frac{\psi'(a, k)}{\psi(a, k)} \right) \right] \quad (\text{D.1})$$

Note that

$$\frac{\partial}{\partial k} \left(\frac{\psi'(a, k)}{\psi(a, k)} \right) = \frac{\dot{\psi}'(a, k)\psi(a, k) - \psi'(a, k)\dot{\psi}(a, k)}{\psi(a, k)^2},$$

where $\frac{\partial \psi}{\partial k} = \dot{\psi}$, and similarly for $\frac{\partial \psi'}{\partial k} = \dot{\psi}'$. Differentiating (2.1), we find that $\dot{\psi}$ satisfies

$$\begin{aligned} -\dot{\psi}'' + V(x)\dot{\psi} &= k^2\dot{\psi} + 2k\psi \quad \text{in } (0, a), \\ \dot{\psi}(0, k) &= \dot{\psi}'(0, k) = 0, \end{aligned} \quad (\text{D.2})$$

where ψ solves (2.1). Multiplying (D.2) by ψ and integrating by parts, we find

$$\dot{\psi}'(a, k)\psi(a, k) = \int_0^a \dot{\psi}'\psi' + (V(x) - k^2)\dot{\psi}\psi - 2k\psi^2 dx.$$

On the other hand, multiplying (2.1) by $\dot{\psi}$ and integrating by parts,

$$\psi'(a, k)\dot{\psi}(a, k) = \int_0^a \psi'\dot{\psi}' + (V(x) - k^2)\psi\dot{\psi} dx.$$

Combining these expressions, we obtain

$$\frac{\partial}{\partial k} \left(\frac{\psi'(a, k)}{\psi(a, k)} \right) = \frac{-2k \int_0^a \psi^2 dx}{\psi^2(a, k)}.$$

Note that when $k^2 < V_0$, all parameters in (2.1) are real, and the solution $\psi(x, k)$ is hence real. Further, because $\psi(0, k) = 1$ and ψ is continuous, we conclude $\int_0^a \psi(x, k)^2 dx > 0$. Finally, we obtain

$$\frac{d}{dk}(iF_B(k)) = k \left(\frac{1}{\sqrt{V_0 - k^2}} + \frac{2 \int_0^a \psi^2(x; k) dx}{\psi^2(a, k)} \right) \neq 0.$$

The factor of k is harmless because it disappears when taking the derivative with respect to the eigenvalue $E = k^2$ instead of with respect to k . (We have assumed that $v(x) > 0$ so that $k_B > 0$, although this is not necessary here.) Since $\psi(x, k_B)$ is exponentially decaying for $x > a$, $\psi(a, k_B) \neq 0$, and we conclude that

$$\frac{d}{dk}(iF_B(k_B)) > 0$$

at each eigenvalue k_B .

Appendix E. Proof that $C_1 \neq 0$.

Let ψ_1 and ψ_2 satisfy $-\psi'' + V(x)\psi - k^2\psi = 0$ with

$$\begin{bmatrix} \psi_1(0) & \psi_2(0) \\ \psi_1'(0) & \psi_2'(0) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

so that $W[\psi_1, \psi_2](x) = \psi_1(x)\psi_2'(x) - \psi_2(x)\psi_1'(x) \equiv 1$.

When the solution ψ_1 satisfies the bound-state condition at $x = a$, it is equal to the bound state ψ_B in $[0, a]$:

$$\psi_B'(a) + \sigma\psi_B(a) = 0 \quad (\psi_B = \psi_1)$$

Consider the initial-value problem

$$\begin{cases} -u'' + V(x)u - k^2u = \psi_B(x), \\ u(0) = u'(0) = 0. \end{cases}$$

By the standard method of variation of parameters, the solution can be written as a variable-coefficient combination of ψ_B and ψ_2 chosen such that

$$\begin{cases} u(x) = \gamma_1(x)\psi_B(x) + \gamma_2(x)\psi_2(x), \\ u'(x) = \gamma_1(x)\psi_B'(x) + \gamma_2(x)\psi_2'(x), \end{cases} \quad (\text{E.1})$$

in which

$$\gamma_1(x) = \int_0^x \psi_B(y)\psi_2(y) dy, \quad \gamma_2(x) = - \int_0^x \psi_B(y)^2 dy. \quad (\text{E.2})$$

For $x \geq a$, the bound state (for $L = \infty$) is $\psi_B(x) = \psi_B(a)e^{-\sigma(x-a)}$, and the equation $-u'' + V(x)u - k^2u = \psi_B(x)$ becomes

$$-u'' + \sigma^2u = \psi_B(a)e^{-\sigma(x-a)}.$$

The general solution of this equation is

$$u(x) = C_1e^{\sigma(x-a)} + \left(C_2 + \frac{\psi_B(a)}{2\sigma}x\right)e^{-\sigma(x-a)}$$

Let us obtain C_1 in terms of $u(a)$ and $u'(a)$:

$$\begin{aligned} u(a) &= C_1 + C_2 + \frac{\psi_B(a)}{2\sigma}a, \\ u'(a) &= \sigma C_1 - \sigma C_2 + \frac{\psi_B(a)}{2\sigma}(1 - \sigma a), \end{aligned}$$

which yields

$$2\sigma C_1 = u'(a) + \sigma u(a) - \frac{\psi_B(a)}{2\sigma}.$$

We will show that this is nonzero. Using (E.1) together with the bound-state condition $\psi'_B(a) + \sigma\psi_B(a) = 0$, we obtain

$$2\sigma C_1 = \gamma_2(a)(\psi'_2(a) + \sigma\psi_2(a)) - \frac{\psi_B(a)}{2\sigma}.$$

The condition $C_1 = 0$ together with the bound-state condition give the pair

$$\begin{cases} \gamma_2(a)(\psi'_2(a) + \sigma\psi_2(a)) - \frac{\psi_B(a)}{2\sigma} = 0, \\ \psi'_B(a) + \sigma\psi_B(a) = 0. \end{cases}$$

Multiplying the first of these equations by $\psi_B(a)$ and the second by $\gamma_2(a)\psi_2(a)$ and subtracting yields

$$\gamma_2(a)(\psi_B(a)\psi'_2(a) - \psi_2(a)\psi'_B(a)) - \frac{\psi_B^2(a)}{2\sigma} = 0.$$

Using the fact that the $W[\psi_B, \psi_2](x) \equiv 1$ and the expression (E.2) for γ_2 , this equality becomes

$$-\int_0^a \psi_B(y)^2 dy - \frac{\psi_B^2(a)}{2\sigma} = 0,$$

which is untenable. This means that C_1 must be nonzero.

Appendix F. WKB analysis.

The formal WKB solution of the initial-value problem (2.1,2.2) is

$$\psi_{\text{WKB}}(x) = \cos\left(kx - \frac{1}{2k} \int_0^x V(y) dy\right) + \mathcal{O}(|k|^{-2})e^{|\text{Im } k|x}, \quad (\text{F.1})$$

in which the $\mathcal{O}(|k|^{-2})$ factor is uniform in x . This can be obtained rigorously as follows. The solution ψ satisfies the integral equation $\psi = \cos(k\cdot) + k^{-1}T\psi$, where the operator T is defined by

$$(T\phi)(x) := \int_0^x V(y)\phi(y) \sin(k(x-y)) dy.$$

This operator is bounded in the weighted uniform norm $\|\phi\|_{|\text{Im } k|} = \sup_{0 < x < L} |\phi(x)e^{-|\text{Im } k|x}|$. Thus, for large enough k , we have an explicit expansion of the solution,

$$\psi = (1 + k^{-1}T + k^{-2}T^2 + \dots) \cos(k\cdot), \quad (\text{F.2})$$

which yields $\psi = \psi_{\text{WKB}}$.

The radiation condition (2.3) applied to the WKB solution,

$$ik \cos\left(kx - \frac{1}{2k} \int_0^x V(y) dy\right) + \left(k - \frac{V_0}{2k}\right) \sin\left(kx - \frac{1}{2k} \int_0^x V(y) dy\right) = 0,$$

yields the resonance equation

$$\exp\left(2ikL - \frac{i}{k} \int_0^L V(y) dy\right) = 1 - \frac{4k^2}{V_0}. \quad (\text{F.3})$$

Excluding a term of order $\mathcal{O}(|k|^{-2})$ that comes from the constant “1”, we obtain

$$k = \frac{\pi(m + 1/2 + ic)}{L} - \frac{i}{L} \log k + \frac{1}{2kL} \int_0^L V(y) dy. \quad (\text{F.4})$$

Observe that, if $V(x) \equiv V_0$, then equation (4.2) is recovered up to order $\mathcal{O}(|k|^{-1})$. As we have learned from the case $V(x) = 0$ for $0 < x < a$, in which solutions of this equation approximate the resonances well only for large enough L , the WKB result should be treated with caution. This subtlety comes from the exponential factor $e^{i\text{Im} k|x}$ in the asymptotics.