A Transparent View on Resonances

Resonances, Transparencies, and their relation in 1D quantum scattering

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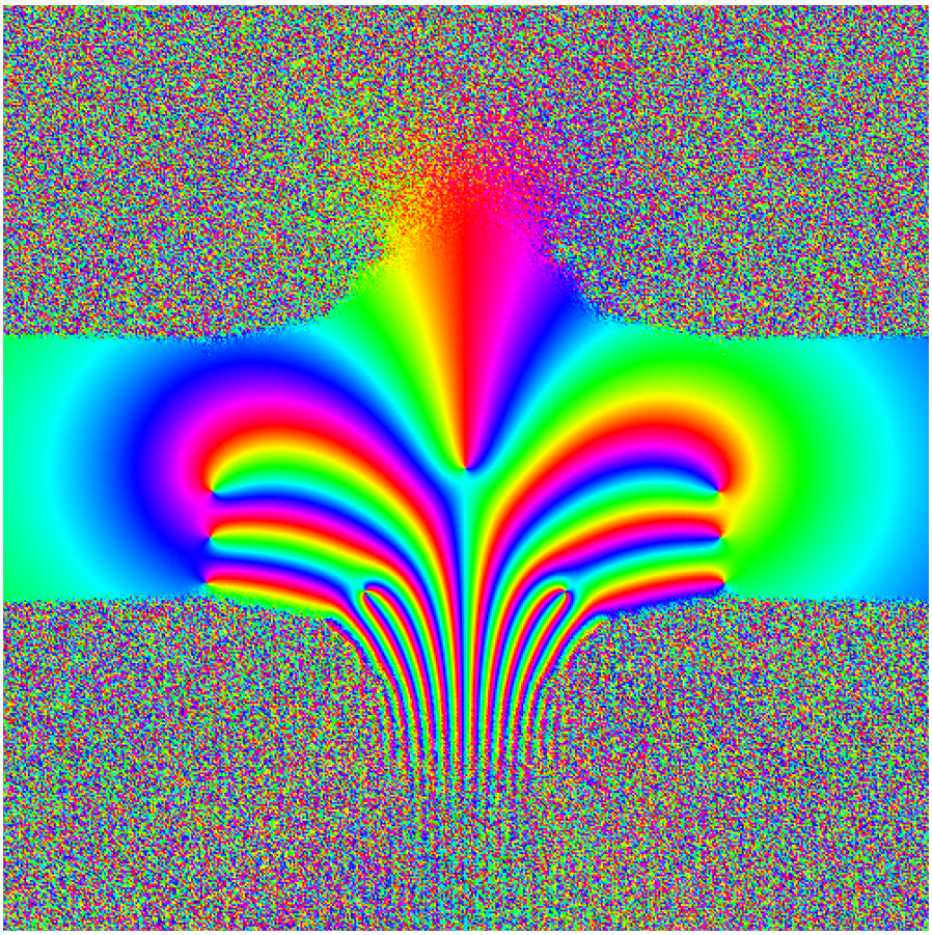

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Abstract

This thesis concerns itself with resonances as arising from 1D scattering experiments in quantum systems, and explores their relation to transparencies. An introduction is given to (the interpretation of) complex energies, and the resolvent operator—whose poles are by definition resonances—is defined. Resonances are then redefined as poles of the transmission amplitude $S(k)$, and some further properties of $S(k)$ are proven. Explicit formulae for $S(k)$ are obtained for i) symmetric piecewise-constant potentials, and ii) symmetric potentials for which WKB may be applied. The latter shows that Bohr-Sommerfeld quantization plays a role despite the exclusion of bound states. Finally, quantum normal forms (QNFs) are discussed, which describe $S(k)$ when the energy is approximately that of a local maximum of the potential. This may bridge the gap between energy various energy regions in which WKB is applicable.

Contents

1 Introduction

In classical mechanics, qualitatively a resonance occurs when a system has the uncanny ability to absorb the energy supplied to it, as a function of some parameter. As the prototypical, we have the damped-driven harmonic oscillator

$$\ddot{x} + \gamma\dot{x} + \omega_0^2 x = F_0 m^{-1} \cos(\omega t). \tag{1.1}$$

We are interested in how much energy this oscillator will have for any given driving frequency ω (with energy given as $E = m\omega_0^2 a^2/2$ for amplitude of oscillation a), once the oscillator has reached equilibrium.

Intuitively, for $\omega \gg \omega_0$, the driving force should have no net effect and the total energy goes to zero due to the damping factor. In contrast, for $\omega \ll \omega_0$ the driving force will be almost constant and we can solve to find that $E = F_0^2/(2m\omega_0^2)$.[1] There is nothing to indicate other than a steady decline of E should take place as ω grows.

It turns out that the energy for general ω is given by

$$E(\omega) = \frac{\omega_0^2 F_0^2}{2m} \frac{1}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2}, \tag{1.2}$$

which agrees with our intuitions on the large and small ω scales (for details, see [15, (9)]). However, we note that there is a local maximum at $\omega = \sqrt{\omega_0^2 - \gamma^2/2}$. At this frequency, the oscillator is able to take "the most advantage" of the driving force and obtain the greatest amount of energy. One says that this choice of driving frequency puts the oscillator *in resonance* with the driving force, at the *resonance frequency* $\omega_{\text{res}} := \sqrt{\omega_0^2 - \gamma^2/2}$.

We can examine the energy around the peak of ω_{res} more closely. Assuming $\gamma \ll 1$, the peak will be around $\omega_{\text{res}} \approx \omega_0$, and $E(\omega)$ takes the form

$$E(\omega) \approx \frac{F_0^2}{2m\gamma^2} \frac{(\gamma/2)^2}{(\omega - \omega_0)^2 + (\gamma/2)^2}. \tag{1.3}$$

Here ω_0 determines the center of the peak, and γ controls the height and width of the peak: the larger γ, the lower and wider the peak will be.

The peak described above has a very particular shape, which is known as a *Fock-Breit-Wigner-* (FBW-) distribution.[2] In its general form, we can write it as

$$\boxed{\text{FBW}(x) = A \times \frac{(\Gamma/2)^2}{(x - x_0)^2 + (\Gamma/2)^2},} \tag{1.4}$$

where A is the maximum height of the distribution. (As is the case in (1.3), A may depend on Γ.) The parameter x_0 determines the center of the peak, and Γ controls its width: the larger Γ, the wider the peak will be—see Figure 1.1 for an illustration. These peaks are most pronounced for smaller values of Γ: the width of the peaks decreases, making the resonance effect more stark a contrast with the "usual" behavior. FBW-distributions occur in many physical situations in which resonances are present, and as such could also be taken as "defining feature" of a resonance.

[1] Notice a particular solution is given by $x_{\text{part}} = Fm^{-1}\omega_0^{-2}$, and that $x_{\text{hom}} \to 0$ as $t \to 0$.

[2] Other names include the *Lorentzian* or *Cauchy* function/distribution.

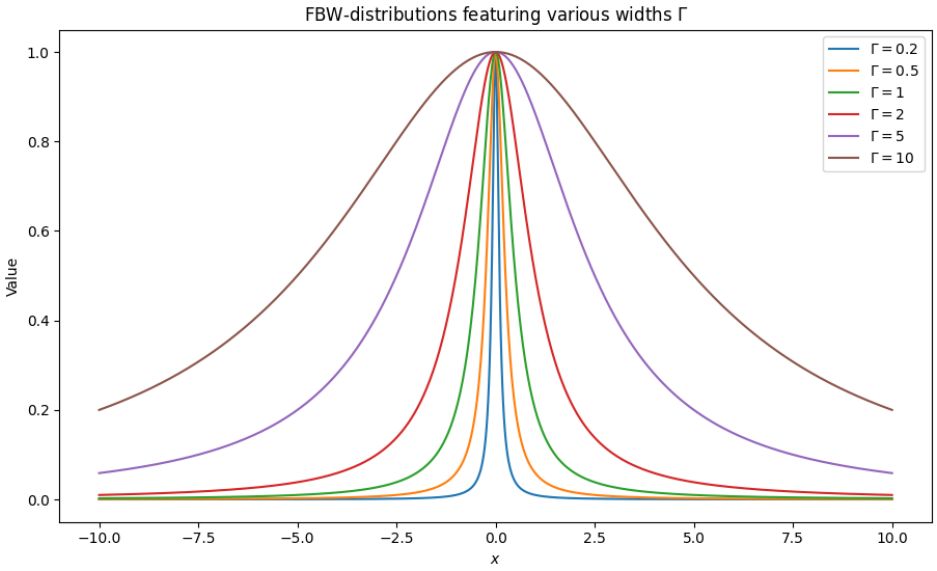
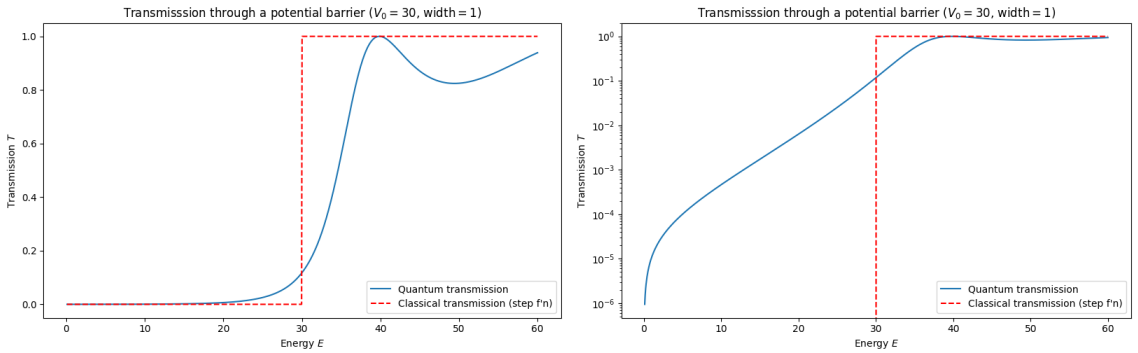


Figure 1.1: FBW distributions around $x_0 = 0$ with $A = 1$, and with different values of Γ to illustrate the peak's width thereupon.



(a) Linear scale (b) Logarithmic scale

Figure 1.2: Transmission through a potential barrier of height $V_0 = 30$ and width 1, both with linear (a) and logarithmic (b) scales for the y-axis.

Systems with uncanny abilities concerning some of their properties are not limited to classical mechanics only. Coming from quantum mechanics, one of the more famous examples is that of particles encountering a potential barrier, in which we are interested in the *transmission*, i.e. the proportion of particles going "through/over," as a function of their energy. Classically, this would be very dull: either the particle has enough energy to make it over, in which transmission would be 1, or it does not, in which case transmission is 0.

However, quantum mechanically things are more interesting. For a shallow barrier, we have the transmission spectrum as in Figure 1.2. We notice foremost the effect of *(quantum) tunneling*, where the transmission is non-zero even though the energy is smaller than the height of the barrier. This is a well-understood phenomenon. However, this makes it more mysterious that full transmission $T = 1$ *can* occur, as it does for $E \approx 40$: should there not also be "anti-tunneling" that would prevent this?

That is to say, if $T > 0$ than zero, indicating there is always tunneling, why is there not always reflection?

Even more intriguing is the phenomenon of *resonant* tunneling, whereby full transmission is reached at an energy (far) lower than the maximum of the potential barrier. This is not seen in this example, as it requires a specific geometry of the potential for it to appear.

These tunneling phenomena turn out to be intimately related to resonances, which in quantum mechanics have a crisp, mathematical definition. The precise relation cannot easily be summed up in a few sentences (indeed, a central tenet of this thesis is the exploration of the relationship between the two), but suffice it to say that to each such full transmission occurrence there is a resonance hiding in the background, effecting it.

Knowledge of resonances in quantum systems (and thus of transmission rates, to some extent) may be used academically for research into the behavior of particles inside complicated, 2- or 3D potential landscapes.

In this thesis, the first order of business will be to introduce some preliminaries that are necessary for (particular parts) of the text, namely some quantum and Hamiltonian mechanics, classical normal form theory, and the WKB approximation.

After this, we shall delineate the model we will use for the rest of this thesis. We will introduce and discuss the concept of complex energies, define resonances by means of the resolvent operator, and link this definition to the transmission amplitude $S(k)$, whose absolute valued-squared is T. Finally, we prove meromorphicity of $S(k)$, and extend the interpretation to a broader class of potentials.

We then find explicit formulae for $S(k)$, for i) piecewise constant & symmetric potentials, and ii) symmetric potentials for which we can apply the WKB approximation. These are found in such a way that they can be applied to all such potentials. By means of some examples (the square well, Gaussian barrier, and sinc potential) we are able to derive properties of the transmission amplitudes for the potentials of which they are representatives, including verifying ones that we had proven in general in the preceding section.

Finally we investigate a method to handle the breakdown of the WKB approximation, which happens when the energy of the particle matches that of a barrier. This we do by means of quantum normal forms. This is an adaptation of classical (Birkhoff-Gustavson) normal form theory, which may be used to analyze motion around a saddle equilibrium in phase space. This we then export to the quantum realm, and are so able to calculate transmission amplitudes. Here too we strive to illustrate the theory by means of examples.

In the appendix we detail how we calculated the scattering matrices (from which the transmission amplitude can be read off) for the calculations performed in this thesis.

2 Preliminaries

2.1 Crash courses

Quantum Mechanics

In quantum mechanics (QM), instead of considering particles as "point-like," they are described using wave mechanics. As such, particles are described by means of a *wavefunction*, commonly denoted as $\Psi(\boldsymbol{x}, t)$, which holds all the information available concerning said particle. Of special importance is the "location" of the particle: this is found using *Born's rule*, which states that $|\Psi(\boldsymbol{x}, t)|^2$ should be interpreted as a probability density function (pdf) for the particle's location at time t. Importantly, this also implies that for all t, $\Psi(\boldsymbol{x}, t)$ should be square integrable in $\boldsymbol{x}$ for it to be a wavefunction. This then allows for a normalization $\Psi \to \widetilde{\Psi}$ s.t. $\int |\widetilde{\Psi}|^2 \, d\boldsymbol{x} = 1$, to complete the interpretation as pdf.

Naturally, we want to know how the wavefunction evolves in space and time—enter the famous *Schrödinger equation*:

$$i\hbar \frac{\partial \Psi}{\partial t} = \mathcal{H}\Psi, \tag{2.1}$$

a linear PDE, first order in time t and (generally) second order in space. Here $\mathcal{H}$ is a self-adjoint operator known as the *Hamiltonian*. As we will stick to a one-dimensional, non-free setting, the Hamiltonian for us will read

$$\mathcal{H} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x), \tag{2.2}$$

so the Schrödinger equation (2.1) becomes

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \Psi, \tag{2.3}$$

where m is the mass of the particle under consideration. The function V is the *potential* function, and it is that which encodes the particular situation we are considering. As such, it will take center stage for the lion's share of the thesis.

Notation 2.1 (Mass normalization)**.** To make our lives easier, we will set $2m \equiv 1$ for the rest of this thesis.

The Schrödinger equation allows a powerful method for solving it, namely by means of *separation of variables*. We make the *ansatz* $\Psi(x, t) = \phi(t)\psi(x)$, and substitute; the result will be two decoupled equations

$$i\hbar \frac{d\phi}{dt} = E\phi \tag{2.4a}$$

and

$$\boxed{-\hbar^2 \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi,} \tag{2.4b}$$

where here E is a separation constant. Due to its appearance as the eigenvalue of the Hamiltonian operator (indeed, (2.4b) is simply $\mathcal{H}\psi = E\psi$), it may be interpreted as

being the *energy* of the system/particle. This is also convenient, as E is guaranteed to be real number due to the self-adjointness of $\mathcal{H}$.

The former equation (2.4a) can readily be solved: $\phi = \exp(-i\hbar^{-1}Et)$. The game then becomes to solve for ψ in equation (2.4b)—a non-trivial task, as there are no conditions put on V at this stage. Crucially, once you have described ψ, you hope that it converges: you divide by the answer to normalize it (as is necessary following Born's rule). We will have then found the *stationary wavefunction* ψ.

Due to the importance of (2.4b), it has its own name: the *time-independent* or *stationary* Schrödinger equation. (Whence also the name for ψ.)

Notation 2.2 (Naming conventions)**.** Since we will be working exclusively in the time-independent domain, we will

- refer to (2.4b) as *the* Schrödinger equation;
- any solving function ψ as its solution; and
- ψ as a wavefunction when it is moreover normalizable.

The solution of the time-independent Schrödinger dictates the evolution of the whole wavefunction in time, as it is an eigenstate and we know its evolution through (2.4a). In that way we can readily propagate (linear combinations, i.e. *superpositions*, of) eigenstates forward and backward in time,

$$\Psi(x,0) = \sum_{j=1}^{N} \alpha_j \psi_j(x) \implies \Psi(x,t) = \sum_{j=1}^{N} \alpha_j \exp\big(-i\hbar^{-1}E_j t\big)\psi_j(x), \tag{2.5}$$

where E_j, ψ_j are such that $\mathcal{H}\psi_j = E_j\psi_j$. In the case of a continuous spectrum of the Hamiltonian, we obtain the so-called *wavepacket* formalism:

$$\Psi(x,0) = \int_{-\infty}^{\infty} \rho(E)\psi_E(x)\,dE \implies \Psi(x,t) = \int_{-\infty}^{\infty} \rho(E)\exp\big(-i\hbar^{-1}Et\big)\psi_E(x)\,dE\,, \tag{2.6}$$

where ψ_E indicates the wavefunction with energy E, and ρ is the initial distribution in energy space.

For further reading, there are many textbooks on introductory quantum mechanics, such as Griffiths [8], Merzbacher [12], and Galindo & Pascual [7].

Hamiltonian Mechanics

We define the quantities $\boldsymbol{q}, \boldsymbol{p} \in \mathbb{R}^d$ to be the *position* and *momentum* of a body, respectively, living in the *phase space* $S := \mathbb{R}^d \times \mathbb{R}^d$. In addition, we define a quantity $H : S \to \mathbb{R}$ as the *Hamiltonian (function)* of our system. The Hamiltonian dictates the motion of the body, in that the derivatives w.r.t. of the phase space quantities are given by

$$\frac{dq_k}{dt} \equiv \frac{\partial H}{\partial p_k} \quad \text{and} \quad \frac{dp_k}{dt} \equiv -\frac{\partial H}{\partial q_k}, \quad \text{for} \quad k = 1, 2, \cdots, d. \tag{2.7}$$

That is to say, the Hamiltonian determines the equations of motion (eoms) of the body. If we create the large vector $\boldsymbol{z} = \begin{pmatrix} q_1 & \cdots & q_d & p_1 & \cdots & p_d \end{pmatrix}^\intercal$, we can summarize the

above Hamiltonian equations by means of a single matrix equation:

$$\frac{d\boldsymbol{z}}{dt} = \begin{pmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{pmatrix} \left(\frac{\partial H}{\partial \boldsymbol{z}}\right)^{\intercal}. \tag{2.8}$$

Naturally we want to say something about the motion of the body, and one approach is by examining the state space S. Namely, if we could find a state space function $A : S \to \mathbb{R}$ which we could show to remain *constant* as the body moves, then we would conclude that the motion has to be restricted to $A^{-1}(a) \subseteq S$, for the particular value $a \in \mathbb{R}$. We then call A a *constant of motion*, and if a is a regular value of A, $A^{-1}(a)$ will be dimension $2d-1$. This is of a lower dimension than the whole phase space S, and hence our problem is simplified.

A particularly important way of viewing integrals of motion arises from taking the time derivative of state space functions along a solution curve generated by the Hamiltonian:

$$\frac{dA}{dt} = \sum_{k=1}^{d} \frac{\partial A}{\partial q_k}\frac{dq_k}{dt} + \frac{\partial A}{\partial p_k}\frac{dp_k}{dt} = \sum_{k=1}^{d} \frac{\partial A}{\partial q_k}\frac{\partial H}{\partial p_k} - \frac{\partial A}{\partial p_k}\frac{\partial H}{\partial q_k} =: \{A, H\}, \tag{2.9}$$

where $\{\cdot,\cdot\}$ is called a *Poisson bracket*. We also write

$$\mathrm{ad}_A\, H \equiv \{A, H\}, \tag{2.10}$$

where we might elect the former notation as it allows us to compose the Poisson bracket more simply. The condition that A be an integral of motion is thus equivalent to whether its Poisson bracket with H is zero—or, that A is *in involution* with the Hamiltonian.

Up to this point we have dealt with $\boldsymbol{q}$ and $\boldsymbol{p}$ living in an arbitrary dimension d. However, in keeping with the general one dimension trend of this thesis, we shall for the remainder assume that $d = 1$, so we have only one q and p with which to contend.

There are many (introductory) treatments available on Hamiltonian mechanics, for instance Wimberger [17, §3].

2.2 Classical (Birkhoff-Gustavson) normal forms

The below construction of the classical normal form is adapted from [16, §2], though other resources also exist that go over this construction, see for instance [14].

In essence, the classical normal form attempts to identify approximate constants of motion, locally around an equilibrium point in phase space. This should then aid in determining the behavior around said equilibrium point. Before giving the precise definition, let us first introduce homogeneous orders, as expansion in terms of the phase space variables q and p is imminent.

Definition 2.3 (Homogeneous orders)**.** We define

$$\mathcal{W}^n := \mathrm{span}\{q^\alpha p^\beta : \alpha, \beta \in \mathbb{N} \text{ and } \alpha + \beta = n\} \text{ over } \mathbb{C} \tag{2.11}$$

as the space of functions of *homogeneous order* (hom. order, ho) n.

Definition 2.4 (Classical Normal Form)**.** Let H have an equilibrium point at z_0, i.e. $\nabla H(z_0) = 0$, and let H_2 be its Taylor expansion up to hom. order 2. We say that H is in *classical normal form (CNF) up to order N around z_0* if

$$\{H_2, H\} = 0 + \mathcal{O}_{\text{ho}}(N+1), \tag{2.12}$$

where we take the order symbol to mean hom. order over q and p.

Hamiltonians are not generally in CNF up to any substantial order. For a concrete example, assume that at $z_0 = (0,0)$ the standard Hamiltonian $H = p^2/(2m) + V(q)$ has an equilibrium, which is to say that $V'(0) = 0$. Making the Maclaurin expansion of H, we see

$$H = \underbrace{\frac{p^2}{2m} + V(0) + \tfrac{1}{2}V''(0)q^2}_{=H_2} + \sum_{j=3}^{\infty} \frac{V^{(j)}(0)}{j!} q^j, \tag{2.13}$$

so we may calculate

$$\{H_2, H\} = \sum_{j=3}^{\infty} \frac{V^{(j)}(0)}{j!} \{H_2, q^j\} = \frac{-p}{m} \sum_{j=3}^{\infty} \frac{V^{(j)}(0)}{(j-1)!} q^{j-1} = \mathcal{O}_{\text{ho}}(3). \tag{2.14}$$

Thus, under the assumption that $V^{(3)}(0) \neq 0$, H is in CNF only up to order 2.

Now the game is to transform the Hamiltonian so that it becomes CNF of arbitrary order, improving the accuracy of our local constant of motion. Or, more methodically, we want to find a *family* of symplectic transformations so that

$$H \longrightarrow H^{(3)} \longrightarrow H^{(4)} \longrightarrow \cdots \longrightarrow H^{(N)}, \tag{2.15}$$

where $H^{(m)}$ is in CNF up to order m. (In this way, we see also that $H = H^{(2)}$, and we use the two interchangeably.) We can think of this number m as the iteration or generation of transformed Hamiltonian.

By transformation we mean transformed by a function $W_m \in \mathcal{W}^m$, $m \geq 3$, generating a flow $\Phi^t_{W_m}$, where t is time. The transformation is then $H^{(m)} := H^{(m-1)} \circ \Phi^{-1}_{W_m}$, i.e. the pullback of the previous Hamiltonian under the time $t = -1$ map. It can then be shown that, as an expansion, the transformation can be written as

$$H^{(m)} = \sum_{j=0}^{\infty} (j!)^{-1} (\text{ad}_{W_m})^j H^{(m-1)}. \tag{2.16}$$

Further context (including the derivation of (2.16)) is discussed in [16, §2.1].

The question then becomes to find that W_m so that $H^{(m)}$ is CNF of order m, for each m. Let us make the following observation, for H_2 as from the standard Hamiltonian, i.e. as indicated in (2.13):

$$A \in \mathcal{W}^n \implies \{H_2, A\} \in \mathcal{W}^n. \tag{2.17}$$

That is to say, if A is hom. order n, then $\{H_2, A\}$ will be of that same hom. order. This also means that if we want to be in CNF up to some certain order, the adjoint with H_2 will have to cancel the Hamiltonian order by order. Letting a subscript h

indicate the hom. order of the term in the Hamiltonian, we make this mathematically concrete by following reasoning:

$$H^{(m)} = \sum_{h=0}^{\infty} H_h^{(m)} \implies \{H_2^{(m)}, H^{(m)}\} = \sum_{h=0}^{\infty} \{H_2^{(m)}, H_h^{(m)}\} \stackrel{!}{=} \mathcal{O}_{\text{ho}}(m+1)$$
$$\implies \{H_2^{(m)}, H_h^{(m)}\} = 0 \quad \text{for } h = 0, 1, \cdots, m. \tag{2.18}$$

This motivates us to find a relation between the Hamiltonians of different generations and different orders—which is done in the following Lemma.

Lemma 2.5 (Relation Hamiltonian terms)**.** *We have that the relation between Hamiltonian terms of different generations and different hom. orders is given by*

$$H_h^{(m)} = \sum_{j=0}^{\lfloor h/(m-2) \rfloor} (j!)^{-1} (\text{ad}_{W_m})^j H_{h-j(m-2)}^{(m-1)}. \tag{2.19}$$

Additionally, we have

(i) $H_h^{(m)} = H_h^{(m-1)}$*, for all* $m \geq 3$ *and* $0 \leq h < m$*, and*

(ii) for $h = 2$*,* $H_2^{(m)} = H_2^{(2)}$ *for all* $m \geq 3$*.*

Proof. Equation (2.19) is (2.36) in [16, §2], and we refer to their reasoning. Also noting that (ii) follows immediately from (i), we need only show subpoint (i).

Eyeing (2.19), the relation holds for $h \leq m-3$: then $\lfloor h/(m-2) \rfloor = 0$, and so the sum runs only over $j = 0$, which yields exactly the relation we want. For $h = m-2$, notice we will have

$$H_{m-2}^{(m)} = H_{m-2}^{(m-1)} + \cancel{\{W_m, H_0^{(m-1)}\}} = H_{m-2}^{(m-1)} \tag{2.20}$$

where cancellation holds as $H_0^{(m-1)}$ is a constant. Finally, for $h = m-1$, we got

$$H_{m-1}^{(m)} = H_{m-1}^{(m-1)} + \{W_m, \cancel{H_1^{(m-1)}}\} = H_{m-1}^{(m-1)}, \tag{2.21}$$

where cancellation now holds as $H_1^{(m-1)} = 0$ for all generations $m-1$. Thus we have shown the relation 2.5(i) for all $h < m$, completing the proof. □

This means that, effectively, the transformations W_m do not touch the lower order homogeneous terms that were previously fixed, and instead only affect the latter terms. See also Table 2.1 for a "pictoral" representation of this iterative fixing of terms. This Lemma thus guarantees that the order of CNF only increases as we apply successively more of the transformations W_m, and moreover that the lower order terms are also part of the higher order CNF. That is to say, we never "undo" part of our CNF as we apply more transformations.

We are now in a position to say something about the W_m.

Proposition 2.6 (Condition on W_N's; homological equation)**.** *Assume that* $H^{(N-1)}$ *is in CNF up to order* $N-1$*,* $N \geq 3$*. In order to guarantee* $H^{(N)}$ *is in CNF up to order* N*,* $W_N \in \mathcal{W}^N$ *needs to satisfy*

$$H_N^{(N-1)} - \mathcal{D}W_N \in \ker \mathcal{D}, \tag{2.22}$$

where $\mathcal{D} := \{H_2^{(2)}, \cdot\} : \mathcal{W}^N \to \mathcal{W}^N$ *is the* homological operator*; the equation* (2.22) *is known as the* homological equation*.*

	H	$=$	$H_{0,1,2}$	$+$	H_3	$+$	H_4	$+$	H_5	$+$	H_6	$+\cdots$
W_3	$\downarrow$											
	$H^{(3)}$	$=$	$H^{(3)}_{0,1,2}$	$+$	$H^{(3)}_3$	$+$	$H^{(3)}_4$	$+$	$H^{(3)}_5$	$+$	$H^{(3)}_6$	$+\cdots$
W_4	$\downarrow$											
	$H^{(4)}$	$=$	$H^{(4)}_{0,1,2}$	$+$	$H^{(4)}_3$	$+$	$H^{(4)}_4$	$+$	$H^{(4)}_5$	$+$	$H^{(4)}_6$	$+\cdots$
W_5	$\downarrow$											
	$H^{(5)}$	$=$	$H^{(5)}_{0,1,2}$	$+$	$H^{(5)}_3$	$+$	$H^{(5)}_4$	$+$	$H^{(5)}_5$	$+$	$H^{(5)}_6$	$+\cdots$
W_6	$\downarrow$											
	$H^{(6)}$	$=$	$H^{(6)}_{0,1,2}$	$+$	$H^{(6)}_3$	$+$	$H^{(6)}_4$	$+$	$H^{(6)}_5$	$+$	$H^{(6)}_6$	$+\cdots$
W_7	$\downarrow$											
	$\vdots$											$\ddots$

Table 2.1: Illustration of how the various transformations W_m affect the generations of Hamiltonians. The terms in like colors (excluding black) are equal to each other.

Proof. By Lemma 2.5 we see that $H^{(N)}_h = H^{(N-1)}_h$ for $h = 0, 1, \cdots, N-1$. So,

$$\{H^{(N)}_2, H^{(N)}_h\} = \{H^{(N-1)}_2, H^{(N-1)}_h\} = 0 \quad \text{for} \quad h = 0, 1, \cdots, N-1. \tag{2.23}$$

We then just need to show that this holds also for $h = N$. By (2.19), we can find an expression for $H^{(N)}_N$:

$$\begin{aligned} H^{(N)}_N = \sum_{j=0}^{1} (j!)^{-1} (\mathrm{ad}_{W_N})^j H^{(b)}_{N-j(N-2)} &= H^{(N-1)}_N + \{W_N, H^{(N)}_2\} \\ &= H^{(N-1)}_N - \{H^{(2)}_2, W_N\} \\ &= H^{(N-1)}_N - \mathcal{D}W_N. \end{aligned} \tag{2.24}$$

As such, the condition for $H^{(N)}$ to be in CNF up to order N becomes

$$H^{(N)} \text{ CNF} \iff \mathcal{D}\left[H^{(N-1)}_N - \mathcal{D}W_N\right] = 0 \iff H^{(N-1)}_N - \mathcal{D}W_N \in \ker \mathcal{D}, \tag{2.25}$$

which completes the proof. □

Remark 2.7 (Dimensionality $\mathcal{D}$)**.** The action of the homological operator depends on the dimension of the space $\mathcal{W}^N$ on which it is acting, yet this is not reflected in the notation. We omit mention of the relevant dimension, as we take it to be implied.

From this point on, whether we can successively find W_N's depends heavily on the nature of the homological operator $\mathcal{D}$. And since it in turn depends non-trivially on the hom. order under consideration, it is tricky to show that the homological equation has a solution for any particular H_2. Such a solution existing for every hom. order is called *solvability*. One particular case in which solvability can be established is if $\mathcal{D}$ can be shown to be diagonal for every hom. order, when expressed as a matrix over the relevant space and in a suitable basis. Then the splitting $\mathcal{W}^m = \mathrm{Im}\,\mathcal{D} \oplus \ker \mathcal{D}$ can be made, and a suitable W_m can be found.

2.3 Scattering

Since we shall be concerned with the influence of a target on an incoming particle, there is a need to discuss the mathematics that models this at its core. This is the mathematics of scattering theory, which aims to describe how the incoming determines the outgoing, whether discrete particles, or, relevantly for us, waves.

To model our situation we shall utilize the Schrödinger equation (2.4b) featuring a potential characterized as

$$V(x) = \begin{cases} 0 & \text{if} \quad x < -\nu \text{ (left)} \\ f(x) & \text{if} \quad -\nu \leq x \leq \nu \\ 0 & \text{if} \quad x > \nu \text{ (right)} \end{cases}, \tag{2.26}$$

where $\nu > 0$ is a parameter that indicates the size of the target. Here f represents the "inner structure" of the target. Though in the later parts of this thesis we will want to focus on this inner structure, for this section any knowledge of it is not relevant.

As we see from (2.26), our potential will be identically zero for $|x| > \nu$, for some parameter ν, so that we have free space to the left and right. In free space, we may readily solve the Schrödinger equation to obtain the solution in these regions. Denoting these by ψ_{left} and ψ_{right} respectively for their validity regions, we see that they will be given by

$$\psi_{\text{left}} = A\exp(ikx) + B\exp(-ikx) \quad \text{and} \quad \psi_{\text{right}} = C\exp(ikx) + D\exp(-ikx), \tag{2.27}$$

for complex constants A, B, C, and D, and where we introduced the *wavenumber* $k := \hbar^{-1}\sqrt{E}$, $E > 0$. Important to note is that these constants are *not* independent of each other: choosing two of these to have specific values fixes the other two. The question of *how*, is precisely that which we intend to answer.

To be able to involve scattering in this story, we need to introduce some notion of incoming and outgoing. This is provided by involving the relevant time evolution operator

$$\mathcal{U}(t) = \exp\bigl(-i\hbar^{-1}\mathcal{H}t\bigr) \overset{\star}{=} \exp\bigl(-i\hbar^{-1}Et\bigr). \tag{2.28}$$

Here $\star$ holds if we are evolving an eigenstate of the Hamiltonian with energy E cf. (2.4a). Supposing we wish to evolve the planar wave $\xi(x) = \exp(ikx)$ in time, this will yield

$$\Xi(x,t) = \xi(x)\exp\bigl(-i\hbar^{-1}Et\bigr) = \exp\bigl(i(kx - \hbar^{-1}Et)\bigr). \tag{2.29}$$

To determine the "direction of motion," we consider where the points of equal phase go under (small) perturbations of x and t. Suppose we choose (x_0, t_0) so that $\Xi(x_0, t_0) = 1$. Then, introducing (small) perturbations Δx and Δt, to maintain $\Xi(x_0+\Delta x, t_0+\Delta t) = 1$ we need

$$k\Delta x = \hbar^{-1}E\Delta t \implies \frac{\Delta x}{\Delta t} = \frac{E}{\hbar k}. \tag{2.30}$$

As such, the "peak" $\Xi = 1$ moves with velocity $E/(\hbar k) > 0$, i.e. to the right. In this way, then, we characterize the planar wave $\exp(ikx)$ as *rightmoving*. In a similar way we can show that $\exp(-ikx)$ is thus *leftmoving*. This allows us to split the wavefunctions ψ_{left} and ψ_{right} into their incoming and outgoing parts—see Table 2.2. We then rewrite (2.27) as

side \ term	$\exp(ikx)$	$\exp(-ikx)$
ψ_{left}	incoming	outgoing
ψ_{right}	outgoing	incoming

Table 2.2: Characterization of the different terms in ψ_{left} and ψ_{right}.

Figure 2.1: Pictoral definition of the scattering matrix $\mathbf{S}$: to give B and C in terms of A and D.

$$\psi_{\text{left}} = A\psi_{\text{left;in}} + B\psi_{\text{left;out}} \quad \text{and} \quad \psi_{\text{right}} = C\psi_{\text{right;out}} + D\psi_{\text{right;in}} \tag{2.31}$$

using said identifications.

To determine the outgoing amplitudes in terms of the incoming ones, then, essentially becomes the problem of finding how B and C depend on A and D. Due to the principle of superposition (equivalently, linearity of the Schrödinger equation), we see that the connection ought to be linear. That is to say, the mapping $(A, D) \mapsto (B, C)$ should be done by means of a matrix. This leads us to the following definition.

Definition 2.8 (Scattering matrix)**.** We define the *scattering matrix* (or *S-matrix*) $\mathbf{S} \in \mathbb{C}^{2\times 2}$ to be the matrix s.t.

$$\mathbf{S} : \text{span}\{\psi_{\text{left;in}}, \psi_{\text{right;in}}\} \longrightarrow \text{span}\{\psi_{\text{left;out}}, \psi_{\text{right;out}}\}, \tag{2.32}$$

and that it sends

$$\mathbf{S}\left[A\psi_{\text{left;in}} + D\psi_{\text{right;in}}\right] = B\psi_{\text{left;out}} + C\psi_{\text{right;out}}. \tag{2.33}$$

To make the dependence of $\mathbf{S}$ on k explicit, we write $\mathbf{S}(k)$.

The scattering matrix only provides the form of the transformation between incoming and outgoing waves; the elements of $\mathbf{S}$ (and thus any scattering calculation) will depend both on the internal structure f of the potential, as well as the wavenumber. Nevertheless, it is possible to make a statement about $\mathbf{S}$ in general, as we shall do in the following Lemma.

Lemma 2.9 (Unitarity of $\mathbf{S}$)**.** *For $k \in \mathbb{R}$, the scattering matrix is unitary.*

Proof. This proof is adapted from [11, §1.2.1]. Let us start from the assumption that the probability current density j, which is defined as

$$j(x) = i\hbar\left(\psi\frac{d\psi^*}{dx} - \psi^*\frac{d\psi}{dx}\right), \tag{2.34}$$

is equal at the boundaries of the potential, which is to say that $j(-\nu) = j(\nu)$. Since we have a description of ψ to the left and right of the target, we may investigate what these quantities are. After some calculation we find that

$$j(-\nu) = i\hbar \left(\psi_{\text{left}} \frac{d\psi^*_{\text{left}}}{dx} - \psi^*_{\text{left}} \frac{d\psi_{\text{left}}}{dx} \right) \Big|_{x=-\nu} = |B|^2 - |A|^2, \tag{2.35a}$$

and similarly

$$j(\nu) = i\hbar \left(\psi_{\text{right}} \frac{d\psi^*_{\text{right}}}{dx} - \psi^*_{\text{right}} \frac{d\psi_{\text{right}}}{dx} \right) \Big|_{x=\nu} = |D|^2 - |C|^2. \tag{2.35b}$$

Rearranging (2.35) thus gives us

$$|A|^2 + |D|^2 = |B|^2 + |C|^2 \iff (A^*\,, D^*) \begin{pmatrix} A \\ D \end{pmatrix} = (B^*\,, C^*) \begin{pmatrix} B \\ C \end{pmatrix}. \tag{2.36}$$

Now, since $\mathbf{S}\,(A\,, D)^\intercal = (B\,, C)^\intercal$, it also holds that $(A^*\,, D^*)\,\mathbf{S}^\dagger = (B^*\,, C^*)$, and so from (2.36) we obtain

$$(A^*\,, D^*)\,\mathbf{S}^\dagger\mathbf{S} \begin{pmatrix} A \\ D \end{pmatrix} = (A^*\,, D^*) \begin{pmatrix} A \\ D \end{pmatrix}. \tag{2.37}$$

This means that $\mathbf{S}$ is an *isometry*, which, since $\mathbf{S}$ is moreover a square matrix, directly implies that it is unitary. □

The scattering matrix being unitary allows us to find an important conservation law. Choosing $(A\,, D)^\intercal = (1\,, 0)^\intercal$, we find that

$$|\mathbf{S}_{11}|^2 + |\mathbf{S}_{21}|^2 = 1. \tag{2.38}$$

The physical interpretation is that, under a steady supply of particles, the proportions that are reflected by and transmitted through the potential are $|\mathbf{S}_{11}|^2$ and $|\mathbf{S}_{21}|^2$, respectively. Based on this interpretation, we make the following definitions.

Definition 2.10 (Reflection and transmission)**.** We name

- $\mathbf{S}_{11}$ and $\mathbf{S}_{21}$ the *reflection* and *transmission amplitude*, respectively, and
- $|\mathbf{S}_{11}|^2$ and $|\mathbf{S}_{21}|^2$ the *reflection* and *transmission coefficient*, respectively. For the transmission coefficient, we will usually write T.

The above quantities will depend on k (or E), and we can parse these as an argument if we wish to make this clear.

Furthermore, when k (or E) is such that $T = 1$, we will call k (or E) a *transparency*.

Remark 2.11. It should be emphasized that the conservation law (2.38), and accordingly the physical interpretation of the reflection and transmission coefficients, only applies in the case where $k \in \mathbb{R}$, as is required for unitarity of $\mathbf{S}$. This stands in contrast to later in the thesis, where we will generally consider $k \in \mathbb{C}$; there we thus lose this model for physical interpretation.

The above choice $(A\,, D)^\intercal = (1\,, 0)^\intercal$ also means that the resultant B and C—which are actually $\mathbf{S}_{11}$ and $\mathbf{S}_{21}$—depend on k *only*. As such, the scattering matrices should be calculable using k and knowledge of the internal structure of the target, i.e. the function f. It should be evident that this will be of great import to the thesis going forward, and as such the practical calculation of scattering matrices requires discussion. This is done in Appendix A, and includes the `Python` program used for computations.

2.4 WKB approximation

Whatever calculation is done in quantum mechanics, it more than likely will involve knowing (the properties of) wavefunctions at some point, to be determined from the associated Schrödinger equation. However, as the Schrödinger equation is second order and involves an arbitrary function (being the potential), finding the solution will in general be a very complicated problem—indeed, often impossible with "pen and paper" methods.

Fortunately, the solution can at least be approximated, for suitable potentials V. One such approximation is the *WKB* approximation—named after Wentzel, Kramers and Brillouin—and is widely used when circumstances allow it. WKB is also known as a *semiclassical* approximation to QM. The idea is that we expand the wavefunction in a power series of $\hbar$, wherein taking the $\hbar \equiv 0$ should then reduce to a classical setting; when we set $\hbar \equiv 0$, we "turn off" quantum mechanics, in a certain sense. In this way, QM can be viewed as a perturbation to an otherwise classical system. This idea will also come back in Section 5 concerning quantum normal forms (QNFs), where it will be applied in a slightly more technical manner.

In this section, we will first derive the WKB approximation by the power series method, after which we discuss the connection formulae to extend its applicability. Finally, we will see how to characterize a certain (WKB-applicable) potential landscape by means of a single matrix.

Further reference to the WKB approximation can be found in for instance [12, §7] and [8, §9].

2.4.1 Derivation

The main observation is that, whenever the potential is constant, $V(x) = V_0$, we have that the solution of the Schrödinger equation is given by

$$\psi_{\text{cst}}(x) = \exp\Big(i\hbar^{-1}x\sqrt{E - V_0}\Big) \tag{2.39}$$

As such, this gives credence to the *ansatz* of the general solving wavefunction also having the form of an exponential function, or at least whenever the potential is "approximately constant"—a qualification we will come back to momentarily. Let us assume that the general solution of the Schrödinger equation ψ_{gen} is given by

$$\psi_{\text{gen}}(x) = \exp\big(i\hbar^{-1}f(x)\big), \tag{2.40}$$

for some yet-unknown, to be determined function f. Plugging this *ansatz* into the Schrödinger equation, we obtain

$$-\hbar^2\psi''_{\text{gen}} + (V(x) - E)\psi_{\text{gen}} = 0 \implies (f')^2 - i\hbar f'' + V(x) - E = 0, \tag{2.41}$$

a differential equation which is seemingly as complicated as the one with which we started, if not more so. However, in the spirit of semiclassics, we now assume that f can be given in terms of a power series in the small/perturbative parameter $\hbar$. That is to say, we assume

$$f = \sum_{j=0}^{\infty} \hbar^j f_j(x), \text{ for functions } f_j(x). \tag{2.42}$$

Plugging this power series into (2.41), we will have to fulfill that equation order by order in $\hbar$; this should yield us expressions for the functions f_j. Observe that the equations we get are

$$\mathcal{O}\big(\hbar^0\big) : (f_0')^2 + V(x) - E = 0 \tag{2.43a}$$
$$\mathcal{O}\big(\hbar^1\big) : 2f_0'f_1' - if_0'' = 0 \tag{2.43b}$$
$$\mathcal{O}\big(\hbar^2\big) : 2f_0'f_2' + (f_1')^2 - if_1'' = 0 \tag{2.43c}$$
$$\vdots$$

Though in principle this allows us to find the functions f_j for whichever j we like, for purposes of this text we will stick only to finding f_0 and f_1. From (2.43a) we find

$$(f_0')^2 = E - V \implies f_0 = \pm \int^x \sqrt{E - V(x')}\, dx' + c_0, \tag{2.44}$$

with c_0 being an integration constant. From (2.43b), in turn, we learn

$$f_1' = \frac{i}{2}\frac{f_0''}{f_0'} = \frac{i}{2}\frac{d}{dx}\ln(f_0') \implies f_1 = \frac{i}{2}\ln(f_0') + c_1 = \frac{i}{4}\ln|E - V| + c_1, \tag{2.45}$$

with c_1 another integration constant. Thus, rolling our calculation back up, we see that

$$\begin{aligned}\psi_{\text{gen}} &= \exp\left(i\hbar^{-1}\sum_{j=0}^{\infty}\hbar^j f_j\right)\\ &= \exp\left(\pm i\hbar^{-1}\int^x \sqrt{E - V(x')}\, dx' - \tfrac{1}{4}\ln|E - V| + \mathcal{O}\big(\hbar^1\big)\right)\\ &= |E - V|^{-1/4}\exp\left(\pm i\hbar^{-1}\int^x \sqrt{E - V(x')}\, dx' + \mathcal{O}\big(\hbar^1\big)\right).\end{aligned} \tag{2.46}$$

In the above we did not take explicitly into account the introduced integration constants $c_{0,1}$. The reason is that their effect would be to provide an additional scale & phase to the overall wavefunction—which addition is moot, as the Schrödinger equation is linear anyway. As such, it is legal to just assume that $c_{0,1} \equiv 0$, and keep the linearity in the back of our minds for use later on.

Finally, the WKB approximation is now formed by disregarding the high order terms in $\hbar$, which is to say that

$$\boxed{\psi_{\text{gen}} \approx \psi_{\text{WKB}}(x) = |E - V|^{-1/4}\exp\left(\pm i\hbar^{-1}\int^x \sqrt{E - V(x')}\, dx'\right).} \tag{2.47}$$

There is one more wrinkle to iron out, which is that of the potential needing to be "approximately constant," an implicit assumption to the validity of the WKB approximation. How to make this concrete? Our set of equations (2.43) was derived assuming that powers of $\hbar$ could indeed be used to indicate the size of the various terms, and hence set each power to zero individually. That is to say, we implicitly

assumed that $\hbar f_1' \not\sim f_0'$ in size, otherwise the $\mathcal{O}(\hbar^0)$-equation would have had to read $2f_0'f_1' + (f_0')^2 + V - E = 0$. As such, we effectively assumed that

$$\begin{aligned} |f_0'| \gg |\hbar f_1'| &\iff |(f_0')^2| \gg \left|-\tfrac{1}{2}i\hbar f_0''\right| \\ &\iff |E-V| \gg \left|\frac{-i\hbar V'}{4\sqrt{E-V}}\right| \\ &\iff |4i\hbar^{-1}| \gg \left|\frac{-V'}{(E-V)^{3/2}}\right|, \end{aligned} \tag{2.48}$$

or more cleanly without signs and the multiplier 4:

$$\boxed{\left|\frac{V'}{(E-V)^{3/2}}\right| \ll \hbar^{-1}.} \tag{2.49}$$

This is the condition which must be fulfilled in order for WKB to be a valid approximation. Note that physically, this means what we already presupposed: that the potential is restricted in how quickly it can vary, and that that restriction depends on the energy of the wave. In other words, it makes concrete the qualification "approximately constant."

On one additional note: the quantity $\int \sqrt{E - V(x')}\, dx'$, or with its proper bounds, has already been making quite an appearance, and will continue to do so for the rest of the text. As such, it will be economical to introduce some notation to shorten this.

Notation 2.12 (WKB-style integral)**.** We denote by $I_{\cdot}^{\cdot}$ the integral

$$I_a^b := \int_a^b \sqrt{E - V(x')}\, dx' \,, \tag{2.50}$$

when it is clear about which potential V we are talking. Furthermore, we keep this same notation when we, later on, complexify the energy $E \to \mathcal{E}$.

One evident flaw of WKB is that it cannot handle the case $E = V(x_0)$ for some x_0: the approximation (and validity condition) explode. We call such x_0 *turning points*, and they are a critical exception to WKB's validity as presented. As such, for WKB to be a useful approximation, we need a way to deal with these turning points. We explore the remedy in the next subsection.

2.4.2 Connection Formulae

When the turning point is isolated (which is to say, when $V'(x_0) \neq 0$, see Figure 2.2), there is a method by which we can get around the problem of WKB blowing up—literally. Namely, comparing the regions just before and just after a turning point, they are both regions where the WKB approximation is valid, albeit that $\sqrt{E-V}$ has switched from real to imaginary (or vice versa).

Since we now explicitly wish to consider the case where $E \leq V(x)$, a convention needs to be chosen for the square root. For reasons that we will get into in section 3.1, we shall use the convention that

$$x < 0 \implies \sqrt{x} = -i\sqrt{-x}. \tag{2.51}$$

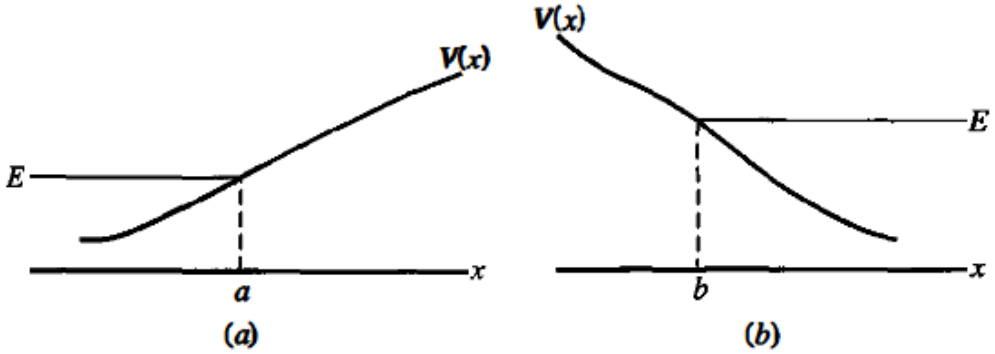


Figure 2.2: Illustration of turning points with $V'(x_0) \neq 0$. (Source: [12, Fig. 7.1])

This also means that some of the WKB-style integrals I_a^b will become complex-valued. That is to say, if $E - V(x)$ is negative over the interval of integration $[a, b]$, then I_a^b will be an imaginary number. We do not introduce additional notation to indicate this.

By the above reasoning, we should be able to deduce what the WKB-approximated wavefunction looks like *after* the turning point, given that we know how it looks *before* it. This is the topic of the following Proposition.

Proposition 2.13 (Connection formulae)**.** *Given the situation as in Figure 2.2, we have that the WKB formula after the relevant turning point in terms of the one before it is given by*

$$\begin{aligned} &A\exp\bigl(i\hbar^{-1}I_x^a\bigr) + B\exp\bigl(-i\hbar^{-1}I_x^a\bigr) \\ &\quad\longleftrightarrow i(e^{-i\pi/4}B - e^{i\pi/4}A)\exp\bigl(i\hbar^{-1}I_a^x\bigr) + \tfrac{1}{2}(Ae^{i\pi/4} + Be^{-i\pi/4})\exp\bigl(-i\hbar^{-1}I_a^x\bigr) \end{aligned} \tag{2.52a}$$

for the turning point a, and

$$\begin{aligned} &A\exp\bigl(i\hbar^{-1}I_x^b\bigr) + B\exp\bigl(-i\hbar^{-1}I_x^b\bigr) \\ &\quad\longleftrightarrow e^{-i\pi/4}(B + iA/2)\exp\bigl(i\hbar^{-1}I_b^x\bigr) + e^{i\pi/4}(B - iA/2)\exp\bigl(-i\hbar^{-1}I_b^x\bigr) \end{aligned} \tag{2.52b}$$

for the turning point b (excluding the scale factors $|E - V|^{-1/4}$ out front). These two formulae are called the connection formulae*.*

Proof. We will not derive these formulae from scratch, instead simply taking them from Merzbacher [12, (7.34) & (7.35)]—a derivation of these can naturally be found there.

Then it rests us to rewrite so that we are left with exponentials instead of sines and cosines. For the turning point a, observe that we can rewrite

$$\begin{aligned} &2A\cos\bigl(\hbar^{-1}I_x^a - \pi/4\bigr) - B\sin\bigl(\hbar^{-1}I_x^a - \pi/4\bigr) \\ &\quad= \underbrace{e^{-i\pi/4}(A + iB/2)}_{\widetilde{A}}\exp\bigl(i\hbar^{-1}I_x^a\bigr) + \underbrace{e^{i\pi/4}(A - iB/2)}_{\widetilde{B}}\exp\bigl(-i\hbar^{-1}I_x^a\bigr), \end{aligned} \tag{2.53}$$

so that we have the transformation

$$\begin{pmatrix}\tilde{A}\\ \tilde{B}\end{pmatrix} = \begin{pmatrix}e^{-i\pi/4} & ie^{-i\pi/4}/2\\ e^{i\pi/4} & -ie^{i\pi/4}/2\end{pmatrix}\begin{pmatrix}A\\ B\end{pmatrix} \iff \begin{pmatrix}A\\ B\end{pmatrix} = -i\begin{pmatrix}ie^{i\pi/4}/2 & ie^{-i\pi/4}/2\\ e^{-i\pi/4} & -e^{-i\pi/4}\end{pmatrix}\begin{pmatrix}\tilde{A}\\ \tilde{B}\end{pmatrix}. \tag{2.54}$$

The first connection formula (2.52a) is then found when replacing the lhs of [12, (7.34)] with (2.53), rewriting into $\widetilde{A}$ and $\widetilde{B}$, and also noting that in Merzbacher $\kappa(x') = ik(x')$. (Final step is to remove the tildes everywhere.)

Regarding the second connection formula (2.52b): observe that from Merzbacher we have that the second connection formula is

$$\begin{aligned} B\exp\bigl(i\hbar^{-1}I_x^b\bigr) + A\exp\bigl(-i\hbar^{-1}I_x^b\bigr) &\longleftrightarrow 2A\cos\bigl(\hbar^{-1}I_b^x - \pi/4\bigr) - B\sin\bigl(\hbar^{-1}I_b^x - \pi/4\bigr) \\ &\overset{\star}{=} e^{-i\pi/4}(A + iB/2)\exp\bigl(i\hbar^{-1}I_b^x\bigr) + e^{i\pi/4}(A - iB/2)\exp\bigl(-i\hbar^{-1}I_b^x\bigr), \end{aligned} \tag{2.55}$$

where for $\star$ we used (2.53). The formula as presented is then recovered by switching $A \leftrightarrow B$. □

Interestingly, the connection formulae do not depend on the slope at the turning point. This is a reflection of the fact that the connection formulae transport the wavefunction from one region where WKB applies to another. And since the WKB approximation does not depend on the slope of the potential (except for the validity condition), neither do the connection formulae.

We also note that the connection formulae as written are linear transformations of the coefficients A and B, between the respective spaces. As such, we can write the connection formulae as matrix operators:

$$\mathbf{A} := \begin{pmatrix} -ie^{i\pi/4} & ie^{-i\pi/4} \\ e^{i\pi/4}/2 & e^{-i\pi/4}/2 \end{pmatrix} \tag{2.56a}$$

for the type-a turning point, and

$$\mathbf{B} := \begin{pmatrix} ie^{-i\pi/4}/2 & e^{-i\pi/4} \\ -ie^{i\pi/4}/2 & e^{i\pi/4} \end{pmatrix} \tag{2.56b}$$

for the type-b turning point, where both matrices transform between the spaces

$$\mathrm{span}\{\exp\bigl(i\hbar^{-1}I_x^p\bigr), \exp\bigl(-i\hbar^{-1}I_x^p\bigr)\} \to \mathrm{span}\{\exp\bigl(i\hbar^{-1}I_p^x\bigr), \exp\bigl(-i\hbar^{-1}I_p^x\bigr)\}, \tag{2.56c}$$

assuming that p is the turning point in question. These matrices are written in the natural of bases of the respective involved spaces.

The matrices invite us to evaluate the effect of passing two turning points as simply multiplying them: calculate $\mathbf{B}(p_2)\mathbf{A}(p_1)$ for two turning points p_1 and p_2, and act with that on the wavefunction. A quick calculation shows that $\mathbf{B}(p_2)\mathbf{A}(p_1) = \mathbf{I}$—life can be this simple!

Alas, too simple. The critical observation debunking our thinking is that the transport of passing through two turning points should depend on what happens in between, which it does not currently. For example, a broad hump in the potential should yield a markedly different effect than a skinny one, yet nowhere does this become apparent currently; we are missing an ingredient. We will remedy this in the following section, and use this remedy to create a matrix representation of the WKB-applicable potential with which we are dealing.

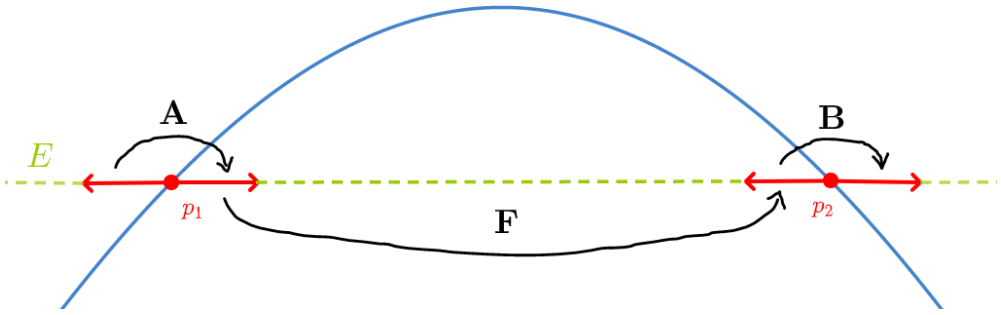


Figure 2.3: Effect of **F**, in conjunction with the matrices **A** and **B**.

2.4.3 Description of potential

The insight is that, after passing turning point p_1, we first have to transport the wavefunction to "before" the turning point p_2 before we can apply operation $\mathbf{B}(p_2)$. In the language of equation (2.56), we still need to find a transformation $\mathcal{F}$ so that

$$\begin{aligned}\mathcal{F}(p_1 \to p_2) : \mathrm{span}\{\exp\big(i\hbar^{-1}I^x_{p_1}\big), \exp\big(-i\hbar^{-1}I^x_{p_1}\big)\} \\ \longrightarrow \mathrm{span}\{\exp\big(i\hbar^{-1}I^{p_2}_x\big), \exp\big(-i\hbar^{-1}I^{p_2}_x\big)\}.\end{aligned} \tag{2.57}$$

Only then can we bona fide transport the wavefunction through both turning points a and b.

We recognize the simple identity

$$I^{p_2}_{p_1} = I^x_{p_1} + I^{p_2}_x \iff I^x_{p_1} = I^{p_2}_{p_1} - I^{p_2}_x. \tag{2.58}$$

So, an element of $\mathrm{span}\{\exp\big(i\hbar^{-1}I^x_{p_1}\big), \exp\big(-i\hbar^{-1}I^x_{p_1}\big)\}$ looks like

$$\begin{aligned}c_1 \exp\big(i\hbar^{-1}I^x_{p_1}\big) + c_2 \exp\big(-i\hbar^{-1}I^x_{p_1}\big) = \big[c_2 \exp\big(-i\hbar^{-1}I^{p_2}_{p_1}\big)\big] \exp\big(i\hbar^{-1}I^{p_2}_x\big) \\ + \big[c_1 \exp\big(i\hbar^{-1}I^{p_2}_{p_2}\big)\big] \exp\big(-i\hbar^{-1}I^{p_2}_x\big)\end{aligned} \tag{2.59}$$

(arbitrary constants $c_{1,2}$). As such, the choice of $\mathcal{F}$ is

$$\mathbf{F}(p_1 \to p_2) := \begin{pmatrix} 0 & \exp\big(-i\hbar^{-1}I^{p_2}_{p_1}\big) \\ \exp\big(i\hbar^{-1}I^{p_2}_{p_1}\big) & 0 \end{pmatrix}, \tag{2.60}$$

which is written in the natural bases of the spaces in equation (2.57). See also Figure 2.3.

There is one more observation to make before we can fully describe the effect of the potential on the solution. Namely, starting from $-\nu$, the first turning point we encounter will be of type a: $V(-\nu) = 0$ and $E > 0$, so V' at the turning point must be positive. The next turning point, then will be type b: we need to come from above in order to meet $V = E$ again at the turning point. Then the next turning point (if any) will be type a again, and so on, and so forth. That is to say, the turning points alternate in appearance. It is moreover not difficult to see that the amount of type a and b turning points needs to be equal (we need to end at $V(\nu) = 0$ again).

For some chosen E, identify the turning points p_j, $j = 1, 2, \ldots, n$, ordered so that $p_1 < p_2 < \cdots < p_n$. Then, we can describe the transform of the solution from $-\nu$ to ν as

$$\boxed{\mathbf{P} := \mathbf{F}(p_N \to \nu)\,\mathbf{B}\,\mathbf{F}(p_{N-1} \to p_N)\,\mathbf{A} \ldots \mathbf{B}\,\mathbf{F}(p_1 \to p_2)\,\mathbf{A}\,\mathbf{F}(-\nu \to p_1).} \tag{2.61}$$

Indeed, the first **F** takes us to the first turning point, which effect, being of type a, is then described by **A**. Following that, the next **F** takes us to the next turning point, which effect we take into account by **B**. Then another **F** for the next turning point, and so, and so forth, until we finally use **F** to go from the final turning point to the exit at ν. Thus, we see that the matrix **P** so constructed is such that

$$\begin{aligned}\mathbf{P} : \psi|_{x\approx -\nu} \longmapsto \psi|_{x\approx \nu} : \operatorname{span}\{\exp\bigl(i\hbar^{-1}I^x_{-\nu}\bigr), \exp\bigl(-i\hbar^{-1}I^x_{-\nu}\bigr)\} \\ \longrightarrow \operatorname{span}\{\exp\bigl(i\hbar^{-1}I^\nu_{x}\bigr), \exp\bigl(-i\hbar^{-1}I^\nu_{x}\bigr)\},\end{aligned} \tag{2.62}$$

written in the natural bases of the involved spaces.

Since we know the anatomy of **P**, we can prove the very useful Lemma below.

Lemma 2.14 (**P** is involutory)**.** *Assume that V is symmetric. Then, the matrix* **P** *is* involutory*, i.e.* $\mathbf{P}^2 = \mathbf{I}$.

Proof. In a symmetric potential, turning points must come in pairs $(p, -p)$: $V(x) = V(-x)$, so if $V(p) = E$, then $V(-p) = E$ as well. Following the earlier identification, this means that $p_n = -p_1$, $p_{n-1} = p_2$, et cetera. This is well-defined (i.e. n is even), as the amount of type a and b turning points are equal to each other and each one is followed by the other.

Now, place two copies of the product (2.61) after each other, and consider the middle section of this product:

$$\mathbf{P}\,\mathbf{P} = \ldots \mathbf{F}(-p_1 \to -p_2)\,\mathbf{A}\,\mathbf{F}(-\nu \to -p_1)\,\mathbf{F}(p_1 \to \nu)\,\mathbf{B}\,\mathbf{F}(p_2 \to p_1)\ldots. \tag{2.63}$$

The middle term evaluates to

$$\begin{aligned}\mathbf{F}(-\nu \to -p_1)\mathbf{F}(p_1 \to \nu) &= \begin{pmatrix} 0 & \exp\bigl(-i\hbar^{-1}I^{-p_1}_{-\nu}\bigr) \\ \exp\bigl(i\hbar^{-1}I^{-p_1}_{-\nu}\bigr) & 0 \end{pmatrix} \begin{pmatrix} 0 & \exp\bigl(-i\hbar^{-1}I^{\nu}_{p_1}\bigr) \\ \exp\bigl(i\hbar^{-1}I^{\nu}_{p_1}\bigr) & 0 \end{pmatrix} \\ &= \begin{pmatrix} \exp\bigl(i\hbar^{-1}[\cancel{I^{\nu}_{p_1} - I^{-p_1}_{-\nu}}]\bigr) & 0 \\ 0 & \exp\bigl(i\hbar^{-1}[\cancel{I^{-p_1}_{-\nu} - I^{\nu}_{p_1}}]\bigr) \end{pmatrix} \\ &= \mathbf{I},\end{aligned} \tag{2.64}$$

where the cancellation holds as

$$\begin{aligned}I^\nu_{p_1} = \int_{p_1}^{\nu} \sqrt{E - V(x)}\,dx &= -\int_{\nu}^{p_1} \sqrt{E - V(x)}\,dx \\ &= \int_{-\nu}^{-p_1} \sqrt{E - V(-y)}\,dy\,, \quad \text{with} \quad y = -x \\ &= \int_{-\nu}^{-p_1} \sqrt{E - V(y)}\,dy \\ &= I^{-p_1}_{-\nu}.\end{aligned} \tag{2.65}$$

So the two **F**s in the middle cancel. The next middle matrix product is $\mathbf{AB} = \mathbf{I}$, so these cancel as well. Then there are two more **F**s which cancel due to symmetry guaranteed by the "opposing" turning points (as above), then another **BA** pair, and so forth. All the matrices will cancel with their (eventual) neighbor, leaving us with a product total of **I**. Hence, $\mathbf{P}^2 = \mathbf{I}$. □

3 Resonances

In this section we will attempt to give meaning to the concept of a "resonance" in a quantum system. How is it defined, and how does that definition relate to other quantities such as the wavefunction of the system?

The mental image we will be relying on is that of a classical, elastic scattering experiment: we shoot a particle at a target, and then we look at its behavior (reflection or transmission) as a function of energy. Or, emulating quantum physics, we consider a stream of particles and look at the proportion that is transmitted through the target.

In particular, we will be interested in the phenomenon of *resonant scattering*. When this happens, the particle and target will form a "whole," in the sense that the entire system may be described by an eigenstate of the Hamiltonian, which then proceeds to decay in time. Or, borrowing the words of Moiseyev, "When the lifetime of the particle—target system in the region of interaction is larger than the collision time in a direct collision process we call the phenomenon a resonance phenomenon" [13].

We shall investigate this using quantum mechanics as described by the Schrödinger equation. In that spirit, we note that we are justified in studying this problem utilizing the time-independent equation only. After all, once we have found the stationary solutions, the time-dependent situation should follow by means of wavepacket constructions.

The model we will be relying on throughout this (and the next) section is delineated below.

1. **Utilize the Schrödinger equation:**

$$-\hbar^2\frac{d^2\psi}{dx^2}+V(x)\psi(x)=E\psi(x), \tag{3.1a}$$

   where we recall the assumption concerning the mass of the particle $2m\equiv 1$.

2. **Assume a real, bounded, compactly supported potential:**

$$V:\mathbb{R}\longrightarrow\mathbb{R}\text{ s.t. }V(x)=0\text{ if }|x|>\nu\text{ for some }\nu>0. \tag{3.1b}$$

   Here by bounded we mean that there exists some $M\geq 0$ s.t. $|V(x)|\leq M$ for all x. This then also excludes potentials like Coulomb, for which $V(x)\propto x^{-2}$.

3. **Split the different regions of the wavefunction as follows:**

$$\psi_{\text{full}}(x)=\begin{cases}\exp(ikx)+L\exp(-ikx) & \text{if}\quad x<-\nu\\ \psi_{\text{int}}(x) & \text{if}\quad x\in[-\nu,\nu]\\ S\exp(ikx) & \text{if}\quad x>\nu\end{cases}, \tag{3.1c}$$

   where k is such that $E=\hbar^2k^2$, and S and L are complex-valued and known as the *transmission* and *reflection* amplitudes, respectively. (Notice also the link back to the scattering matrix $\mathbf{S}$, as discussed in section 2.3.)

We will be interested in L and S, as these tell us about the result of the interaction between particle and target. We can immediately deduce that to each k there corresponds only one unique $S,L\in\mathbb{C}$, due to uniqueness of solutions of ODEs. As such, we recognize $S=S(k)$ and $L=L(k)$ as generally complex-valued functions of k.

Figure 3.1: Sketch of our scattering model, in which we are interested in the (properties of the) complex-valued functions $S(k)$ and $L(k)$.

There are two footnotes that need to be made concerning this model. The first is that the ψ we are so deriving will not be a normalizable function, so that it is also not a bona fide wavefunction. More pressingly, we need to reconsider the implicit assumption of E being a strictly real number. Let us illustrate this by means of an example. Consider a Hamiltonian permitting two eigenstates $|\psi_{1,2}\rangle$ with associated energies $E_{1,2}$. Starting from a normalized superposition $|\alpha\rangle = c_1 |\psi_1\rangle + c_2 |\psi_2\rangle$, the probability to measure $|\alpha\rangle$ after time t is

$$\begin{aligned}
\Pr(\text{measure } \alpha \text{ after time } t) &= |\langle\alpha|\mathcal{U}(t)|\alpha\rangle|^2 \\
&= |c_1^* \langle\psi_1| + c_2^* \langle\psi_2|) \\
&\qquad \times (c_1 \exp\bigl(-i\hbar^{-1}E_1 t\bigr) |\psi_1\rangle + c_2 \exp\bigl(-i\hbar^{-1}E_2 t\bigr) |\psi_2\rangle)|^2 \\
&= ||c_1|^2 \exp\bigl(-i\hbar^{-1}E_1 t\bigr) + |c_2|^2 \exp\bigl(-i\hbar^{-1}E_2 t\bigr)|^2 \\
&= |c_1|^4 + |c_2|^4 + 2|c_1 c_2|^2 \cos((E_2 - E_1)t/\hbar), \qquad (3.2)
\end{aligned}$$

which is *periodic*: when we start in $|\alpha\rangle$, we are guaranteed to return to it after time $T = 2\pi\hbar/|E_2 - E_1|$. However, for modeling decay we specifically do not want any manner of periodicity; characteristic of a decay is that it is a one-way process.

The solution to this contradiction is to consider the energy to be *complex* instead; this will allow for decay of states to occur. Exploring this idea will be the first order of business in the rest of this section. After that, we shall by means of the resolvent operator formally define what is meant by a resonance, and see that it is related to the function $S(k)$ that we introduced above. In fact, we will make the case to define resonances in terms of poles of (the meromorphic continuation of) $S(k)$. After giving some more properties of the function $S(k)$, we close this section by showing that the derived properties also hold for potentials which are decreasing sufficiently quickly.

3.1 Complexifying energy

To codify that we are now (generally) dealing with complex energies, we will from now on use the symbol $\mathcal{E}$ to emphasize this fact. However, since the real part of these energies will still be important, we maintain E to indicate whenever we consider our energies purely real. Let us additionally introduce the following notation, simplifying indicating real and imaginary parts.

Notation 3.1 (Shorthand real and imaginary part)**.** For any $z \in \mathbb{C}$, we write

$$z_{\mathrm{R}} := \operatorname{Re} z \quad \text{and} \quad z_{\mathrm{I}} := \operatorname{Im} z. \tag{3.3}$$

Let us make the decomposition $\mathcal{E} = \mathcal{E}_{\mathrm{R}} + i\mathcal{E}_{\mathrm{I}}$. The role of $\mathcal{E}_{\mathrm{R}}$ should be clear; what does adding an imaginary part to the energy mean? To illustrate, consider $|\psi\rangle$ as an eigenstate of the Hamiltonian with said complex energy $\mathcal{E}$. The probability of measuring this state after some time $t > 0$ has elapsed is given by

$$\Pr(\text{measure } \psi \text{ after time } t) = |\,\langle\psi|\,\mathcal{U}(t)|\psi\rangle\,|^2, \tag{3.4}$$

where $\mathcal{U}(t) := \exp(-i\hbar^{-1}t\,\mathcal{H})$ is the time-evolution operator, with $\mathcal{H}$ the time-independent Hamiltonian operator cf. (2.2). Working this out, we have

$$|\,\langle\psi|\,\mathcal{U}(t)|\psi\rangle\,|^2 = |\exp\!\big(-i\hbar^{-1}\mathcal{E}t\big)\,\langle\psi|\psi\rangle\,|^2 = \exp\!\big(2\hbar^{-1}\mathcal{E}_{\mathrm{I}}t\big). \tag{3.5}$$

So, with time, the probability of measuring our original state will decay—even though it is an eigenstate, which is persistent over time for real energies (indeed, for $\mathcal{E}_{\mathrm{I}} = 0$ the probability equals 1 for all time).

Thus we conclude that the introduced imaginary component of the energy makes it so that even if we start out in an eigenstate, we may not observe this anymore later in time. That is to say, the state "decays" in time. Note that for this mental picture to make sense, we need to enforce that $\mathcal{E}_{\mathrm{I}} \leq 0$; should the opposite be true, the relevant probability would increase and exceed 1, which is absurd.

The above realizations thus motivate us to make the following definition.

Definition 3.2 (Decay rate & lifetime)**.** We define $\Gamma > 0$ to be

$$\Gamma := -2\hbar^{-1}\mathcal{E}_{\mathrm{I}} \iff \mathcal{E}_{\mathrm{I}} = -\hbar\Gamma/2 \tag{3.6}$$

to be the *decay rate* of the state with energy $\mathcal{E}$. The quantity Γ^{-1} is the *lifetime* of the state.

In this way, the rhs of (3.5) may be rewritten to $\exp(-\Gamma t)$, which naturally justifies the name given to Γ (and also justifies the additional factor of $1/2$). The complex energy $\mathcal{E}$ can now be written as

$$\boxed{\mathcal{E} = E - i\hbar\Gamma/2,} \tag{3.7}$$

where E is the energy of the particle-target compound and Γ says something about the lifetime of the interaction. This is the form of the complexified energy that is also commonly found in literature.

Complexifying the energy also implies, through the relation $\mathcal{E} = \hbar^2k^2$, that the wavenumber must be taken complex. We write $k = k_{\mathrm{R}} + ik_{\mathrm{I}}$ and substitute into the above relation to find

$$E = \hbar^2(k_{\mathrm{R}}^2 - k_{\mathrm{I}}^2) \quad \text{and} \quad \Gamma = -4\hbar k_{\mathrm{R}}k_{\mathrm{I}}. \tag{3.8}$$

Since we defined $\Gamma < 0$, this means that k_{R} and k_{I} should be of differing signs. However, whether we need to choose $k_{\mathrm{R}} > 0 > k_{\mathrm{I}}$ or $k_{\mathrm{I}} > 0 > k_{\mathrm{R}}$, or whether the choice matters at all, we cannot establish from this information alone.

With the aim of making a clear choice between $k_\mathrm{R} > 0 > k_\mathrm{I}$ or $k_\mathrm{I} > 0 > k_\mathrm{R}$, let us consider the probability density $\rho(x,t) = |\Psi(x,t)|^2$ associated with the solution we are assuming. The probability density is, following Born's rule, associated with the location of the particle, in the closest allowable sense. By multiplying the time evolution on the wavefunction ψ_full and simplifying, we find that in the limit of $x \to \infty$,

$$\rho(x,t) = |\Psi(x,t)|^2 = |\exp\bigl(-i\hbar^{-1}\mathcal{E}t\bigr)\psi_\mathrm{full}|^2 = |S|^2 \exp\left(-\Gamma\left[t - \frac{x}{2\hbar k_\mathrm{R}}\right]\right). \tag{3.9}$$

(Full calculation may be found in Appendix B.) This equation describes that, with time, the probability density is being translated in space with velocity $v := 2k_\mathrm{R}$; the factor of Γ here controls the "width" of the probability density. Considering Born's rule, this expression only makes sense if we consider $v > 0$; after all, for $x > \nu$ there should only be particles which have come through the target, and these are traveling towards $+\infty$. Therefore, we must choose $k_\mathrm{R} > 0$ and consequently $0 > k_\mathrm{I}$ for the real and imaginary parts of our wavenumbers.

Our choice should be consistent with what is going on on the other side, i.e. where $x \to -\infty$. There, we have two terms with which to contend instead of just one. By the same strategy of finding the probability density and simplifying as above, we find for $x \to -\infty$

$$\rho(x,t) = \exp\left(-\Gamma\left[t - \frac{x}{2\hbar k_\mathrm{R}}\right]\right) + |L|^2 \exp\left(-\Gamma\left[t + \frac{x}{2\hbar k_\mathrm{R}}\right]\right) + \text{osc.} \tag{3.10}$$

(Once more, full calculation can be found in Appendix B). By the choice $k_\mathrm{R} > 0 > k_\mathrm{I}$ and the same logic as above, we now identify *two* waves: the first term is right-moving, and hence towards to the target, and the second is left-moving, towards $-\infty$. This is also consistent with the roles accorded to the several terms in the solution of the wavefunction.

In the spirit of scattering theory, another way to characterize the above probability densities is by their direction of motion with respect to the target. The density for $x \to \infty$, in (3.9), is right-moving, and so it is *outgoing* with respect to the target. For $x \to -\infty$, which density is given in (3.10), the first term is right-moving also, so it is *incoming* to the target. Naturally, then, the second term is also characterized as outgoing, since it is left-moving away from the potential.

The notions of complex energy and incoming/outgoing states are brought together in the following definition.

Definition 3.3 (Gamow-Siegert states)**.** An eigenstate ψ of $\mathcal{H}$ is called a *Gamow-Siegert* (GS) state if it

1. satisfies $\mathcal{H}\psi = \mathcal{E}\psi$ with $\mathcal{E}_\mathrm{R} > 0 > \mathcal{E}_\mathrm{I}$, and
2. is *purely outgoing* at large distance, i.e.

$$\psi' \overset{x\to\pm\infty}{\sim} \pm ik\psi. \tag{3.11}$$

One point that warrants an explanation is why we want to consider only *purely* outgoing states, instead of states which also have an incoming part like in (3.10). The reason is that purely outgoing states exist without the presence of a "particle gun" which is supplying particles into the system. This makes them a "true" model of natural decay, in which we do not assume that particles are supplied from outside.

Remark 3.4 (Optical model; target as sink/source)**.** There is an alternative interpretation of complex eigenvalues, based on shifting the imaginary part to the potential:

$$-\hbar^2\frac{d^2\psi}{dx^2}+V(x)\psi=(E-i\hbar\Gamma/2)\psi \iff -\hbar^2\frac{d^2\psi}{dx^2}+\left\{V(x)+\frac{i\hbar\Gamma}{2}\right\}\psi=E\psi. \quad (3.12)$$

Complex potentials break the continuity relation for the probability density, in- or decreasing it instead over time. Interpreting the total amount of probability to be (proportional to) the total amount of particles under consideration, one can derive the following relation:

$$\frac{dN}{dt}=2\int V_{\mathrm{I}}(x)\rho(x)\,dx\,, \quad (3.13)$$

where N is the total number of particles and ρ the density. (see [15, (64)] and the discussion there for further detail). In this sense, the target acts as a *source* of particles, which then is counteracted by particles dissipating off to infinity. This is called the *optical model* of studying resonances, as this view can also be utilized to study reflection/refraction of optical waves interacting at interfaces.

3.1.1 The relation $\mathcal{E}\leftrightarrow k$

Throughout the previous subsection we have related k to $\mathcal{E}$ by means of $\mathcal{E}=\hbar^2k^2$, allowing us to map $k\mapsto\mathcal{E}$ without any trouble. It is the reverse relation, $\mathcal{E}\mapsto k$, that is troublesome and so requires some attention. Naively that mapping would be given by $k=\hbar^{-1}\sqrt{\mathcal{E}}$. However, the two choices we have for $\sqrt{\mathcal{E}}$—related by $\pm$—are *not* equivalent in this case. As an illustration of why, we need not look further than the definition of GS states. Here only one choice of k leads to an outgoing state, whilst the other will definitely *not* lead to one. As such, ambiguity has arisen when attempting to relate $\mathcal{E}$ to k.

To resolve this ambiguity, we need to somehow "attach" to $\mathcal{E}$ the declaration of which choice of square root (i.e. which choice of k) we need to take when we need to. Mathematically this means that we should consider $\mathcal{E}$ to live on a *Riemann surface*, consisting of two *(Riemann) sheets*, corresponding to the two possible choices of preimage of $\mathcal{E}$. There is a great deal of literature concerning Riemann surfaces (see for instance [6], or [18] for a more gentle treatment), but it comes down to being a way to "sew together" copies of the complex plane to make for a natural codomain of a certain function. For our energy Riemann surface, we sew the two copies along the positive real axis, recognizing 0 to be the branch point ($\mathcal{E}=0\mapsto k=0$, regardless of which sheet we should be on). This yields a mental image like in Figure 3.2.

For our purposes, though, it will be good enough to simplify the Riemann surface at hand by means of $\mathbb{C}\times\{\mathrm{I},\mathrm{II}\}$, where the Roman numerals indicate which sheet we are on, and consequently which k to associate with $\mathcal{E}$—see Figure 3.3. Thus, effectively the positive axis is a "portal" by which we can traverse between the two sheets.

It then remains us to define the square root for the two sheets, which we do next.

Definition 3.5 (Definition of square roots)**.** On the Riemann surface of the function $k(\mathcal{E})=\hbar^{-1}\sqrt{\mathcal{E}}$, on the two sheets we define the square roots as follows.

1. On sheet I, we have $\arg\sqrt{\mathcal{E}}\in[0,\pi) \iff \operatorname{Im}\sqrt{\mathcal{E}}>0$ for $\mathcal{E}\notin(0,\infty)$.

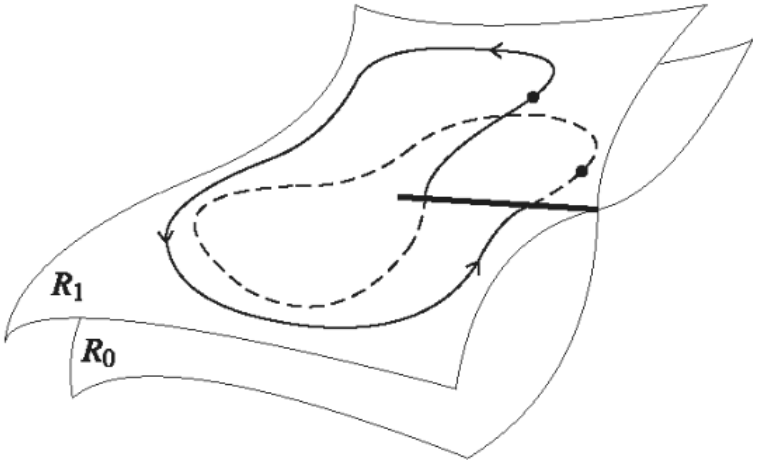


Figure 3.2: "Sewed together" picture of the Riemann surface for the function $k = \hbar^{-1}\sqrt{\mathcal{E}}$. (Source: [15, Fig. 4])

2. On sheet II, we have $\arg\sqrt{\mathcal{E}} \in [\pi, 2\pi) \iff \mathrm{Im}\sqrt{\mathcal{E}} < 0$ for $\mathcal{E} \notin (0, \infty)$.

An observation to make is that on the first sheet, the purely outgoing solutions will be square-integrable: $k_\mathrm{I} > 0$ implies $\pm ikx$ has negative real part for $x \to \pm\infty$, so $|\psi|^2$ will decay exponentially. That is to say that any wavefunction will have to have its energy on the first sheet. (We will also see later that here is where bound states live.) For this reason, the first sheet is also known as the *physical* sheet.

In contrast, the alias of the second sheet is the *unphysical* sheet, as there the outgoing solutions grow exponentially for extreme x, making it so they will definitely not be wavefunctions. Despite this inconvenience, the unphysical sheet will be getting most of our attention, as that is where the situation $k_\mathrm{R} > 0 > k_\mathrm{I}$ can occur, and where the interesting, yet-to-be-defined resonances are located.

3.2 Resolving the definition

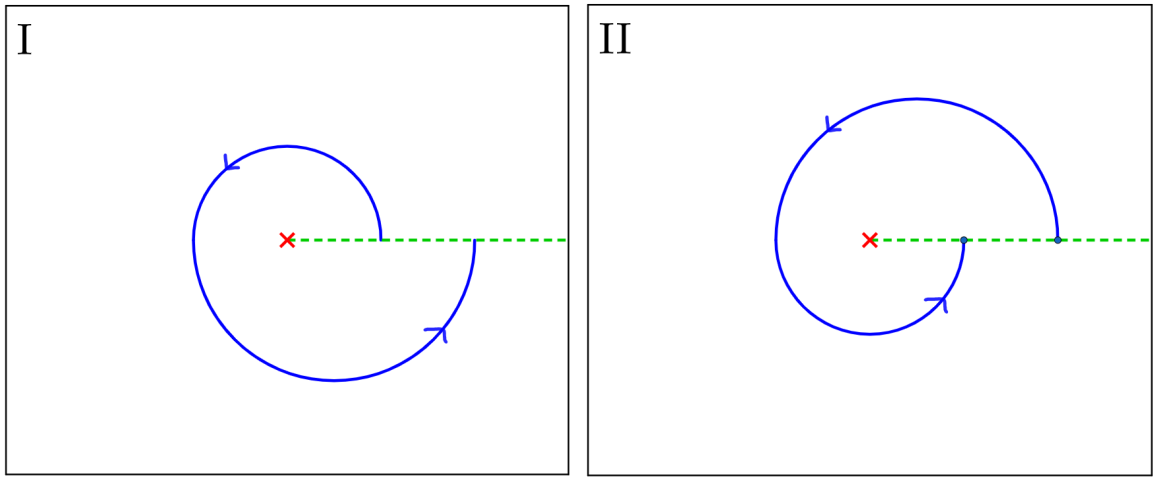
With what we have learned about $S(k)$ in the above, we can almost make a working definition of resonances. Since this working definition is dependent on the formal definition, though, we need to first spend some time on learning about it. To do this, we have to get acquainted with the *resolvent* operator of a certain system.

Definition 3.6 (Resolvent operator v1)**.** For $\mathcal{E} \in \mathbb{C}$, we define as the *resolvent* $\mathcal{R}(\mathcal{E})$ to be the operator which satisfies

$$(\mathcal{H} - \mathcal{E})\mathcal{R}(\mathcal{E})\psi = \mathcal{R}(\mathcal{E})(\mathcal{H} - \mathcal{E})\psi = \psi, \tag{3.14}$$

for all $\psi \in L^2$.

In effect, the resolvent is the "inverse" of the Schrödinger operator $\mathcal{H} - \mathcal{E}$. The above describes the resolvent operator, but it does not give us a concrete expression to calculate it. This we address in the following Lemma, which relates the resolvent to the time-evolution operator, and so may also provide some intuition for it.



(a) Sheet I (b) Sheet II

Figure 3.3: Two separate complex planes picture. Each plane represents a sheet of the Riemann surface, with an example loop traversing both sheets. The green dashed horizontal is the branch cut $(0, \infty)$, and the red cross is the branch point 0.

Lemma 3.7 (Resolvent as Laplace transform)**.** *We have that*

$$\mathcal{R}(\mathcal{E}) = i\hbar^{-1} \int_0^\infty \exp\big(i\hbar^{-1}\mathcal{E}s\big)\mathcal{U}(s)\,ds \quad \textit{for} \quad \mathcal{E}_{\mathrm{I}} > 0, \tag{3.15}$$

where $\mathcal{U}(t) := \exp(-i\hbar^{-1}t\,\mathcal{H})$ *is the time evolution operator. In this way, it is the* Laplace transform *of said time evolution operator.*

Proof. This proof is heavily inspired by [10, §2.2]. We shall show that for the rhs of (3.15), it commutes with $\mathcal{H} - \mathcal{E}$ and their product yields identity $\mathcal{I}$.

Let us define $\mathcal{U}_\mathcal{E}(t) := \exp(-i\hbar^{-1}t(\mathcal{H} - \mathcal{E}))$. Now observe that

$$\begin{aligned}
-i\hbar^{-1}(\mathcal{H} - \mathcal{E}) \int_0^\infty \exp\big(i\hbar^{-1}\mathcal{E}s\big)\mathcal{U}(s)\,ds &= \lim_{\epsilon\to 0} \frac{\mathcal{U}_\mathcal{E}(\epsilon) - \mathcal{I}}{\epsilon} \int_0^\infty \mathcal{U}_\mathcal{E}(s)\,ds \\
&\overset{\star}{=} \lim_{\epsilon\to 0} \frac{1}{\epsilon}\left[\int_0^\infty \mathcal{U}_\mathcal{E}(s+\epsilon)\,ds - \int_0^\infty \mathcal{U}_\mathcal{E}(s)\,ds\right] \\
&= \lim_{\epsilon\to 0} \frac{1}{\epsilon}\left[\int_\epsilon^\infty \mathcal{U}_\mathcal{E}(s)\,ds - \int_0^\infty \mathcal{U}_\mathcal{E}(s)\,ds\right] \\
&= \lim_{\epsilon\to 0} \frac{-1}{\epsilon} \int_0^\epsilon \mathcal{U}_\mathcal{E}(s)\,ds \\
&= -\mathcal{I},
\end{aligned} \tag{3.16}$$

where in $\star$ we utilized the identity

$$\mathcal{U}_\mathcal{E}(t_1)\mathcal{U}_\mathcal{E}(t_2) = \mathcal{U}_\mathcal{E}(t_2)\mathcal{U}_\mathcal{E}(t_1) = \mathcal{U}_\mathcal{E}(t_1 + t_2). \tag{3.17}$$

This identity also shows that $\mathcal{H} - \mathcal{E}$ and the integral commute. As such, we see that indeed

$$\mathcal{R}(\mathcal{E}) = (\mathcal{H} - \mathcal{E})^{-1} = i\hbar^{-1} \int_0^\infty \mathcal{U}(s) e^{i\hbar^{-1}\mathcal{E}s}\,ds\,, \tag{3.18}$$

as we intended to show. □

As a result of this Lemma, we can study the effect of the resolvent operator on a state by means of the time-evolution operator. Assume that we have a Hamiltonian $\mathcal{H}_0$ which admits discrete bound states ψ_j with corresponding energies $E_j < 0$, and has continuous spectrum for $E > 0$. We can decompose some $\psi \in L^2$ in terms of the bound states, $\psi = \sum_j \alpha_j \psi_j$, and evaluate the effect of the resolvent:

$$\begin{aligned}\mathcal{R}(\mathcal{E})\psi &= i\hbar^{-1} \int_0^\infty \exp\bigl(-i\hbar^{-1}\mathcal{E}s\bigr) \left[\sum_j \alpha_j \psi_j\right] ds \\ &= i\hbar^{-1} \sum_j \alpha_j \psi_j \int_0^\infty \exp\bigl(i\hbar^{-1}(\mathcal{E} - E_j)s\bigr)\, ds\,. \end{aligned} \tag{3.19}$$

There is a problem appearing in this expression: it will diverge if either i) $\mathcal{E}_\mathrm{I} \leq 0$, or ii) $\mathcal{E} = E_j$ for some j. Since the case i) includes ii), we can solve this problem by requiring in the definition of the resolvent that $\mathcal{E}_\mathrm{I} > 0$.

However, this restriction creates another problem. We have defined above that GS states require $\mathcal{E}_\mathrm{I} < 0$, and so with the restriction $\mathcal{E}_\mathrm{I} > 0$, the resolvent operator cannot work on GS states. This could be solved by means of a continuation of the resolvent operator into $\mathcal{E}_\mathrm{I} \leq 0$, but there is a fundamental issue here. Suppose that $E > 0$ lies in the continuous part of the spectrum of $\mathcal{H}_0$ and that ψ_E is its corresponding eigenfunction. Then we find that

$$\mathcal{R}(E)(\mathcal{H}_0 - E)\psi_E = \mathcal{R}(E)\mathbf{0} = \mathbf{0} \neq \psi_E, \tag{3.20}$$

where $\mathbf{0}$ is the zero function. This means that the resolvent operator has a pole at the energy E. However, since E was arbitrary and lies in the continuous spectrum of $\mathcal{H}_0$, the resolvent in fact has a continuum of poles along the positive real axis. As such, the resolvent would not be able to be *meromorphically* continued (for which all poles must be isolated).

We could now be at peace with a resolvent operator continued into $\mathcal{E}_\mathrm{I} < 0$ that is not meromorphic. However, that means additional trouble in the continuation itself. Declaring this definition too problematic, we need to reconsider it.

The resolution is to augment the definition of the resolvent operator with an additional condition. For clarity, this is written down below in a new Definition.

Definition 3.8 (Resolvent operator v2)**.** For $k \in \mathbb{C} : k_\mathrm{I} > 0$, we redefine the resolvent operator $\mathcal{R}(k) : L^2 \to L^2$ to be the operator satisfying

1. $(\mathcal{H} - \hbar^2 k^2)\mathcal{R}(k)\psi = \mathcal{R}(k)(\mathcal{H} - \hbar^2 k^2)\psi = \psi$ for all $\psi \in L^2$
2. $\mathcal{R}(k)\phi$ is purely *outgoing*, i.e.

$$\mathcal{R}(k)\phi \propto \begin{cases} \exp(ikx) & \text{for} \quad x > \nu \\ \exp(-ikx) & \text{for} \quad x < -\nu \end{cases}. \tag{3.21}$$

As it turns out, with this definition a meromorphic continuation is possible, as is the topic of the following Theorem.

Theorem 3.9 (Meromorphic continuation of the resolvent)**.** *The resolvent operator $\mathcal{R}(k)$ can be extended to a meromorphic family of operators for $k \in \mathbb{C}$, when considering it to run over the spaces*

$$\boxed{\mathcal{R}(k) : L^2_{\text{com}} \longrightarrow L^2_{\text{loc}},} \tag{3.22}$$

instead of $L^2 \to L^2$. Here, L^2_{com} is the space of L^2 functions with compact support, and L^2_{loc} the space of functions locally in L^2, which is to say

$$L^2_{\text{loc}} = \left\{ q : \mathbb{R} \to \mathbb{R} : \int_{-A}^{A} |q|^2 \, dx < \infty \text{ for all } A > 0 \right\}. \tag{3.23}$$

Proof. For a formal proof, see [3, §2.2]. □

Why do the spaces need to be chosen in this particular way to furnish the continuation? Let us try to gain an intuition by considering the case on the positive real line. That the image now should be L^2_{loc} instead of L^2 comes from the outgoing condition: the outgoing waves are clearly in L^2_{loc} for $k_{\text{I}} \leq 0$, but not in L^2. In turn, then, that the domain is curtailed to L^2_{com} stems from the fact that when operated on by $\mathcal{H} - \hbar^2 k^2$, a purely outgoing function will have a compact support. That is to say,

$$\mathcal{H} - \hbar^2 k^2 : \{\phi : \phi \in L^2_{\text{loc}} \;\&\; \phi \text{ purely outgoing}\} \longrightarrow L^2_{\text{com}}, \tag{3.24}$$

as purely outgoing functions satisfy the Schrödinger equation outside of the support of V. This does not constitute a full proof of the chosen spaces, but should show the interplay between the two.

With this construction done, we can finally properly define resonances.

Definition 3.10 (Resonance)**.** A *resonance* is a pole of the resolvent $\mathcal{R}$ (as defined in Definition 3.8, and including in its meromorphic continuation to the lower-half k-plane). More concretely, for $\phi, \psi \in L^2_{\text{com}}$, a resonance is a pole of the meromorphic continuation of the inner product $\langle \phi, \mathcal{R}(k)\psi \rangle$.

Owing to the problem ii) identified for equation (3.19), we would suspect that there are poles occurring there where the energy corresponds to one of the bound states of the Hamiltonian. This is indeed correct, as we will show in the next Proposition.

Proposition 3.11 (Bound states)**.** *A resonance located at k with $k_{\text{I}} > 0$ must have that it is purely imaginary, i.e. $k = i\kappa$ for some $\kappa > 0$. The associated state is called a* bound state*, and its energy $E = \hbar^2 k^2 < 0$ is a* bound state energy*.*

Proof. Let $k : k_{\text{I}} > 0$ be such that a resonance occurs, which means that there is a solution of the Schrödinger equation which is purely outgoing. Moreover, since $k_{\text{I}} > 0$, the real part of the exponent $\pm ikx$ will be negative for $x \to \pm\infty$, so that the solution will exhibit exponential decay to both sides, making it square-integrable. As such, the solution is a bona fide wavefunction solution to the Schrödinger equation.

The existence of a wavefunction as eigenfunction of the Hamiltonian means that the associated energy $\mathcal{E}$ must be a real number, due to self-adjoint-ness. Then, $k_{\text{I}} > 0$ and $\mathcal{E}$ being real can only be unified if we conclude that $\mathcal{E} < 0$ and k is purely imaginary. □

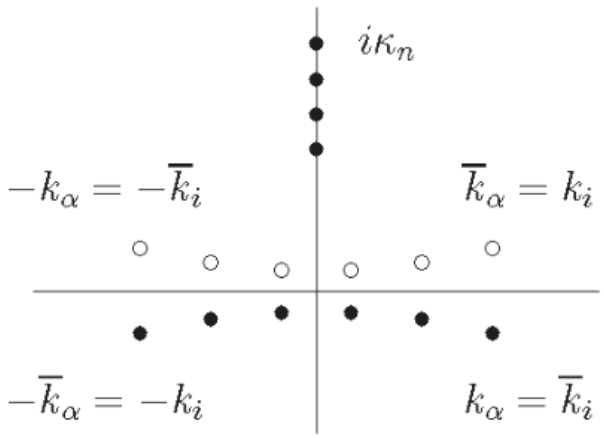


Figure 3.4: Example of locations of resonances in the k-plane (indicated by solid black dots). The resonances on the vertical axis represent bound states. (Source: [15, Fig. 4].)

Bound states are called this way as their negative energy does not allow them to exist "outside" of the potential, thus binding them inside.

Furthermore, the resolvent has a symmetry property which is also carried over in the meromorphic continuation. This comes from the observation that, for some $\phi \in L^2_{\text{com}}$, we have

$$[\mathcal{R}(k)\phi]^* \overset{x>\nu}{\propto} \exp(ikx)^* = \exp(i(-k^*)x) \propto \mathcal{R}(-k^*)\phi, \tag{3.25}$$

and similarly for $x < -\nu$. Combined with linearity, this suggests that $\mathcal{R}(-k^*) \propto [\mathcal{R}(k)]^*$ as operators, over the whole real line. In fact equality can be shown, for which details see [3, (2.2.13)]. As such, we expect resonances to come in pairs, which lie symmetrically around the imaginary axis.

The above two considerations thus describe where resonances could be located in the complex k-plane: either on the positive imaginary axis, or in pairs in the lower half plane mirrored in the imaginary axis. The resulting structure is sketched in Figure 3.4. In addition, the various resonances have names owing the way in which they appear in the calculation, i.e. from which feature of the potential they are "derived." A representative sketch of these may be found in Figure 3.5, but we will not delve further into the specific meaning of the different types of poles than we have done thusfar.

So far we have defined resonances and see where they have to be located in the complex k-plane, but how can we actually locate these? We introduce the following crucial Proposition.

Proposition 3.12 (Resonances and linear (in)dependence)**.** *Let $\phi_{1,2}$ be the solutions to $\mathcal{H}\psi = \hbar^2 k^2 \psi$ for some k, such that*

$$\phi_1 = \exp(ikx) \text{ for } x > \nu \quad \text{and} \quad \phi_2 = \exp(-ikx) \text{ for } x < -\nu. \tag{3.26}$$

Then, the resolvent will have a pole at k if and only if the solutions $\phi_{1,2}$ are linearly dependent.

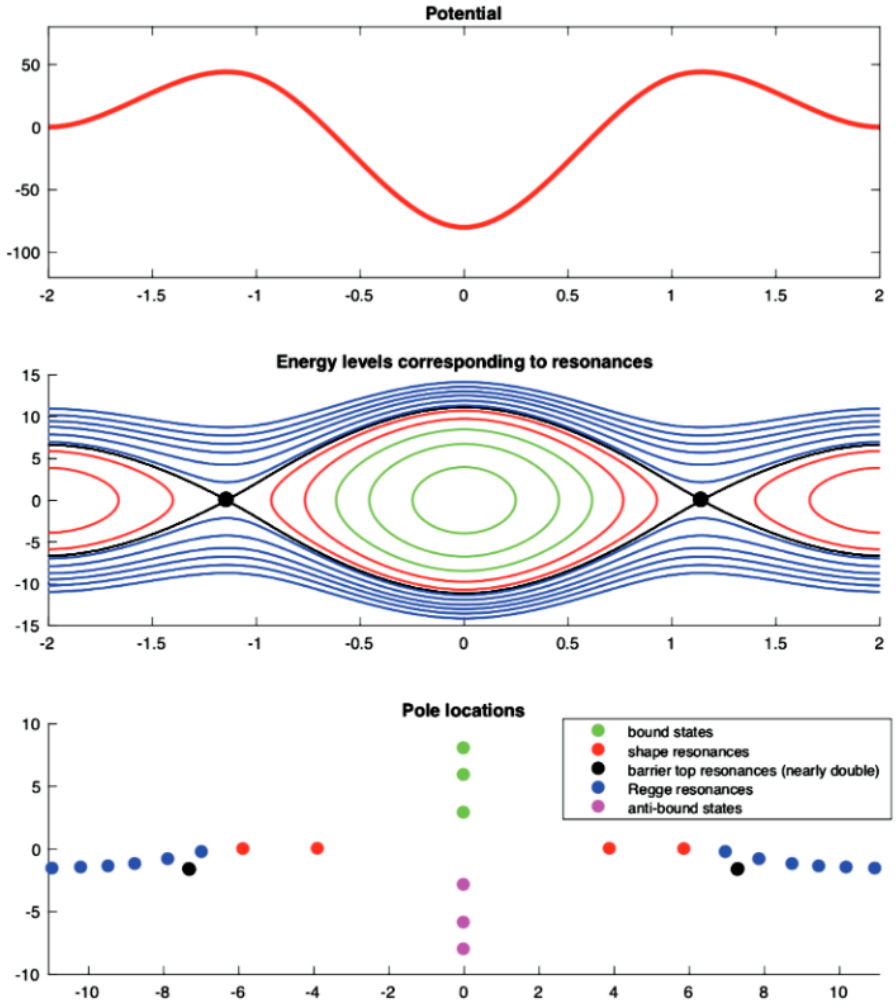


Figure 3.5: Pole names in the k-plane, classified by means of classical mechanics (in **green** are the discussed bound states) (Source: [3, Fig. 1.8]).

Proof. Let us prove both directions separately, though they have many steps in common.

$\Longrightarrow$ Suppose $\phi_{1,2}$ are linearly independent. Then it follows that neither is purely outgoing; indeed, if w.l.o.g. ϕ_1 were purely outgoing, then $\phi_1 \propto \phi_2$ for $x < -\nu$, which by uniqueness implies $\phi_1 \propto \phi_2$ everywhere. As such, we can write

$$\begin{aligned}(\mathcal{H} - \hbar^2 k^2)\mathcal{R}(k)\mathbf{0} = \mathbf{0} &\implies \mathcal{R}(k)\mathbf{0} \in \ker(\mathcal{H} - \hbar^2 k^2) \\ &\implies \mathcal{R}(k)\mathbf{0} \in \operatorname{span}\{\phi_1, \phi_2\} \\ &\implies \mathcal{R}(k)\mathbf{0} = \mathbf{0}. \end{aligned} \tag{3.27}$$

The last line follows as $\mathbf{0}$ is the only element in $\operatorname{span}\{\phi_1, \phi_2\}$ which is purely outgoing. As such, we conclude that no pole occurs in this case. Thus, by contrapositive, a pole occurring implies that $\phi_{1,2}$ are linearly dependent.

$\Longleftarrow$ Now suppose that $\phi_{1,2}$ are linearly dependent. This means that $\phi_1 \propto \phi_2$, and as

such that both are purely outgoing. We repeat the reasoning from above:

$$\begin{aligned}\mathcal{R}(k)(\mathcal{H}-\hbar^2k^2)\mathbf{0}=\mathbf{0} &\implies \mathcal{R}(k)\mathbf{0}\in\ker(\mathcal{H}-\hbar^2k^2)\\ &\implies \mathcal{R}(k)\mathbf{0}\in\operatorname{span}\{\phi_1\}.\end{aligned}\tag{3.28}$$

This is as far as we can get with determining what $\mathcal{R}(k)\mathbf{0}$ equals; in principle the resolvent of $\mathbf{0}$ could be any solution to the Schrödinger equation, not necessarily needing to be zero. As such, we encounter a pole of the resolvent, and hence a resonance.

Since we have now shown both directions, the proof is complete. □

This Proposition shows that the occurrence of resonances is linked with the (non-)degeneracy of the space of solutions to the Schrödinger equation: when it becomes one-dimensional, a resonance occurs.

Checking linear (in)dependence of solutions of the Schrödinger equation is not a very scalable method, though, not in the least because we would first need to solve the equation to find them. For this reason, we aim to find a simple formula or condition from which we can deduce (in)dependence of the solutions. As we shall discuss in the upcoming section, this will be accomplished by means of the Wronskian, and relating it to the scattering amplitude $S(k)$.

3.3 The function $S(k)$

It is here that we want to reintroduce the function $S(k)$, first defined in the model (3.1c), but tucked away since then. Besides being able to tell us something about the solution (in)dependence (as we will show momentarily), its use also lies in the fact that we can find an algebraic expression to define it, not just a numerical one (as we had shown in the preliminaries to be the case). This will allow us to—later in the section—derive properties of $S(k)$.

3.3.1 Dependence relation

Following up from Proposition 3.12, let us recall the two solutions of the Schrödinger equation $\phi_{1,2}$, and let us emphasize the dependence on k by parsing this as an argument: $\phi_{1,2}\equiv\phi_{1,2}(k)$. In the limit of $|x|>\nu$, these solutions exhibit the behaviors

$$\phi_1(k)=\exp(ikx)\text{ for }x>\nu\quad\text{and}\quad\phi_2(k)=\exp(-ikx)\text{ for }x<-\nu.\tag{3.29}$$

We note that, due to these behaviors, these functions can be used as bases for every other solution by looking at their behavior for $|x|>\nu$. For example, if $\chi(x)$ is a solution, then

$$\chi(x)|_{\text{right}}=\chi_+\exp(ikx)+\chi_-\exp(-ikx)=\chi_+\phi_1(k)+\chi_-\phi_1(-k),\tag{3.30}$$

for relevant constants $\chi_+,\chi_-\in\mathbb{C}$. Thus, we can express χ for $x>\nu$ as a superposition of $\phi_1(k)$ and $\phi_1(-k)$. Similarly, we can express $\chi|_{\text{left}}$ in the basis $\{\phi_2(k),\phi_2(-k)\}$.

In fact, this expression in terms of a basis locally (i.e. only for $|x|>\nu$) holds globally, due to the uniqueness. This pivotal fact we use to our advantage. Let us

establish that in the case we are considering (referring back to (3.1c)), we can make the identifications $\phi_1(\pm k) = \exp(\pm ikx)$ on $x > \nu$ and $\phi_2(\pm k) = \exp(\mp ikx)$ on $x < -\nu$. We then observe that

$$\psi_{\text{full}}|_{x>\nu} = S(k)\phi_1(k)|_{x>\nu} \overset{\star}{\Longrightarrow} \psi_{\text{full}} = S(k)\phi_1(k) \tag{3.31a}$$

and

$$\psi_{\text{full}}|_{x<-\nu} = \phi_2(-k) + L(k)\phi_2(k) \overset{\star}{\Longrightarrow} \psi_{\text{full}} = \phi_2(-k) + L(k)\phi_2(k), \tag{3.31b}$$

which combination implies directly that we must have

$$S(k)\phi_1(k) = \phi_2(-k) + L(k)\phi_2(k). \tag{3.32}$$

The implications $\star$ in (3.31) hold because of uniqueness of solution to ODEs. From this equality, then, we can directly show the following crucial Lemma.

Lemma 3.13 (Solution (in)dependence)**.** *We have that*

$$\boxed{S(k)^{-1} = -(2ik)^{-1}[\phi_1(k), \phi_2(k)] \quad \textit{for} \quad |x| > \nu \textit{ and } k \neq 0,} \tag{3.33}$$

where $[f, g] := fg' - f'g$ *is the* Wronskian (determinant) *of functions* f *and* g*, and prime indicates differentiation w.r.t.* x*. (Cf. [2, §2.3].)*

Proof. Let us prove this first for $x < -\nu$. We calculate:

$$\begin{aligned}
[\phi_1(k), \phi_2(k)] &= S(k)^{-1}[S(k)\phi_1(k), \phi_2(k)] \\
&= S(k)^{-1}[\phi_2(-k) + L(k)\phi_2(k), \phi_2(k)] \\
&= S(k)^{-1}\left(\{\phi_2(-k) + \cancel{L(k)\phi_2(k)}\}\phi_2'(k) - \{\phi_2'(-k) + \cancel{L(k)\phi_2'(k)}\}\phi_2(k)\right) \\
&= S(k)^{-1}\left(\phi_2(-k)\phi_2'(k) - \phi_2'(-k)\phi_2(k)\right).
\end{aligned} \tag{3.34}$$

Now we invoke the assumption of $x < -\nu$, so we have $\phi_2(k) = \exp(-ikx)$. Hence:

$$\begin{aligned}
\phi_2(-k)\phi_2'(k) - \phi_2'(-k)\phi_2(k) &= \exp(ikx) \times -ik\exp(-ikx) - ik\exp(ikx) \times \exp(-ikx) \\
&= -2ik,
\end{aligned} \tag{3.35}$$

which we can then combine with (3.34) to find

$$[\phi_1(k), \phi_2(k)] = -2ikS(k)^{-1}, \tag{3.36}$$

completing the proof for $x < -\nu$.

For the case $x > \nu$, note that by the reasoning leading up to (3.32) and making the substitution $x \to -x$, we can derive the relation

$$S(k)\phi_2(k) = \phi_1(-k) + L(k)\phi_1(k) = \psi_{\text{full}}(-x) \tag{3.37}$$

Starting from this relation, we follow the steps as for the case $x < -\nu$ to show $x > \nu$. □

It follows directly that if $S(k)^{-1} = 0$ for some k, the solutions $\phi_{1,2}(k)$ must be linearly dependent on each other, i.e. $\phi_1(k) \propto \phi_2(k)$. And, following from Proposition 3.12, we have that in the case of linearly dependent solutions, a resonance is encountered for that specific k. This invites us to fuse the result of Lemma 3.13 with Proposition 3.12 in order to form a condition for resonances based *solely* on the transmission amplitude $S(k)$. The result is the below definition.

Definition 3.14 (Resonance through $S(k)$)**.** We shall call a pole of the function $S(k)$, as defined through (3.1c), a *resonance*.

This definition will prove valuable to the later parts of this thesis, as computing $S(k)$ is easier than finding the resolvent.

Up to this point, though, the function $S(k)$ has only been defined implicitly from the setting we are studying. This we will strive to remedy in the next subsection, where we intend to describe $S(k)$ algebraically. Concretely, we will show that $S(k)$ is meromorphic on the upper half of the complex k plane. This will then furnish a continuation to the entire k-plane, just like for the resolvent, to give us a full description.

3.3.2 Meromorphic structure

To show that the function $S(k)$ is meromorphic, we will stick closely to the analysis as presented in [2, §2.1-3]. We once more bring to mind the solutions $\phi_{1,2}(k)$, chosen so as to exhibit

$$\phi_1(\pm k) = \exp(\pm ikx) \text{ for } x > \nu \quad \text{and} \quad \phi_2(\pm k) = \exp(\mp ikx) \text{ for } x < -\nu. \tag{3.38}$$

We have already established that $\{\phi_{1,2}(k), \phi_{1,2}(-k)\}$ are bases of the solution space in the regions $x > \nu$ resp. $x < -\nu$. In the spirit of regarding these functions more like a basis, let us simplify them by removing their oscillatory behavior.

Definition 3.15 (Jost function)**.** We define the *Jost functions* to be

$$m_{1,2}(x,k) := \exp(\mp ikx)\phi_{1,2}(k). \tag{3.39}$$

As a consequence, $m_{1,2}$ will satisfy the Schrödinger-esque equations

$$-\hbar^2\phi''_{1,2} + V(x)\phi_{1,2} = \mathcal{E}\phi_{1,2} \iff m''_{1,2} \pm 2ikm'_{1,2} = \hbar^{-2}V(x)m_{1,2}, \tag{3.40}$$

where the prime indicates differentiation w.r.t. x. Furthermore $m_{1,2} = 1$ for $x > \nu$ resp. $x < -\nu$, as is apparent from the definition.

Lemma 3.16 (Properties Jost functions)**.** *We have the following properties concerning* $m_{1,2}(x,k)$.

1. *They satisfy the integral equation relations*

$$m_1(x,k) = 1 + \hbar^{-2}\int_x^\infty \frac{\exp(2ik(t-x)) - 1}{2ik} V(t)m_1(t,k)\,dt\,, \tag{3.41a}$$

and

$$m_2(x,k) = 1 + \hbar^{-2}\int_{-\infty}^x \frac{\exp(2ik(x-t)) - 1}{2ik} V(t)m_2(t,k)\,dt\,, \tag{3.41b}$$

for all k *with* $k_{\mathrm{I}} \geq 0$.

2. *We have that for all x, $m_{1,2}(x,k)$ are analytic for $k : k_{\mathrm{I}} > 0$ and continuous for $k_{\mathrm{I}} \geq 0$.*

Remark 3.17 (On the restriction on k)**.** The restriction on item 1. in the above Lemma is not strictly necessary for the case of V with bounded support. We choose to add this restriction, though, to anticipate the validity of this result also for a broader class of V—see subsection 3.4 below for further details.

Proof of Lemma 3.16. Since item 2 is more technical and involved, we shall prove only item 1. For a proof of item 2, refer to [2, Lem. 1].

Observe that from the hypothesis, we have

$$\begin{aligned}
\hbar^2 m_1' &= \frac{d}{dx}\left[\hbar^2 + \int_x^\infty \frac{\exp(2ik(t-x))-1}{2ik} V(t)m_1(t,k)\,dt\right] \\
&= \frac{d}{dx}\left[\frac{\exp(-2ikx)}{2ik}\int_x^\infty \exp(2ikt)V(t)m_1(t,k)\,dt - \frac{1}{2ik}\int_x^\infty V(t)m_1(t,k)\,dt\right] \\
&= -\exp(-2ikx)\int_x^\infty \exp(2ikt)V(t)m_1(t,k)\,dt - \cancel{\frac{V(x)m_1(x,k)}{2ik}} + \cancel{\frac{V(x)m_1(x,k)}{2ik}} \\
&= \exp(-2ikx)\int_x^\infty \exp(2ikt)V(t)m_1(t,k)\,dt\,, \qquad (3.42)
\end{aligned}$$

and consequently

$$\begin{aligned}
\hbar^2 m_1'' &= \frac{d}{dx}\left[\exp(-2ikx)\int_x^\infty \exp(2ikt)V(t)m_1(t,k)\,dt\right] \\
&= -2ik\underbrace{\exp(-2ikx)\int_x^\infty \exp(2ikt)V(t)m_1(t,k)\,dt}_{=\hbar^2 m_1'} + V(x)m_1(x,k). \qquad (3.43)
\end{aligned}$$

From this last equation, we recognize that (3.40) is fulfilled for m_1. Furthermore, as $x \to +\infty$ the integral will vanish, so that $m_1 \to 1$, fulfilling also that requirement.

For m_2, the same steps may be followed as above to reach that it too satisfies the given relation, and $m_2 \to 1$ as $x \to -\infty$. □

Let us now try to reconnect to the situation at hand. Remembering equality (3.32), we have that

$$\begin{aligned}
S(k)\phi_1(k) &= \phi_2(-k) + L(k)\phi_2(k) \\
&\implies S(k)m_1(k) = \exp(-ikx)\phi_2(-k) + \exp(-ikx)L(k)\phi_2(k) \\
&\implies m_1(k) = S(k)^{-1}[\exp(-ikx)\phi_2(-k) + \exp(-ikx)L(k)\phi_2(k)] \\
&\overset{x<-\nu}{\implies} m_1(k) = S(k)^{-1}[1 + L(k)\exp(-2ikx)]. \qquad (3.44)
\end{aligned}$$

However, thanks to Lemma 3.16, we also have the relation

$$\begin{aligned}
m_1(k) = \exp(-2ikx) \times \frac{\hbar^{-2}}{2ik}\int_x^\infty \exp(2ikt)V(t)m_1(t,k)\,dt \\
+ \left\{1 - \frac{\hbar^{-2}}{2ik}\int_x^\infty V(t)m_1(t,k)\,dt\right\}. \qquad (3.45)
\end{aligned}$$

Comparing terms between (3.44) and (3.45), we thus obtain the pair of equalities

$$\frac{L(k)}{S(k)} = \frac{\hbar^{-2}}{2ik}\int_x^\infty e^{2ikt}V(t)m_1(t,k)\,dt \tag{3.46a}$$

and

$$\frac{1}{S(k)} = 1 - \frac{\hbar^{-2}}{2ik}\int_x^\infty V(t)m_1(t,k)\,dt\,, \tag{3.46b}$$

where we emphasize that $x < -\nu$. We note that the rhs's of the above two equations depend on x, while the lhs's do not. This is not an error, though: as long as we choose $x < -\nu$ the specific value does not matter, as the integration from x to $-\nu$ yields zero due to the bounded support of V. This fact allows us to make the expression completely x-independent either by choosing $x = -\nu$, or sending $x \to -\infty$. For reasons that will become clear in the next section (where we will tinker with the potential function), we choose the latter of these two. As such, going from (3.46b), we find an expression for $S(k)$:

$$\boxed{\frac{1}{S(k)} = 1 - \frac{\hbar^{-2}}{2ik}\int_{-\infty}^\infty V(t)m_1(t,k)\,dt\,, \quad k_\mathrm{I} \geq 0.} \tag{3.47}$$

Now, by Lemma 3.16, we know that m_1 is an analytic function on $k_\mathrm{I} > 0$. This guarantees that $S(k)^{-1}$ is analytic also provided that the integral expression actually converges—which it does, as we assume that V has compact support. Thus, $S(k)^{-1}$ is analytic on the domain $k_\mathrm{I} > 0$. As such, its inverse $S(k)$ will in general be a *meromorphic* function on that same domain: we cannot exclude the possibility of $S(k)^{-1}$ having zeros, potentially giving it poles.

Since the function $S(k)$ is meromorphic, it also permits a meromorphic continuation to the lower-half of the k-plane. However, we shall not spend so much time on how precisely we choose to make this continuation. As we will see in Section 4—where we intend to find $S(k)$ as a bona fide function of k for various situations—the functions we end up with already allow k to be chosen in the lower half plane without hassle. Or, put differently, we continue the function $S(k)$ meromorphically by keeping the expression and simply discarding the condition $k_\mathrm{I} > 0$. It is also good to mention that, like analytic continuation, meromorphic continuation is unique (see for instance [9, §4.1]). As such, the choice of continuation we are making is unambiguous.

To recap our efforts in this section: we deduced in Lemma 3.13 that $S(k)$ will have a pole whenever the solutions $\phi_{1,2}$ are linearly dependent, which allowed us to redefine resonances in terms of $S(k)$. We were then able to find the algebraic expression (3.47) for the transmission amplitude, showing that it is meromorphic, and valid for $k_\mathrm{I} > 0$. By meromorphic continuation, then, we can extend the validity of this expression to all of $\mathbb{C}$, and hence also extend our new definition of resonances there.

3.4 Unlocking potentials

So far, in accordance with (3.1b), we only considered bounded potentials $V(x)$ with compact support, i.e. so that $\operatorname{supp} V \subseteq [-\nu, \nu]$ for some $\nu > 0$. In the above it is clear that the presented equations hold and make sense whenever this is the case. However, this does not mean that *only* such functions would make sense in the above

equations; we might be able to allow a broader class of potentials into our model, and still maintain what we have derived above.

Namely, seeing that V only shows up inside an integral, we suspect that instead of requiring V to have compact support, perhaps only its integral over $\mathbb{R}$ needs to converge. We introduce the spaces

$$L^1_a := \left\{ q : \mathbb{R} \to \mathbb{R} : \int_{-\infty}^{\infty} (1+|x|)^a \, |q(x)| \, dx < \infty \right\} \quad \text{for} \quad a \geq 0. \tag{3.48}$$

That is to say, an element of L^1_a needs to decrease "fast enough" in order to counteract the growing of the term $(1+|x|)^a$. Bounded functions with compact support as we have considered them above form a subset of L^1_a for any a: the bounded support makes the interval of integration finite, which makes the integral finite.

Let us assume now that instead of V being real, bounded, and compactly supported, we take $V \in L^1_1$. Does the above derived, in particular equation (3.47), still make sense? To answer this, we need to consider the information that the assumption gives us about the Jost functions $m_{1,2}$; as the Jost functions are effectively the solutions under the new potential, they will also be influenced. Once more we refer to [2] as bringing us this line of reasoning. Starting from (3.41), observe we have for m_1 and under the assumption of $k_{\mathrm{I}} \geq 0$:

$$\begin{aligned} \frac{m_1(x,k)}{1+|x|} &= \frac{1}{1+|x|} \left(1 + \hbar^{-2} \int_x^{\infty} \frac{\exp(2ik(t-x))-1}{2ik} V(t) m_1(t,k) \, dt \right) \\ &\leq 1 + \hbar^{-2} \int_x^{\infty} \frac{\exp(2ik(t-x))-1}{2ik} V(t) m_1(t,k) \, dt \, , \end{aligned} \tag{3.49}$$

from which we derive

$$\begin{aligned} \frac{|m_1(x,k)|}{1+|x|} &\leq 1 + \hbar^{-2} \left| \int_x^{\infty} \frac{\exp(2ik(t-x))-1}{2ik} V(t) m_1(t,k) \, dt \right| \\ &\leq 1 + \frac{\hbar^{-2}}{2|k|} \int_x^{\infty} \underbrace{|\exp(2ik(t-x))-1|}_{\leq 2} \, |V(t)| \, |m_1(t,k)| \, dt \\ &\leq 1 + \frac{\hbar^{-2}}{|k|} \int_x^{\infty} (1+|t|) |V(t)| \, \frac{|m_1(t,k)|}{1+|t|} \, dt \, . \end{aligned} \tag{3.50}$$

The bound as presented in the second step holds only for $k_{\mathrm{I}} \geq 0$; if this restriction is not maintained, the bounded term could in principle become arbitrarily large in size (for suitable k). From here we start an iteration procedure. Substitute the inequality back into itself to obtain

$$\begin{aligned} \frac{|m_1(x,k)|}{1+|x|} &\leq 1 + \frac{\hbar^{-2}}{|k|} \int_x^{\infty} (1+|t_1|) |V(t_1)| \left[1 + \frac{\hbar^{-2}}{|k|} \int_{t_1}^{\infty} (1+|t_2|) |V(t_2)| \frac{|m_1(t_2,k)|}{1+|t_2|} \, dt_2 \right] dt_1 \\ &= 1 + \frac{\hbar^{-2}}{|k|} \int_x^{\infty} (1+|t_1|) |V(t_1)| \, dt_1 \\ &\quad + \frac{\hbar^{-4}}{|k|^2} \int_x^{\infty} \int_{t_1}^{\infty} (1+|t_1|)(1+|t_2|) |V(t_1)| \, |V(t_2)| \frac{m_1(t_2,k)}{1+|t_2|} \, dt_2 \, dt_1 \, , \end{aligned} \tag{3.51}$$

and if we re-substitute this *ad infinitum*, we obtain the inequality

$$\frac{|m_1(x,k)|}{1+|x|} \leq 1 + \sum_{n=1}^{\infty} \frac{\hbar^{-2n}}{|k|^n} \int_x^\infty \int_{t_1}^\infty \cdots \int_{t_{n-1}}^\infty \prod_{j=1}^{n} (1+|t_j|)|V(t_j)|\, dt_j\,. \tag{3.52}$$

This expression makes sense as the iteration of a Volterra integral equation. However, convergence of the rhs of this equation is not yet established. To this end, we introduce a helpful Lemma which allows us to simplify the above.

Lemma 3.18 (Lots of integrals)**.** *Let q be some function such that $\int_{-\infty}^{\infty} |q(t)|\, dt < \infty$. Then, we have that*

$$\int_x^\infty \int_{x_1}^\infty \cdots \int_{x_{n-1}}^\infty |q(x_1)| \cdots |q(x_n)|\, dx_n \cdots dx_1 = \frac{1}{n!} \left(\int_x^\infty |q(t)|\, dt \right)^n, \tag{3.53}$$

for all $n \in \mathbb{N}$ and all $x \in \mathbb{R}$.

Proof. The proof may be found in Appendix B. □

Continuing from (3.52) and applying the above Lemma, we thus get

$$\begin{aligned}
\frac{|m_1(x,k)|}{1+|x|} &\leq 1 + \sum_{n=1}^{\infty} \frac{\hbar^{-2n}}{|k|^n \times n!} \left(\int_x^\infty (1+|t|)|V(t)|\, dt \right)^n \\
&\leq 1 + \sum_{n=1}^{\infty} \frac{\hbar^{-2n}}{|k|^n \times n!} \left(\int_{-\infty}^\infty (1+|t|)|V(t)|\, dt \right)^n \\
&= \exp\left(\frac{\hbar^{-2}}{|k|} \int_{-\infty}^\infty (1+|t|)|V(t)|\, dt \right) \\
&< \infty.
\end{aligned} \tag{3.54}$$

The final strict inequality follows as $V \in L_1^1$, so the integral will be finite. Therefore, we reach the conclusion that

$$\boxed{|m_1(x,k)| \leq K^{1/|k|}(1+|x|),} \tag{3.55}$$

where

$$K := \exp\left(\hbar^{-2} \int_{-\infty}^\infty (1+|t|)|V(t)|\, dt \right) > 1 \tag{3.56}$$

is a constant. Now we utilize this in equation (3.47) to find:

$$\begin{aligned}
|S(k)^{-1}| &\leq 1 + \frac{\hbar^{-2}}{2|k|} \int_{-\infty}^\infty |V(t)|\, |m_1(t,k)|\, dt \\
&\leq 1 + \frac{K^{1/|k|}\hbar^{-2}}{|k|} \int_{-\infty}^\infty (1+|t|)|V(t)|\, dt \\
&= 1 + \frac{K^{1/|k|} \ln K}{|k|}.
\end{aligned} \tag{3.57}$$

Since $|S(k)^{-1}|$ remains finite on the set $k_{\mathrm{I}} \geq 0$, we conclude as in the previous subsection that the function $S(k)^{-1}$ is analytic on the domain $k_{\mathrm{I}} > 0$ and hence $S(k)$ is meromorphic for $k_{\mathrm{I}} > 0$. By the same argument as previously, then, we can employ a meromorphic continuation in order to

This is all to say that if instead of a $V(x)$ with bounded support we choose $V \in L_1^1$, the equation (3.47) still has the desired properties. That is to say, that $S(k)$ still is a meromorphic function.

To conclude

In this section we laid out the model which we are going to use for the rest of this thesis, and then proceeded to introduce and give meaning to the complex energies which will appear. Then we mathematically defined resonances (through the resolvent operator), and determined some basic symmetry properties. Through Proposition 3.12 and Lemma 3.13, we were able to redefine resonances as being poles of the transmission amplitude $S(k)$. We then proceeded to give an algebraic form of $S(k)$ in the form of (3.47), and used it to show that $S(k)$ is meromorphic on $k_{\mathrm{I}} > 0$ (and could thus be continued meromorphically to all of $\mathbb{C}$). Finally, we showed that the derived relation (3.47) also made sense when viewing the potential V not as bounded and compactly supported, but instead as being an element of L^1_1.

In the next section we will attempt to derive explicitly the transmission amplitude $S(k)$ for specific classes of potentials. This will not use the relation (3.47), as it relies on knowing the solution to the Schrödinger equation everywhere, and in some sense finding out the solution is what we want to avoid.

4 Particular transmission solutions

In this section and the next we aim to explore more concretely where resonances are found for certain classes of potentials. In particular, in this section we will see that resonances are closely related to the phenomenon of *resonant tunneling*: a specific configuration of potential and energy leading to bona fide full transmission $T = 1$, even when the relevant energy is far lower than would classically be required for (near) full transmission.

Firstly, we will reiterate the model in which we are working, and derive from it a general formula for the transmission amplitude $S(k)$ (not involving integrals!). We then apply this formula to the case of square potentials, i.e. potentials which consist of square wells and barriers, which can be solved exactly. As a special case, we will study the simple square well in depth. Finally, we consider potentials which lend themselves to application of the WKB approximation. We shall utilize the matrix $\mathbf{P}$ as introduced in subsection 2.4.3 to find a simplified formula for $S(k)$, and consider some representative case studies.

4.1 Towards a general formulation

Let us reiterate that the potentials we consider here are members of the class L^1_1, cf. equation (3.48). That is to say, potentials which fall off suitably quickly, so that far from the origin we can consider the potential zero and so be left with a planar wave. As we have shown in the previous section, the mathematical machinery will work with these potentials.

However, for our ease of calculation, we will maintain the assumption of potential as made in our model (3.1b), which is to say that V should be real, bounded, and have compact support. Furthermore, we will from now on assume that V is an *even* (or *symmetric*) potential, i.e. that $V(-x) = V(x)$ for all x.

Assuming energy $\mathcal{E} = \hbar^2 k^2$, the solution outside of $[-\nu, \nu]$ will be a superposition of $\exp(\pm ikx)$, whereas inside it will be some function $\psi(x)$ cf. (3.1c). Supposing that $\psi(x)$ indeed solves Schrödinger inside, then given our symmetry assumption we can also find a second solution: for $\psi(-x)$ it holds that

$$\begin{aligned} -\hbar^2 \frac{d^2}{dx^2}\psi(-x) + V(x)\psi(-x) &= \mathcal{E}\psi(-x) \\ \iff \hbar^2 \frac{d^2}{d(-x)^2}\psi(-x) + V(-x)\psi(-x) &= \mathcal{E}\psi(-x) \\ \iff -\hbar^2 \frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) &= \mathcal{E}\psi(x), \end{aligned} \tag{4.1}$$

meaning that $\psi(-x)$ is also a solution. We can then define

$$\psi_{\mathrm{e}}(x) := \tfrac{1}{2}(\psi(x) + \psi(-x)) \quad \text{and} \quad \psi_{\mathrm{o}}(x) := \tfrac{1}{2}(\psi(x) - \psi(-x)), \tag{4.2}$$

which will be, respectively, *even* and *odd* solutions to the Schrödinger equation. We then adapt the presumed full solution of (3.1c) to read instead

$$\psi_{\mathrm{full}}(x) = \begin{cases} \psi_+ + L\psi_- & \text{if} \quad x < -\nu \\ A\psi_{\mathrm{e}} + B\psi_{\mathrm{o}} & \text{if} \quad x \in [-\nu, \nu] \\ S\psi_+ & \text{if} \quad x > \nu \end{cases}, \tag{4.3}$$

where $\psi_\pm(x) := \exp(\pm ikx)$ and for complex-valued functions $A(k), B(k), L(k), S(k)$.

Fixing k fixes these functions as constants. This means that for each k, we have four unknown constants and four matching conditions (function values and their derivatives) which they need to satisfy. Thus, in principle, we should be able to solve for all four constants and obtain non-trivial solutions depending only on k. This we do in the following Proposition, but only for $S(k)$. After all, that is the prime quantity in which we are interested.

Proposition 4.1 (1D transmission amplitude)**.** *The value of $S(k)$ in equation* (4.3) *is given by*

$$S(k) = \frac{ik(\psi'_{\mathrm{e}}\psi_{\mathrm{o}} - \psi_{\mathrm{e}}\psi'_{\mathrm{o}})\exp(-2ik\nu)}{\Delta(k)}\Big|_{x=\nu}, \tag{4.4}$$

cf. [4, §5.1], where $\Delta(k)$ is given by

$$\Delta(k) = (\psi'_{\mathrm{e}} - ik\psi_{\mathrm{e}})(\psi'_{\mathrm{o}} - ik\psi_{\mathrm{o}})|_{x=\nu}. \tag{4.5}$$

Proof. From matching the function values and their derivatives at the boundaries $-\nu$ and ν, the following equations can be found:

$$\begin{cases} \psi_+ + L\psi_- = A\psi_{\mathrm{e}} + B\psi_{\mathrm{o}} & \text{at} \quad x = -\nu \\ ik\psi_+ - ikL\psi_- = A\psi'_{\mathrm{e}} + B\psi'_{\mathrm{o}} & \text{at} \quad x = -\nu \\ A\psi_{\mathrm{e}} + B\psi_{\mathrm{o}} = S\psi_+ & \text{at} \quad x = \nu \\ A\psi'_{\mathrm{e}} + B\psi'_{\mathrm{o}} = ikS\psi_+ & \text{at} \quad x = \nu \end{cases}. \tag{4.6}$$

We "move" the first two equations to $x = \nu$ by recognizing that for the even and odd solutions we have

$$\psi_{\mathrm{e}}(-\nu) = \psi_{\mathrm{e}}(\nu),\ \psi_{\mathrm{o}}(-\nu) = -\psi_{\mathrm{o}}(\nu),\ \psi'_{\mathrm{e}}(-\nu) = -\psi'_{\mathrm{e}}(\nu),\ \text{and}\ \psi'_{\mathrm{o}}(-\nu) = \psi'_{\mathrm{o}}(\nu), \tag{4.7}$$

and additionally $\psi_+(-\nu) = \psi_-(\nu)$. Thus, we obtain the matrix system of equations

$$\begin{pmatrix} \psi_{\mathrm{e}} & -\psi_{\mathrm{o}} & -\psi_+ & 0 \\ -\psi'_{\mathrm{e}} & \psi'_{\mathrm{o}} & ik\psi_+ & 0 \\ \psi_{\mathrm{e}} & \psi_{\mathrm{o}} & 0 & -\psi_+ \\ \psi'_{\mathrm{e}} & \psi'_{\mathrm{o}} & 0 & -ik\psi_+ \end{pmatrix} \begin{pmatrix} A \\ B \\ L \\ S \end{pmatrix} = \begin{pmatrix} \psi_- \\ ik\psi_- \\ 0 \\ 0 \end{pmatrix}, \quad \text{at} \quad x = \nu. \tag{4.8}$$

Then we can apply Cramer's rule to find the value of S. Observe:

$$\begin{aligned} \begin{vmatrix} \psi_{\mathrm{e}} & -\psi_{\mathrm{o}} & -\psi_+ & 0 \\ -\psi'_{\mathrm{e}} & \psi'_{\mathrm{o}} & ik\psi_+ & 0 \\ \psi_{\mathrm{e}} & \psi_{\mathrm{o}} & 0 & -\psi_+ \\ \psi'_{\mathrm{e}} & \psi'_{\mathrm{o}} & 0 & -ik\psi_+ \end{vmatrix} &= \begin{vmatrix} \psi_{\mathrm{e}} + ik^{-1}\psi'_{\mathrm{e}} & -\psi_{\mathrm{o}} - ik^{-1}\psi'_{\mathrm{o}} & 0 & 0 \\ -\psi'_{\mathrm{e}} & \psi'_{\mathrm{o}} & ik\psi_+ & 0 \\ \psi_{\mathrm{e}} + ik^{-1}\psi'_{\mathrm{e}} & \psi_{\mathrm{o}} + ik^{-1}\psi'_{\mathrm{o}} & 0 & 0 \\ \psi'_{\mathrm{e}} & \psi'_{\mathrm{o}} & 0 & -ik\psi_+ \end{vmatrix} \\ &= -2k^2\psi_+^2(\psi_{\mathrm{e}} + ik^{-1}\psi'_{\mathrm{e}})(\psi_{\mathrm{o}} + ik^{-1}\psi'_{\mathrm{o}}), \end{aligned} \tag{4.9}$$

and

$$\begin{aligned} \begin{vmatrix} \psi_{\mathrm{e}} & -\psi_{\mathrm{o}} & -\psi_+ & \psi_- \\ -\psi'_{\mathrm{e}} & \psi'_{\mathrm{o}} & ik\psi_+ & ik\psi_- \\ \psi_{\mathrm{e}} & \psi_{\mathrm{o}} & 0 & 0 \\ \psi'_{\mathrm{e}} & \psi'_{\mathrm{o}} & 0 & 0 \end{vmatrix} &= \begin{vmatrix} \psi_{\mathrm{e}} - ik^{-1}\psi'_{\mathrm{e}} & -\psi_{\mathrm{o}} + ik^{-1}\psi'_{\mathrm{o}} & -2\psi_+ & 0 \\ -\psi'_{\mathrm{e}} & \psi'_{\mathrm{o}} & ik\psi_+ & ik\psi_- \\ \psi_{\mathrm{e}} & \psi_{\mathrm{o}} & 0 & 0 \\ \psi'_{\mathrm{e}} & \psi'_{\mathrm{o}} & 0 & 0 \end{vmatrix} \\ &= -2ik(\psi_{\mathrm{e}}\psi'_{\mathrm{o}} - \psi'_{\mathrm{e}}\psi_{\mathrm{o}}). \end{aligned} \tag{4.10}$$

Now combine equations (4.9) and (4.10) and simplify:

$$S = \frac{-2ik(\psi_{\mathrm{e}}\psi'_{\mathrm{o}} - \psi'_{\mathrm{e}}\psi_{\mathrm{o}})}{-2k^2\psi_+^2(\psi_{\mathrm{e}} + ik^{-1}\psi'_{\mathrm{e}})(\psi_{\mathrm{o}} + ik^{-1}\psi'_{\mathrm{o}})} = \frac{-ik(\psi_{\mathrm{e}}\psi'_{\mathrm{o}} - \psi'_{\mathrm{e}}\psi_{\mathrm{o}})\psi_-^2}{(\psi'_{\mathrm{e}} - ik\psi_{\mathrm{e}})(\psi'_{\mathrm{o}} - ik\psi_{\mathrm{o}})}, \tag{4.11}$$

where also used that $\psi_+^{-1} = \psi_-$. The desired result is then obtained by recognizing $\psi_- = \exp(-ikx)$, and evaluating it at $x = \nu$. □

Remark 4.2 (Link to bound states)**.** By linearity, the wavefunction

$$\Delta(k)\psi_{\mathrm{full}}(x) = \begin{cases} \Delta(k)\psi_+ + L\Delta(k)\psi_- & \text{if} \quad x < -\nu \\ A\Delta(k)\psi_{\mathrm{e}} + B\Delta(k)\psi_{\mathrm{o}} & \text{if} \quad x \in [-\nu, \nu]\,, \\ S\Delta(k)\psi_+ & \text{if} \quad x > \nu \end{cases} \tag{4.12}$$

where $\Delta(k)$ is as in (4.5), is also a solution to the Schrödinger equation for every value of k. By the same methodology as in Proposition 4.1, we can find that $L, A, B \propto \Delta(k)^{-1}$. Thus, if there exists a k_0 so that $\Delta(k_0) \to 0$, the various products $S\Delta(k_0)$ etc. will generally not explode—though $\Delta(k_0)\psi_+$ will go to zero. Assuming no explosions take place and $(k_0)_{\mathrm{I}} > 0$, then, the solution ψ_{full} will have exponential decay as $x \to \pm\infty$, meaning it is square-integrable and so a wavefunction.

This illustrates the emergence of bound states under the same conditions as in subsection 3.3.1, albeit in a more ad hoc fashion. For further details see [4, §5.2].

Eyeing the mix of $\psi_{\mathrm{e,o}}$ and their derivatives, we can make a simplification of the found expression by introducing

$$\theta_{\mathrm{e,o}} := \frac{\psi'_{\mathrm{e,o}}}{\psi_{\mathrm{e,o}}}\Big|_{x=\nu} = \frac{d}{dx}\Big|_{x=\nu} \ln(\psi_{\mathrm{e,o}}) \tag{4.13}$$

with which we simplify the formula for $S(k)$ as derived in Proposition 4.1:

$$\boxed{S(k) = \frac{ik(\theta_{\mathrm{e}} - \theta_{\mathrm{o}})e^{-2ik\nu}}{(\theta_{\mathrm{e}} - ik)(\theta_{\mathrm{o}} - ik)}.} \tag{4.14}$$

The $\theta_{\mathrm{e,o}}$ represent the motions of the even and odd components of the wavefunction as it emerges from the potential.

Notable is that the expression of $S(k)$ has dependence on ν, even though intuitively it should not: ν is merely a cutoff, and traversal through any additional free space should not change the value of $S(k)$. The reason is that $\theta_{e,o}$ each also depend on ν, presumably nontrivially so. The additional exponential $e^{-2ik\nu}$ is then a "compensation" factor for this $\theta_{e,o}$ dependence on ν. Additionally, if one considers sufficiently large energies (for which we will always be in the approximately free case for our bounded potentials), the $e^{-2ik\nu}$ is necessary in order to guarantee $S(k) \to 1$, as we would expect for free space. This is also touched upon in Remark 4.14.

With this, in a certain sense we have now solved the transmission problem in 1 dimension: we know the transmission amplitude $S(k)$, which contains all the information we need. However, this formula relies on us knowing the solution to the Schrödinger equation inside the potential, which renders our formula kind of moot. After all, if we already know the solution, the transmission amplitude follows *trivially*.

Nevertheless, equation (4.14) has a right to exist: if we could somehow find $\theta_{\mathrm{e,o}}$ in a more clever way than solving the Schrödinger equation computationally, we will know $S(k)$ immediately without a lot of (computer) work. Additionally, we may find the structure of $S(k)$ and draw general conclusions from that structure about a broad class of potentials, or learn how $S(k)$ depends on various parameters. This is what we shall attempt to do for the remainder of this section.

The next subsection will concern itself with the case of piecewise constant potentials (i.e. consisting of square wells and barriers), which may be solved exactly. Thereafter we shall consider potentials for which WKB is applicable, for which we utilize the approximation discussed in the above.

4.2 Piecewise constant potentials

Notice that if we declare initial conditions of the wavefunction at a, then we can find the value and derivative of the wavefunction at some b by

$$\begin{pmatrix}\psi(b)\\ \psi'(b)\end{pmatrix} = \mathcal{P}\exp\left[\int_a^b \begin{pmatrix}0 & 1\\ \hbar^{-2}(V(x')-\mathcal{E}) & 0\end{pmatrix} dx'\right]\begin{pmatrix}\psi(a)\\ \psi'(a)\end{pmatrix}, \tag{4.15}$$

where $\mathcal{P}\exp$ indicates that we are talking about the path-ordered exponential. This is just the statement of "integrate the Schrödinger equation from a to b." Though there is an expression for how to solve path-ordered exponentials, this would be a pain to solve for general potentials. As such, for general V, computers would be needed to evaluate this path-ordered exponential, and hence solve the Schrödinger equation.

However, if we assume that V is *constant*, then we do not have to worry anymore about the path-ordering of this integral; as it were, the "$\mathcal{P}$" disappears, and we are left with a regular matrix exponential. Since we consider 2×2 matrices, these can be calculated with little effort, and so we can aim to find a closed, "simple" expression for the wavefunction and its derivative at the target point. From this we can then derive $\theta_{\mathrm{e,o}}$, and so $S(k)$.

Let us make things concrete in the following Definition.

Definition 4.3. (Piecewise constant (pc) potentials) Let $\{x_j\}_{j=0}^{n+1}\subset\mathbb{R}$ with $-\nu\leq x_j<x_{j+1}\leq\nu$ for all $j\neq n+1$. Then, if $V(x)$ is such that

$$V(x)=V_j\in\mathbb{R} \text{ if } x\in(x_j,x_{j+1}), \tag{4.16}$$

we will call $V(x)$ *piecewise constant* (pc). Effectively, (a subset of) the region $[-\nu,\nu]$ is partitioned into n regions, on each of which there is a constant potential.

Now, observe that for the region (x_0,x_{n+1}) and by the properties of the path-ordered exponential, we can say that for pc potentials,

$$\begin{aligned}\mathcal{P}\exp\left[\int_{x_0}^{x_{n+1}} \begin{pmatrix}0 & 1\\ \hbar^{-2}(V(x')-\mathcal{E}) & 0\end{pmatrix} dx'\right] &= \prod_{j=0}^{n}\mathcal{P}\exp\left[\int_{x_j}^{x_{j+1}} \begin{pmatrix}0 & 1\\ \hbar^{-2}(V(x')-\mathcal{E}) & 0\end{pmatrix} dx'\right]\\ &= \prod_{j=0}^{n}\exp\left[\int_{x_j}^{x_{j+1}} \begin{pmatrix}0 & 1\\ \hbar^{-2}(V_j-\mathcal{E}) & 0\end{pmatrix} dx'\right]\\ &= \prod_{j=0}^{n}\exp\left[(x_{j+1}-x_j)\begin{pmatrix}0 & 1\\ \hbar^{-2}(V_j-\mathcal{E}) & 0\end{pmatrix}\right]\end{aligned} \tag{4.17}$$

Here the order of the matrix product is important: the *rightmost* matrix is $j = 0$, then $j = 1$, and so on. Due to the exponents being particularly simple, these exponentials have nice expressions, as we learn from the following Lemma.

Lemma 4.4 (Particular matrix exponential)**.** *For $A \neq 0$, we have that*

$$\exp\left[\begin{pmatrix} 0 & \ell \\ \ell A & 0 \end{pmatrix}\right] = \begin{pmatrix} \cosh\bigl(\ell A^{1/2}\bigr) & A^{-1/2}\sinh\bigl(\ell A^{1/2}\bigr) \\ A^{1/2}\sinh\bigl(\ell A^{1/2}\bigr) & \cosh\bigl(\ell A^{1/2}\bigr) \end{pmatrix}. \tag{4.18}$$

Proof. The proof may be found in Appendix B. □

As such, we can characterize any pc potential using a matrix (or rather a product of various matrices), which describes how the wavefunction will move through these. In principle, this is already enough information to find the transmission amplitude corresponding to any such potential. However, as we have been considering symmetric potentials so far (and know how to find $S(k)$ for those), it should pay off to consider now symmetric pc potentials.

To utilize the expression (4.14) for $S(k)$, we need to know something about the even and odd wavefunctions which solve the Schrödinger equation for symmetric potentials. This we address in the following Proposition.

Proposition 4.5 (Construction even/odd solutions)**.** *Assume the potential V is piecewise constant and symmetric. Then, we have that*

1. *The solution ϕ_e, which is defined by*

$$\begin{pmatrix} \phi_e(x) \\ \phi_e'(x) \end{pmatrix} := \mathcal{P}\exp\left[\int_0^x \begin{pmatrix} 0 & 1 \\ \hbar^{-2}(V(x') - \mathcal{E}) & 0 \end{pmatrix} dx'\right] \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{4.19a}$$

   is an even *solution.*

2. *The solution ϕ_o, which is defined by*

$$\begin{pmatrix} \phi_o(x) \\ \phi_o'(x) \end{pmatrix} := \mathcal{P}\exp\left[\int_0^x \begin{pmatrix} 0 & 1 \\ \hbar^{-2}(V(x') - \mathcal{E}) & 0 \end{pmatrix} dx'\right] \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{4.19b}$$

   is an odd *solution.*

Proof. By symmetry of V, we have

$$\mathbf{C} := \mathcal{P}\exp\left[\int_0^x \ldots\right] = \mathcal{P}\exp\left[-\int_0^{-x} \ldots\right] = \mathcal{P}\exp\left[\int_{-x}^0 \ldots\right]. \tag{4.20}$$

Additionally, since we can decompose $\mathbf{C}$ in the manner of (4.17), each individual matrix exponential's exponent has trace zero, and $\det\exp M = \exp\operatorname{Tr} M$ for any matrix, we conclude that $\det\mathbf{C} = 1$, and that $\mathbf{C}$ is invertible. Let us now prove the separate parts.

1. Observe that, in addition to the hypothesis (4.19a), we also have that

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \mathbf{C}\begin{pmatrix} \phi_{\mathrm{e}}(-x) \\ \phi_{\mathrm{e}}'(-x) \end{pmatrix} \iff \begin{pmatrix} \phi_{\mathrm{e}}(-x) \\ \phi_{\mathrm{e}}'(-x) \end{pmatrix} = \mathbf{C}^{-1}\begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{4.21}$$

This holds because ϕ_{e} as defined by (4.19a) is the *unique* solution to the Schrodinger equation, with the given initial condition at the origin. We find

$$\begin{pmatrix}\phi_{\mathrm{e}}(x)\\ \phi'_{\mathrm{e}}(x)\end{pmatrix} = \mathbf{C}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}\mathbf{C}_{11}\\ \mathbf{C}_{21}\end{pmatrix} \quad \text{and} \quad \begin{pmatrix}\phi_{\mathrm{e}}(-x)\\ \phi'_{\mathrm{e}}(-x)\end{pmatrix} = \mathbf{C}^{-1}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}\mathbf{C}_{22}\\ -\mathbf{C}_{21}\end{pmatrix}, \tag{4.22}$$

from which we importantly conclude that $\phi'_{\mathrm{e}}(x) = -\phi'_{\mathrm{e}}(-x)$ for all x. Finally, we do

$$\phi_{\mathrm{e}}(y) - \phi_{\mathrm{e}}(-y) = \int_{-y}^{y} \phi'_{\mathrm{e}}(x)\,dx = 0 \implies \phi_{\mathrm{e}}(y) = \phi_{\mathrm{e}}(-y) \text{ for all } y, \tag{4.23}$$

which is to say that ϕ_{e} is even.

2. In much the same way as above, observe that

$$\begin{pmatrix}\phi_{\mathrm{o}}(x)\\ \phi'_{\mathrm{o}}(x)\end{pmatrix} = \mathbf{C}\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}\mathbf{C}_{12}\\ \mathbf{C}_{22}\end{pmatrix} \quad \text{and} \quad \begin{pmatrix}\phi_{\mathrm{o}}(-x)\\ \phi'_{\mathrm{o}}(-x)\end{pmatrix} = \mathbf{C}^{-1}\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}-\mathbf{C}_{12}\\ \mathbf{C}_{22}\end{pmatrix}. \tag{4.24}$$

We thus conclude that $\phi_{\mathrm{o}}(x) = -\phi_{\mathrm{o}}(-x)$ for all x, i.e. that ϕ_{o} is indeed an odd function.

Both parts have been proven, so we are now done. □

With all the above in mind, we can now exactly determine the parameters $\theta_{\mathrm{e,o}}$ needed to apply equation (4.14) in a systematic manner, for every symmetric pc potential. This is the content of the following Algorithm.

Algorithm 4.6 (Symmetric pc potential $\theta_{\mathrm{e,o}}$)**.** For a symmetric, piecewise constant potential V, in order to find $\theta_{\mathrm{e,o}}$ we have the following steps.

1. Write the path-ordered exponential from 0 to ν, and split this up into regular matrix exponentials using equation (4.17).
2. For each resultant matrix, evaluate it using Lemma 4.4.
3. Multiply each of the evaluated matrices together (preserving order) to find the full evolution. Call the resulting matrix $\mathbf{W}$.
4. Then we find the desired quantities by

$$\begin{pmatrix}\phi_{\mathrm{e}}(\nu)\\ \phi'_{\mathrm{e}}(\nu)\end{pmatrix} = \mathbf{W}\begin{pmatrix}1\\0\end{pmatrix} \quad \text{and} \quad \begin{pmatrix}\phi_{\mathrm{o}}(\nu)\\ \phi'_{\mathrm{o}}(\nu)\end{pmatrix} = \mathbf{W}\begin{pmatrix}0\\1\end{pmatrix}, \tag{4.25}$$

   as a result from Proposition 4.5.
5. Finally, we find $\theta_{\mathrm{e,o}}$ by using

$$\theta_e = \frac{\phi'_{\mathrm{e}}(\nu)}{\phi_{\mathrm{e}}(\nu)} = \frac{\begin{pmatrix}0 & 1\end{pmatrix}\mathbf{W}\begin{pmatrix}1\\0\end{pmatrix}}{\begin{pmatrix}1 & 0\end{pmatrix}\mathbf{W}\begin{pmatrix}1\\0\end{pmatrix}} \quad \text{and} \quad \theta_o = \frac{\phi'_{\mathrm{o}}(\nu)}{\phi_{\mathrm{o}}(\nu)} = \frac{\begin{pmatrix}0 & 1\end{pmatrix}\mathbf{W}\begin{pmatrix}0\\1\end{pmatrix}}{\begin{pmatrix}1 & 0\end{pmatrix}\mathbf{W}\begin{pmatrix}0\\1\end{pmatrix}} \tag{4.26}$$

This sets us up perfectly for use of expression (4.14), to find the transmission amplitude. We work this out in the following Corollary, which is also the main result of this section.

Corollary 4.7 ($S(k)$ for square pc potentials)**.** *Let V be symmetric and piecewise constant, and $\mathbf{W}$ the matrix as resulting from Algorithm 4.6. Then,*

$$S(k) = \frac{-ik\exp(-2ik\nu)}{(\mathbf{W}_{21} - ik\mathbf{W}_{11})(\mathbf{W}_{22} - ik\mathbf{W}_{12})}. \tag{4.27}$$

Proof. Substitute the expressions for $\theta_{\mathrm{e,o}}$ from equation (4.26) into the formula for $S(k)$ (4.14) and behold

$$\begin{aligned} S(k) &= ik\exp(-2ik\nu)\left[\begin{pmatrix}0 & 1\end{pmatrix}\mathbf{W}\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix}\mathbf{W}\begin{pmatrix}0\\1\end{pmatrix} - \begin{pmatrix}0 & 1\end{pmatrix}\mathbf{W}\begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix}\mathbf{W}\begin{pmatrix}1\\0\end{pmatrix}\right] \\ &\quad\times\left[\begin{pmatrix}-ik & 1\end{pmatrix}\mathbf{W}\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}-ik & 1\end{pmatrix}\mathbf{W}\begin{pmatrix}0\\1\end{pmatrix}\right]^{-1} \\ &\overset{\star}{=} ik\exp(-2ik\nu)\left|\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\mathbf{W}\right|^{-1}[(\mathbf{W}_{21} - ik\mathbf{W}_{11})(\mathbf{W}_{22} - ik\mathbf{W}_{12})]^{-1} \\ &= \frac{-ik\exp(-2ik\nu)}{(\mathbf{W}_{21} - ik\mathbf{W}_{11})(\mathbf{W}_{22} - ik\mathbf{W}_{12})}, \end{aligned} \tag{4.28}$$

where in $\star$ we used that $\det\mathbf{W} = 1$. □

As such, we can now in all generality find the transmission amplitude for any square symmetric potential, through the matrix $\mathbf{W}$. The remainder of this subsection will be dedicated to studying arguably the simplest square potential, being the square well.

4.2.1 Square well

Let us consider the square well, i.e. the potential

$$V_{\mathrm{well}}(x) = \begin{cases} V_0 & \text{if} \quad x \in [-\nu, \nu] \\ 0 & \text{otherwise} \end{cases}, \tag{4.29}$$

for $V_0 < 0$. The associated $\mathbf{W}$ matrix is found in one step by

$$\begin{aligned} \mathbf{W} = \mathcal{P}\exp\left[\int_0^\nu \begin{pmatrix}0 & 1\\ \hbar^{-2}(V(x') - \mathcal{E}) & 0\end{pmatrix}dx'\right] &= \exp\left[\begin{pmatrix}0 & \nu\\ \nu\hbar^{-2}(V_0 - \mathcal{E}) & 0\end{pmatrix}\right] \\ &= \begin{pmatrix}\cosh(q\nu) & q^{-1}\sinh(q\nu)\\ q\sinh(q\nu) & \cosh(q\nu)\end{pmatrix}, \end{aligned} \tag{4.30}$$

where we introduced $q := \hbar^{-1}\sqrt{V_0 - \mathcal{E}}$. Thus, we find

$$\begin{aligned} S(k) &= \frac{-ik\exp(-2ik\nu)}{(q\sinh(q\nu) - ik\cosh(q\nu))(\cosh(q\nu) - ikq^{-1}\sinh(q\nu))} \\ &= \frac{-ik\exp(-2ik\nu)}{-ik[\cosh^2(q\nu) + \sinh^2(q\nu)] + \cosh(q\nu)\sinh(q\nu)[q - k^2q^{-1}]} \\ &= \frac{-ik\exp(-2ik\nu)}{\frac{1}{2}[q - k^2q^{-1}]\sinh(2q\nu) - ik\cosh(2q\nu)} \end{aligned} \tag{4.31}$$

As a sanity check, we would like to investigate the large-k behavior of the amplitude. This we do in the following Proposition.

Proposition 4.8 (Large-k behavior $S(k)$ for square well/barrier)**.** *Assume* $|k|^2 \gg |\hbar^{-2}V_0|$ *and* $|k_\mathrm{I}| \gg 1$*. Then, we have the following behaviors for the transmission amplitude* (4.31)*.*

1. *For* $\operatorname{sgn} k_\mathrm{I} = 1$*, we have that*
$$S(k) \sim 1. \tag{4.32}$$
2. *For* $\operatorname{sgn} k_\mathrm{I} = -1$ *and* $|k_\mathrm{I}| \gg |k_\mathrm{R}|$*, we have that*
$$S(k) \sim -|k|^4 \exp(-4ik\nu). \tag{4.33}$$

Proof. Observe that

$$q = \hbar^{-1}\sqrt{V_0 - \hbar^2 k^2} = -i\sqrt{k^2 - \hbar^{-2}V_0} \approx -ik\left(1 - \frac{\hbar^{-2}V_0}{2k^2}\right) = -ik + \sigma, \tag{4.34}$$

for $\sigma := -\hbar^{-2}V_0/(2ik)$. We recognize that σ is the error between q and its limit $-ik$, and it vanishes as we consider larger k. Now, calculate

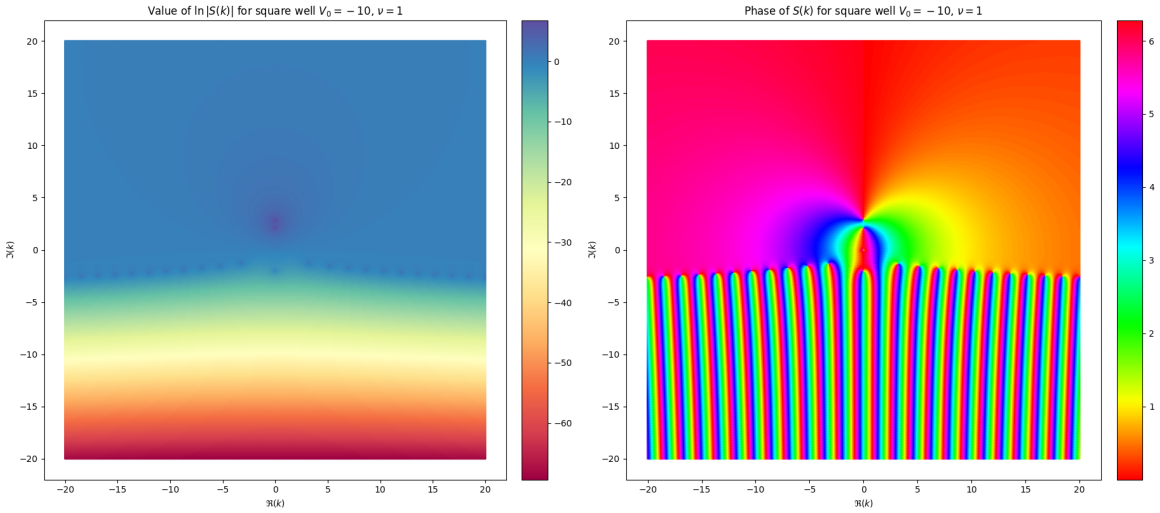
$$\begin{aligned}
\frac{1}{2}\left(q - \frac{k^2}{q}\right) &= \frac{1}{2}\left(-ik + \sigma - \frac{k^2}{-ik + \sigma}\right) \\
&= \frac{1}{2}\left(-ik + \sigma - \frac{k^2}{-ik}\frac{1}{1 - \sigma/(ik)}\right) \\
&= \frac{1}{2}\left(-ik + \sigma - ik\left[1 + \frac{\sigma}{ik} + \left(\frac{\sigma}{ik}\right)^2 + \mathcal{O}(\sigma^3)\right]\right) \qquad (4.35) \\
&= -ik - \frac{\sigma^2}{2ik} + \mathcal{O}(\sigma^3). \qquad (4.36)
\end{aligned}$$

We then calculate the denominator of (4.31) as

$$\begin{aligned}
&\frac{1}{2}\left(q - \frac{k^2}{q}\right)\sinh(2q\nu) - ik\cosh(2q\nu) \\
&\quad= \left(-ik - \frac{\sigma^2}{2ik} + \mathcal{O}(\sigma^3)\right)\sinh(-2ik\nu + 2\sigma\nu) - ik\cosh(-2ik\nu + 2\sigma\nu) \\
&\quad= -ik\left(\cosh(-2ik\nu + 2\sigma\nu) + \sinh(-2ik\nu + 2\sigma\nu) - \frac{\sigma^2}{2k^2}\sinh(-2ik\nu + 2\sigma\nu) + \mathcal{O}(\sigma^3)\right) \\
&\quad= -ik\left(\exp(-2ik\nu + 2\sigma\nu) - \frac{\sigma^2}{2k^2}\sinh(-2ik\nu + 2\sigma\nu) + \mathcal{O}(\sigma^3)\right), \qquad (4.37)
\end{aligned}$$

and so obtain an expression for $S(k)$:

$$\begin{aligned}
S(k) &\sim \left(\exp(2\sigma\nu) - \frac{\sigma^2}{2k^2}\sinh(-2ik\nu + 2\sigma\nu)\exp(2ik\nu)\right)^{-1} \\
&= \left(\exp(2\sigma\nu)\left[1 - \frac{\sigma^2}{4k^2}\right] + \frac{\sigma^2}{4k^2}\exp(4ik\nu - 2\sigma\nu)\right)^{-1}. \qquad (4.38)
\end{aligned}$$



(a) Value of $\ln|S(k)|$ (b) Phase of $S(k)$

Figure 4.1: Phase and size of $S(k)$ as in (4.31), with $V_0 = -10$ and $\nu = 1$ ($\hbar \equiv 1$). Note that these are *not* from a simulation, but the implementation of (4.31).

Now we split cases. For $\operatorname{sgn} k_\mathrm{I} = 1$, $|\sigma| \to 0$ and $|\exp(4ik\nu)| \to 0$ as well. Hence, the denominator reduces to 1, and we have shown $S(k) \sim 1$.

For $\operatorname{sgn} k_\mathrm{I} = -1$, $|\sigma| \to 0$ still, but now $|\exp(4ik\nu)| \gg 1$. Hence, the second term will dominate the first, and we can write the estimation as

$$\begin{aligned} S(k) &\sim \frac{4k^2}{\sigma^2}\exp(-4ik\nu + 2\sigma\nu) \\ &= \left|\frac{4k^2\exp(4k_\mathrm{I}\nu)\exp(2\sigma_\mathrm{R}\nu)}{\sigma^2}\right| \times \frac{\sigma^2/(4k^2)\exp(2i\sigma_\mathrm{I}\nu)\exp(-4ik_\mathrm{R}\nu)}{|\sigma^2/(4k^2)|}, \end{aligned} \tag{4.39}$$

where the first factor represents the size of $S_{k_\mathrm{I}\ll 0}$ and the second its phase. The size will decay like $|k|^4\exp(4k_\mathrm{I}\nu)$, as can be seen from the above.

Concerning the phase, we see

$$\begin{aligned} \operatorname{phase}(S) &= \exp(-4ik_\mathrm{R}\nu)\cancel{\exp(2i\sigma_\mathrm{I}\nu)}\operatorname{phase}(\sigma^2/(4k^2)) \\ &= \exp(-4ik_\mathrm{R}\nu)\operatorname{phase}(-k^4) \\ &\sim -\exp(-4ik_\mathrm{R}\nu)\operatorname{phase}(k_\mathrm{I}^4) \\ &= -\exp(-4ik_\mathrm{R}\nu). \end{aligned} \tag{4.40}$$

Thus, (4.39) will come to read

$$S(k) \sim -\exp(4k_\mathrm{I}\nu)\exp(-4ik_\mathrm{R}\nu) = -\exp(-4ik\nu), \tag{4.41}$$

and so we have shown this case. □

An illustration of this Proposition in action is given in Figure 4.1. Notice that in the Figure we can identify the bound and antibound states, as well as resonances. The transition from $\operatorname{sgn} k_\mathrm{I} = +$ to $-$ results in the appearance of the "wavefronts" in the phase. This partially explains the reason for resonances to exist: all these "wavefronts" need to terminate for some k_I as $S \to 1$ for k with large imaginary parts, and the termination will results in poles.

Remark 4.9 (Square barrier applicability)**.** Up to now, the assumption that $V_0 < 0$ has not been utilized yet. As such, the found expression (4.31) can equally be applied to square barriers, where one would choose $V_0 > 0$ instead.

We can also use the above expression (4.31) to calculate the transmission coefficient $T = |S|^2$. Since this is somewhat tricky for complex k, let us for simplicity assume real $\mathcal{E} \equiv E > 0$, so q is purely imaginary. Then, the term involving sinh is purely real, and the term involving cosh is purely imaginary. We can thus calculate

$$\begin{aligned} T(E) = S(k)\overline{S(k)} &= \frac{k^2}{k^2\cosh^2(2q\nu) + \frac{1}{4}[q - k^2q^{-1}]^2\sinh^2(2q\nu)} \\ &= \frac{1}{1 + \{\frac{1}{4}[qk^{-1} - kq^{-1}]^2 + 1\}\sinh^2(2q\nu)} \\ &= \frac{1}{1 + \cosh^2(\ln q - \ln k)\sinh^2(2q\nu)} \\ &= \frac{1}{1 + \sinh^2(\ln|q| - \ln k)\sin^2(2|q|\nu)}. \end{aligned} \tag{4.42}$$

Eyeing this expression, we notice that when

$$2|q|\nu = n\pi \iff \sqrt{E - V_0} = \frac{\hbar n\pi}{2\nu} \iff E = \left(\frac{\hbar n\pi}{2\nu}\right)^2 + V_0 \text{ for some } n \in \mathbb{Z}, \tag{4.43}$$

we will have $T = 1$. Such energies are thus transparency energies for the square well. In Figure 4.2, we have the transmission spectra for the square well, both from a simulation (the "computed" line) and this theoretical prediction. Notice that the peaks line up almost perfectly with our theoretical calculation, as well as with the predictions for the locations of the transparency energies. This also bolsters the confidence in the correctness of the program written to compute the spectrum.

Remark 4.10 (Bohr-Sommerfeld quantization I)**.** The expression (4.43) is recognized precisely as the *Bohr-Sommerfeld quantization condition* for the square well. This is an interesting observation, as normally Bohr-Sommerfeld only applies for bound states of certain systems, whilst here we are decidedly not dealing with bound states.

Curiously, from Figure 4.2 we learn that T may become very low for certain values of the energy—for instance, $T \approx 0.1$ for $E \approx 11$. This stands in contrast to what we would expect in the classical case: since $E > 0$ and we encounter a well, classically we would expect full transparency. The mathematical cause is that for such energies at which a local minimum is reached, the product $\sinh(\cdot)\sin(\cdot)$ is very large, driving down T. From a physical perspective, this shows the influence of the interface that is the "drop" into the square well.

We also notice that the peaks get wider as the energy increases. This is most clearly demonstrated algebraically if we rewrite the transmission coefficient around a transparency energy E_{trans}. Upon a slight perturbation,

$$E_{\text{trans}} \to E_{\text{trans}} + \delta E \implies |q| \to |q| + \frac{\hbar^{-1}\delta E}{2\sqrt{E_{\text{trans}} - V_0}} \quad \text{and} \quad k \to k + \frac{\hbar^{-1}\delta E}{2\sqrt{E_{\text{trans}}}}, \tag{4.44}$$

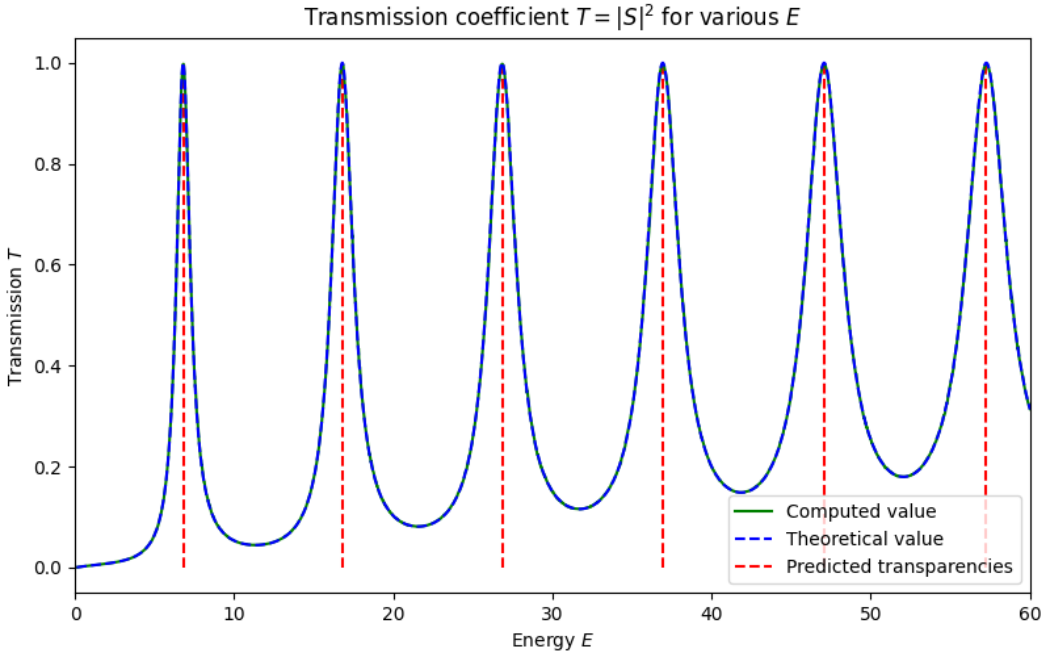


Figure 4.2: Comparison of the theoretical transmission coefficient derived from (4.31) to simulated (computed) value, for square well with $V_0 = -1000$ and $\nu = 10$ cf. (4.29) ($\hbar \equiv 1$). The locations of the predicted transparencies are from (4.43). The **green** (computed) curve lies under the dashed **blue** (theoretical) one.

so that

$$\begin{aligned}\sin^2(2|q|\nu) \longrightarrow \sin^2\big(2|q|\nu + \delta E\,\hbar^{-1}\nu[E_{\text{trans}} - V_0]^{-1/2}\big) \\ \approx \left(\cancel{\sin(2|q|\nu)} + \delta E\,\hbar^{-1}\nu[E_{\text{trans}} - V_0]^{-1/2}\cancel{\cos(2|q|\nu)}^{\pm 1} + \mathcal{O}\big(\delta E^3\big)\right)^2 \\ \approx \frac{\hbar^{-2}\nu^2}{E_{\text{trans}} - V_0}\delta E^2 + \mathcal{O}\big(\delta E^4\big). \qquad (4.45)\end{aligned}$$

and

$$\begin{aligned}\sinh^2(\ln|q| - \ln k) \longrightarrow \sinh^2(\ln|q| + \ln(1 + f_1\delta E) - \ln k - \ln(1 + f_2\delta E)) \\ \approx \sinh^2\big(\ln|q| - \ln k + \delta E\{f_1 \ln|q| - f_2 \ln k\} + \mathcal{O}\big(\delta E^2\big)\big) \\ \approx \sinh^2(\ln|q| - \ln k) + \mathcal{O}(\delta E), \qquad (4.46)\end{aligned}$$

for the appropriate factors $f_{1,2}$. As such, to lowest order in δE, we write the transmission coefficient around a transparency energy as

$$\begin{aligned}T(E_{\text{trans}} + \delta E) \approx \left[1 + \frac{\hbar^{-2}\nu^2\sinh^2(\ln|q| - \ln k)}{E_{\text{trans}} - V_0}\,\delta E^2\right]^{-1} \\ = \frac{E_{\text{trans}} - V_0}{\hbar^{-2}\nu^2\sinh^2(\ln|q| - \ln k)}\left[\frac{E_{\text{trans}} - V_0}{\hbar^{-2}\nu^2\sinh^2(\ln|q| - \ln k)} + \delta E^2\right]^{-1}. \qquad (4.47)\end{aligned}$$

Finally making the substitution

$$\Gamma := \frac{2\hbar\sqrt{E_{\text{trans}} - V_0}}{\nu\sinh(\ln|q| - \ln k)}, \qquad (4.48)$$

we see that the transmission coefficient has the form

$$\boxed{T(E_{\text{trans}} + \delta E) \approx \frac{(\Gamma/2)^2}{(\Gamma/2)^2 + \delta E^2}} \tag{4.49}$$

around the transparency E_{trans}. As such, the peaks of the transmission spectrum follow FBW distributions, as introduced in the Introduction (1.4). The parameter Γ dictates the width of the peaks: the larger Γ is, the wider the peak will be. In our case, for increasing E_{trans}, we have that $\ln|q| - \ln|k| \to 0 \implies \sinh^2(\cdot) \to 0$ and $\sqrt{E_{\text{trans}} - V_0} \not\to 0$. As such, for the square well, Γ should grow without bound as we consider larger transparency energies. This is the effect we see happening in Figure 4.2.

The transmission spectrum can be viewed to be composed of many of the above-defied FBW-distributions summed together, one for each transparency:

$$T(E) = \sum_{m=0} \frac{(\Gamma_m/2)^2}{(E - E_m)^2 + (\Gamma_m/2)^2}, \tag{4.50}$$

where

$$E_m = \left(\frac{\hbar(N+m)\pi}{2\nu}\right)^2 + V_0 \tag{4.51}$$

and N is the minimal positive integer so that $E_0 \geq 0$. This is *almost* the true form of the transmission spectrum. Namely, the peaks need to be well-defined enough in order for each of them to count as a FBW-distribution. In other words, if the peaks become too wide, then peaks start to interfere with each other and they will no longer be FBW-distributions. Quoting from [5, §2.2], mathematically we make this condition concrete as

$$\frac{\Gamma/2}{\Delta E} \ll 1, \tag{4.52}$$

where ΔE is the distance between two adjacent transparencies. Furthermore noting that $\Delta E \sim m < E_m \sim m^2$, we can extend (4.52) by writing

$$\frac{\Gamma_m/2}{E_m} < \frac{\Gamma_m/2}{\Delta E} \ll 1. \tag{4.53}$$

On its resonances

The fact that the transmission coefficient has an FBW-distribution around each peak allows us to locate resonances in a friendlier way. To illustrate: since a resonance is a pole of the transmission amplitude, following (4.31) resonances are located at those k where

$$\frac{q - k^2 q^{-1}}{2}\sinh(2q\nu) = ik\cosh(2q\nu) \iff \coth(2q\nu) = \frac{qk^{-1} - kq^{-1}}{2i}, \tag{4.54}$$

which is a transcendental and uninsightful equation.

Let us instead assume that we expand T around transparency E_m, so that we obtain

$$T(E_m + \delta E) \approx \frac{(\Gamma_m/2)^2}{\delta E^2 + (\Gamma_m/2)^2}, \tag{4.55}$$

featuring Γ_m as in (4.48) (with $E_{\text{trans}} \equiv E_m$). Now, if we allow *complex* perturbations δE, then the choice $\delta E = \pm i\Gamma_m/2$ will lead to

$$T(E_m \pm i\Gamma_m/2) \approx \frac{(\Gamma_m/2)^2}{-(\Gamma_m/2)^2 + (\Gamma_m/2)^2} \to \infty. \tag{4.56}$$

This will only work for Γ_m sufficiently small, as T is only FBW for small δE. Nevertheless, the above means that for $k_m := \hbar^{-1}\sqrt{E_m - i\Gamma_m/2}$, we must have that $|S(k_m)| \to \infty$ as well—a resonance is located.

Remark 4.11 (Relation resonances $\leftrightarrow$ transparencies)**.** The above construction works in *every* case in which a transparency along the real energy axis can be rewritten as a FBW distribution. This means that, as long as that is the case, one can find a close (albeit slightly approximate) relation between resonances and transparencies.

There is one subtlety: for the square root, we *must* choose the one whose image lies in the lower half plane. That is to say, we *must* assume our complex energy to be on the second sheet of the Riemann surface on which the energy lives cf. section 3.1.1. That this should be the case follows as the converse of Proposition 3.11, but since we have a concrete formula at our disposal we should also be able to make this derivation utilizing it. This is the topic of the following Proposition.

Proposition 4.12 (Location of resonances)**.** *For the square well, the resonances with $E_m > 0$ are all located in the* lower half *of the complex k-plane, or correspondingly, on the second sheet of the energy Riemann surface.*

Proof. Let $\mathcal{E}_m = E_m \pm i\Gamma_m/2$ be a resonance of the square well. It lies in the right half of the complex plane, as $E_m > 0$. Let us for now consider the + case, so $\mathcal{E}_m$ lies in the first quadrant.

The proof will be by contrapositive: we will show that, assuming

$$\sqrt{\cdot} : \arg\sqrt{z} \in [0, \pi), \tag{4.57}$$

the resonance equation (4.54) cannot be satisfied. To this end, notice that since $\mathcal{E}_m$ lies in first quadrant, so will $k_m = \hbar^{-1}\sqrt{\mathcal{E}_m}$. Furthermore, since $V_0 - \mathcal{E}_m$ lies in the third quadrant, $q_m = \hbar^{-1}\sqrt{V_0 - \mathcal{E}_m}$ will lie in the second quadrant. For simplicity, let

$$q_m = -a + bi \quad \text{and} \quad k_m = c + di, \tag{4.58}$$

for $a, b, c, d > 0$. We now analyse both lhs and rhs of (4.54).

lhs: Utilizing some hypertrigonometric identities, we may derive that

$$\coth(2\nu q_m) = \coth(2\nu(-a+bi)) = \frac{\coth(-2\nu a)[1 + \cot^2(2\nu b)]}{\coth^2(-2\nu a) + \cot^2(2\nu b)} + i\,\frac{\cot(2\nu b)[1 - \coth^2(-2\nu a)]}{\coth^2(-2\nu a) + \cot^2(2\nu b)}. \tag{4.59}$$

We cannot say anything about the sign of the imaginary part. The real part, however, will have negative sign: the denominator is positive, coth of a negative number is negative, and the term in brackets is positive. Hence, we conclude that the lhs lies on the *left* side of the complex plane.

rhs: We have that

$$\frac{q_m}{k_m} = \frac{-a+bi}{c+di} = \frac{1}{c^2+d^2}\left[(bd-ac)+i(ad+bc)\right]. \tag{4.60}$$

so it lies on the upper half of the complex plane, and

$$\frac{k_m}{q_m} = \frac{c+di}{-a+bi} = \frac{1}{a^2+b^2}\left[(bd-ac)-i(ad+bc)\right], \tag{4.61}$$

lies on the lower half. For the rhs we need the difference of these two numbers and then divided by $2i$:

$$\begin{aligned}\frac{1}{2i}\left[\frac{q_m}{k_m}-\frac{k_m}{q_m}\right] = -i\frac{(bd-ac)}{2}\left[\frac{1}{c^2+d^2}-\frac{1}{a^2+b^2}\right] \\ + \frac{(ad+bc)}{2}\left[\frac{1}{c^2+d^2}+\frac{1}{a^2+b^2}\right].\end{aligned} \tag{4.62}$$

Evidently, the real part of this quantity is positive, so that this number lives on the *right* side of the complex plane.

Thus, under the assumption (4.57), the lhs and rhs lie in different halves of the complex plane, and so the equation (4.54) cannot possibly be satisfied.

In the case of $-$, i.e. where $\mathcal{E}_m = E_m - i\Gamma_m/2$, a similar reasoning as the above can be followed, yielding the same conclusion (albeit that then the lhs lives on the right half, and the rhs on the left).

Taken together, then, we must have that if k_m is a resonance, i.e. satisfies the equation (4.54), we must have that

$$\arg k_m = \arg\sqrt{E_m \pm i\Gamma_m/2} \in [\pi, 2\pi). \tag{4.63}$$

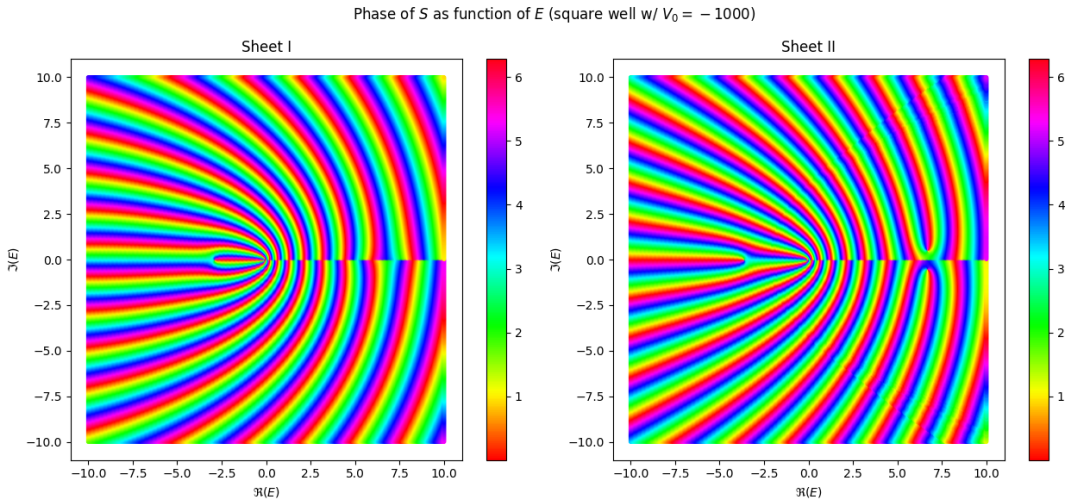
That is to say k_m must live on the lower half of the complex plane, and so that the corresponding energy must live on the second Riemann sheet. □

We may confirm the result of the above Proposition by evaluating the transmission amplitude over the energy Riemann surface. The result of this is the Figure 4.3. On the first sheet (which corresponds to upper half of the k plane) we see only one pole, which is located on the negative real axis around -3. This pole corresponds to a bound state of the square well.

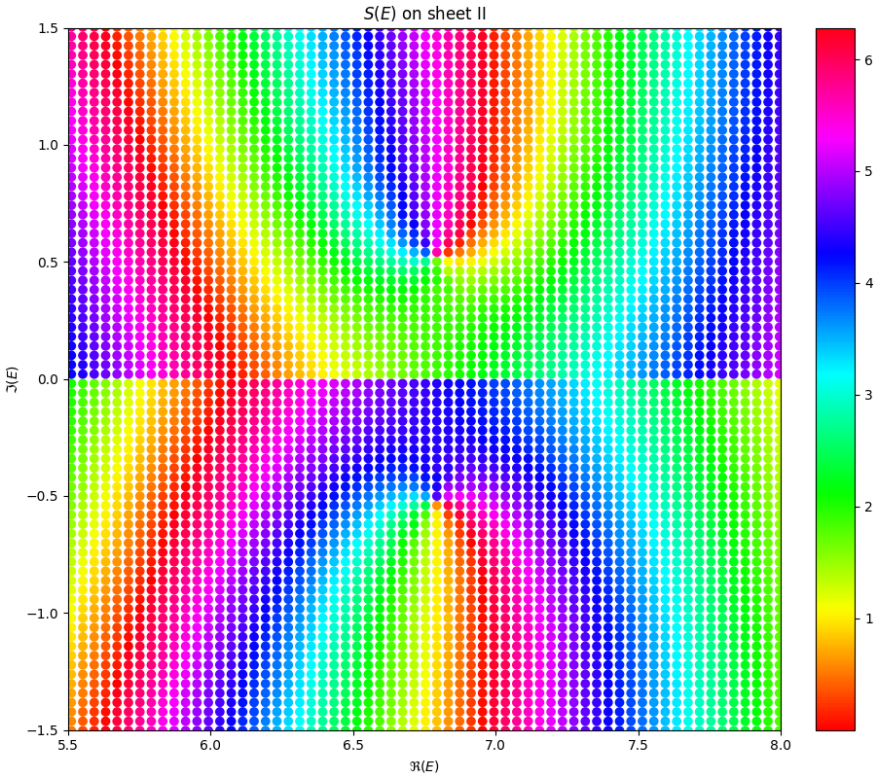
On the second sheet, however, we see three poles: one again on the negative real axis, and two off-axis in the right side of the plane. The former here is known as an *antibound* state (also present in Figure 3.5), and corresponds to k-values on the negative imaginary axis. These we shall not further discuss in this thesis.

The two off-axis poles, though, are the highlights of Figure 4.3. These are the resonances which we hypothesized existed by the construction of equation (4.56), now confirmed to be there. Indeed, the real part of this conjugate pair of energies is approximately 6.7, which is the first transparency energy. If the bounds of this image were larger, we would see more of these resonances on the second sheet belonging to larger transparency energies.

Finally, we note that even though to each transparency energy E_m there belong two resonances $E_m \pm i\Gamma_m/2$, only the minus variant constitutes a Gamow-Siegert type.



(a) Large-scale view of the two sheets of the Riemann surface.



(b) Zoomed view on the second sheet, around the two resonances.

Figure 4.3: Phase of $S(\mathcal{E})$ for the square well ($V_0 = -1000$, $\nu = 10$) over a subset of the Riemann surface ($\hbar \equiv 1$). Where all colors come together (once on sheet I, three times on sheet II), there is a pole.

4.3 WKB Potentials

In this section we will strive to simplify the expression for $S(k)$ in (4.14) as much as possible, under the assumption that the potential-energy combination allows us to use the WKB approximation for the solution of the Schrödinger equation. In fact, we will attempt to eliminate any dependence on the solution, as represented by $\theta_{\mathrm{e,o}}$. This should then yield a transmission amplitude based solely on the (geometry of the) potential we are dealing with, which is the best we can do.

The basis for the simplification will be the following Proposition, relating $\theta_{\mathrm{e,o}}$ directly to the potential as encoded in $\mathbf{P}$.

Proposition 4.13 ($\theta_{\mathrm{e,o}}$ in case of WKB)**.** *Assume that we can approximate the wavefunction using WKB, except possibly at some turning points. Then, we have that*

$$\boxed{\theta_{\mathrm{e,o}} = -ik \times \frac{(1\,,-1)\,\boldsymbol{v}^{\pm}}{(1\,,1)\,\boldsymbol{v}^{\pm}},} \tag{4.64}$$

where $\boldsymbol{v}^{\pm}$ are the eigenvectors of $\mathbf{P}$ such that $\mathbf{P}\boldsymbol{v}^{\pm} = \pm\boldsymbol{v}^{\pm}$.

Proof. Following its definition, effectively what we need to calculate is

$$\theta_{\mathrm{e,o}} = \frac{\psi'(\nu) \mp \psi'(-\nu)}{\psi(\nu) \pm \psi(-\nu)}. \tag{4.65}$$

Naturally we invoke WKB; let us first worry about the front factor of the wavefunction:

$$\psi_{\mathrm{WKB}}(x) = |\mathcal{E} - V(x)|^{-1/4} \times \mathrm{stuff}_1 \implies \psi_{\mathrm{e,o}}(x) = |\mathcal{E} - V(x)|^{-1/4} \times \mathrm{stuff}_2. \tag{4.66}$$

As such,

$$\theta_{\mathrm{e,o}} = \frac{d}{dx}\Big|_{x=\pm\nu} \ln(\psi_{\mathrm{e,o}}) = \frac{-1}{\cancel{4}} \frac{\cancel{|V'(\pm\nu)|}}{\cancel{|\mathcal{E} - V(\pm\nu)|}} + \mathrm{stuff}_3, \tag{4.67}$$

by virtue of V being continuous, so the derivative at the start and end of the intervals must vanish (or otherwise be of small size). Therefore, the front factor is not relevant to finding $\theta_{\mathrm{e,o}}$, and so we will disregard it.

Now, assume that around $x \approx -\nu$, we have the wavefunction $\psi(x)$ approximated via WKB as

$$\psi|_{x\approx-\nu}(x) = A\exp\big(i\hbar^{-1}I^{x}_{-\nu}\big) + B\exp\big(-i\hbar^{-1}I^{x}_{-\nu}\big), \tag{4.68}$$

for some $A, B \in \mathbb{C}$, and we use the $I^{\cdot}_{\cdot}$ as introduced in Notation 2.12. Evidently, $\psi(-\nu) = A + B$ and

$$\begin{aligned}\psi'(-\nu) &= i\hbar^{-1}\sqrt{\mathcal{E} - \cancel{V(-\nu)}}\,\big[A\exp\big(i\hbar^{-1}I^{-\nu}_{-\nu}\big) - B\exp\big(-i\hbar^{-1}I^{-\nu}_{-\nu}\big)\big] \\ &= ik(A - B).\end{aligned} \tag{4.69}$$

Near $x \approx \nu$, the wavefunction will be given by $\psi|_{x\approx\nu} = \mathbf{P}\psi|_{x\approx-\nu}$ cf. (2.62). As such,

$$\psi|_{x\approx\nu}(x) = \widetilde{A}\exp\big(i\hbar^{-1}I^{\nu}_{x}\big) + \widetilde{B}\exp\big(-i\hbar^{-1}I^{\nu}_{x}\big), \text{ with } \begin{pmatrix}\tilde{A}\\ \tilde{B}\end{pmatrix} = \mathbf{P}\begin{pmatrix}A\\ B\end{pmatrix}. \tag{4.70}$$

Then, $\psi(\nu) = \widetilde{A} + \widetilde{B}$, and

$$\begin{aligned}\psi'(\nu) &= -i\hbar^{-1}\sqrt{\mathcal{E} - \cancel{V(\nu)}}\left[\widetilde{A}\exp\bigl(i\hbar^{-1}I_\nu^\nu\bigr) - \widetilde{B}\exp\bigl(i\hbar^{-1}I_\nu^\nu\bigr)\right] \\ &= ik(\widetilde{B} - \widetilde{A})\end{aligned} \tag{4.71}$$

(note here that x was the lower bound on the integral, hence differentiation incurred an additional minus sign). Collecting the relevant info, we have

$$\theta_{\mathrm{e,o}} = ik \times \frac{(\widetilde{B} - \widetilde{A}) \mp (A - B)}{(\widetilde{A} + \widetilde{B}) \pm (A + B)}. \tag{4.72}$$

We can compactify the expression somewhat by noticing that

$$\widetilde{B} - \widetilde{A} = (1\,,-1)\,(-\mathbf{P})\begin{pmatrix}A\\B\end{pmatrix} \quad \text{and} \quad A - B = (1\,,-1)\begin{pmatrix}A\\B\end{pmatrix}, \tag{4.73}$$

from which it follows

$$(\widetilde{B} - \widetilde{A}) \mp (A - B) = (1\,,-1)\,[-\mathbf{P} \mp \mathbf{I}]\begin{pmatrix}A\\B\end{pmatrix} = -\,(1\,,-1)\,[\mathbf{P} \pm \mathbf{I}]\begin{pmatrix}A\\B\end{pmatrix}. \tag{4.74}$$

Here, $\mathbf{I}$ is the identity matrix. Similarly, we find

$$(\widetilde{A} + \widetilde{B}) \pm (A + B) = (1\,,1)\,[\mathbf{P} \pm \mathbf{I}]\begin{pmatrix}A\\B\end{pmatrix}, \tag{4.75}$$

so that we obtain

$$\theta_{\mathrm{e,o}} = -ik \times \frac{(1\,,-1)\,[\mathbf{P} \pm \mathbf{I}]\begin{pmatrix}A\\B\end{pmatrix}}{(1\,,1)\,[\mathbf{P} \pm \mathbf{I}]\begin{pmatrix}A\\B\end{pmatrix}} \tag{4.76}$$

Now, we make the observation that

$$\mathbf{P}\,[\mathbf{P} \pm \mathbf{I}]\begin{pmatrix}A\\B\end{pmatrix} = \pm\,[\mathbf{P} \pm \mathbf{I}]\begin{pmatrix}A\\B\end{pmatrix}, \tag{4.77}$$

for all vectors $(A\,,B)^{\intercal}$, as $\mathbf{P}$ is involutory by Lemma 2.14. As such, we have that $[\mathbf{P} \pm \mathbf{I}]\,(A\,,B)^{\intercal}$ are eigenvectors of $\mathbf{P}$ with eigenvalues ± 1. Defining

$$\boldsymbol{v}^{\pm} := [\mathbf{P} \pm \mathbf{I}]\begin{pmatrix}A\\B\end{pmatrix}, \tag{4.78}$$

we substitute this into (4.76) to obtain the query, and so complete the proof. □

In fact, it can be verified that the eigenvectors of $\mathbf{P}$ are

$$\boldsymbol{v}^{\pm} = \begin{pmatrix}1\\ v_2^{\pm}\end{pmatrix} = \begin{pmatrix}1\\ [\pm 1 - \mathbf{P}_{11}]\mathbf{P}_{12}^{-1}\end{pmatrix}, \tag{4.79}$$

under the assumption that $\mathbf{P}_{12} \neq 0$. Then, we can fill in the formula (4.14) using (4.64) and obtain

$$\begin{aligned} S(k) &= -\exp(-2ik\nu)\left(\frac{(1\,,-1)\,\boldsymbol{v}^+}{(1\,,1)\,\boldsymbol{v}^+} - \frac{(1\,,-1)\,\boldsymbol{v}^-}{(1\,,1)\,\boldsymbol{v}^-}\right) \\ &\quad \times \left[\left(\frac{(1\,,-1)\,\boldsymbol{v}^+}{(1\,,1)\,\boldsymbol{v}^+}+1\right)\left(\frac{(1\,,-1)\,\boldsymbol{v}^-}{(1\,,1)\,\boldsymbol{v}^-}+1\right)\right]^{-1} \\ &= -\exp(-2ik\nu)\frac{(1\,,-1)\,\boldsymbol{v}^+\,(1\,,1)\,\boldsymbol{v}^- - (1\,,-1)\,\boldsymbol{v}^-\,(1\,,1)\,\boldsymbol{v}^-}{\underbrace{(2\,,0)\,\boldsymbol{v}^+\,(2\,,0)\,\boldsymbol{v}^-}_{=4}} \\ &= \frac{-\exp(-2ik\nu)}{4}\left|\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}^2 (\boldsymbol{v}^+\,,\boldsymbol{v}^-)\right| \\ &= \frac{-\exp(-2ik\nu)}{2}(v_2^- - v_2^+). \end{aligned} \tag{4.80}$$

We see from (4.79) that

$$v_2^- - v_2^+ = \frac{-1-\mathbf{P}_{11}}{\mathbf{P}_{12}} - \frac{1-\mathbf{P}_{11}}{\mathbf{P}_{12}} = -\frac{2}{\mathbf{P}_{12}}, \tag{4.81}$$

so that we can finally write

$$\boxed{S(k) = \frac{\exp(-2ik\nu)}{\mathbf{P}_{12}}} \tag{4.82}$$

as the general transmission amplitude in the case that we can apply the WKB approximation.

Let us explore what this formula can give us in terms of concrete results. To keep things organized, I will do this in the following sections, in which cases will be treated by count of turning points for the specific energy-potential combination. An illustration of each energy-potential combination giving rise to the amount of turning points is given in Figure 4.4

4.3.1 No turning points

In the case of there being no turning points (e.g. the **dashed black** line in Figure 4.4), we can do the calculation easily. Namely, in this case, $\mathbf{P}$ is simply the forward transport of the wavefunction by means of $\mathbf{F}$:

$$\mathbf{P} = \mathbf{F}(-\nu \to \nu) = \begin{pmatrix} 0 & \exp(-i\hbar^{-1}I) \\ \exp(i\hbar^{-1}I) & 0 \end{pmatrix}, \tag{4.83}$$

for $I := I^{\nu}_{-\nu}$. Then employ (4.82) to directly get

$$S(k) = \frac{\exp(-2ik\nu)}{\exp(-i\hbar^{-1}I)} = \exp\big(i\left[\hbar^{-1}I - 2k\nu\right]\big) \tag{4.84}$$

After staring at this expression for a bit, we notice that for $\mathcal{E} > 0$, whatever is inside the exponent is purely imaginary. In turn, this means that $|S(k)|^2 = 1$ regardless of the

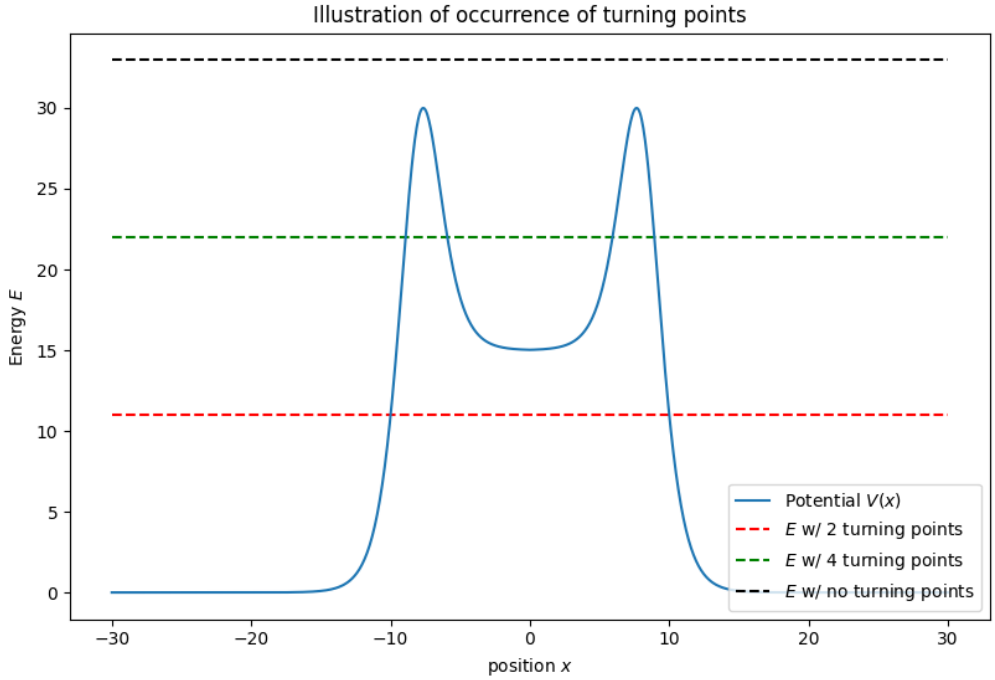


Figure 4.4: Illustration of the occurrence of different amounts of turning points for various energy levels (here presented for the same potential for all energies).

specific geometry of the potential or the size of the energy. As such, we have effectively shown that when there are no turning points in a WKB-applicable situation, we will always have full transmission!

This conclusion should not be wholly unexpected. The gradually varying potential ensures that the incoming wave is not reflected back; only at an interface, i.e. a sudden change in the potential, should we have a reflected wave created. Since there are no turning points, there are no such interfaces, and hence no reflected waves. The only effect then that the potential could have is to induce a phase into the transmitted wave, which is perfectly allowed by the above expression.

Remark 4.14 (Notes on physicality)**.** The derived expression for $S(k)$ (4.84) is also good on two key fronts necessary for physicality.

1. *It is independent of increase of ν.* Since ν is nothing more than a cutoff for our potential landscape, we should be able to increase it to an arbitrary size and still end up with the same physics, that is to say, with the same transmission *amplitude*. Fortunately, this is covered in the expression. Observe that if we parse ν explicitly as an argument into $S(k)$, we can derive

$$\begin{aligned} S(k,\nu+\delta\nu) &= \exp\big(i\left[\hbar^{-1}I^{\nu+\delta\nu}_{-\nu-\delta\nu} - 2k(\nu+\delta\nu)\right]\big) \\ &= \exp\big(i\left[\hbar^{-1}I^{\nu}_{-\nu} - 2k\nu\right]\big)\exp\big(i\left[\hbar^{-1}\left\{I^{-\nu}_{-\nu-\delta\nu} + I^{\nu+\delta\nu}_{\nu}\right\} - 2k\,\delta\nu\right]\big) \\ &= S(k,\nu)\exp\big(i\left[\hbar^{-1}\left\{I^{-\nu}_{-\nu-\delta\nu} + I^{\nu+\delta\nu}_{\nu}\right\} - 2k\,\delta\nu\right]\big). \end{aligned} \tag{4.85}$$

Now, since $V(x) \equiv 0$ for $x > \nu$, we have that

$$I^{\nu+\delta\nu}_{\nu} = \int_{\nu}^{\nu+\delta\nu} \sqrt{\mathcal{E}}\,dx' = \delta\nu\,\sqrt{\mathcal{E}} = \hbar k\,\delta\nu. \tag{4.86}$$

Similarly, $I^{-\nu}_{-\nu-\delta\nu} = \hbar k\,\delta\nu$ also. We then see that the exponential factor in (4.85) simplifies to 1, so that we have indeed $S(k, \nu + \delta\nu) = S(k, \nu)$ for $\delta\nu \geq 0$.

2. *As $|k|$ grows, $S(k) \to 1$.* That is to say, if we increase the energy of our particle, it should care less and less about the potential, and instead just fly through. This too is satisfied: for large $|k|$, the exponent becomes

$$i\left[\hbar^{-1}\int_{-\nu}^{\nu}\sqrt{\mathcal{E}-V(x')}\,dx' - 2k\nu\right] \xrightarrow{|k|\to\infty} i\left[2k\nu - 2k\nu\right] = 0, \tag{4.87}$$

so that $S(k) \to 1$.

Point 2. of the above Remark in fact holds for *any* system, as in the limit of large $|k| \leftrightarrow |\mathcal{E}|$ the WKB condition will always be satisfied and there will be no more turning points. As such, we (re)produce the result that any system will become transparent as long as you "shoot hard enough."

4.3.2 Two turning points; one hill

The next step up is to consider a potential hill, i.e. a situation where we have two turning points (e.g. the **dashed red** line in Figure 4.4). Qualitatively, we would not expect to find much here: the hill should simply force some exponential decay of the wavefunction, and as such make it impossible to obtain full transmission.

Assume that the turning points are located at $-q$ and q with $0 < q < \nu$, and define $Q := \exp\!\big(-i\hbar^{-1}I^q_{-q}\big)$ and $\alpha := \exp\!\big(-i\hbar^{-1}I^\nu_q\big)$. We find the **P**-matrix thusly:

$$\begin{aligned}
\mathbf{P} &= \mathbf{F}(q\to\nu)\,\mathbf{B}\,\mathbf{F}(-q\to q)\,\mathbf{A}\,\mathbf{F}(-\nu\to -q)\\
&= \begin{pmatrix} 0 & \alpha \\ \alpha^{-1} & 0 \end{pmatrix}\begin{pmatrix} ie^{-i\pi/4}/2 & e^{-i\pi/4} \\ -ie^{i\pi/4}/2 & e^{i\pi/4}\end{pmatrix}\begin{pmatrix} 0 & Q \\ Q^{-1} & 0\end{pmatrix}\begin{pmatrix} -ie^{i\pi/4} & ie^{-i\pi/4} \\ e^{i\pi/4}/2 & e^{-i\pi/4}/2\end{pmatrix}\begin{pmatrix} 0 & \alpha \\ \alpha^{-1} & 0\end{pmatrix}\\
&= \begin{pmatrix} 0 & \alpha \\ \alpha^{-1} & 0 \end{pmatrix}\begin{pmatrix} i(Q/4 - Q^{-1}) & Q^{-1} + Q/4 \\ Q^{-1} + Q/4 & i(Q^{-1} - Q/4)\end{pmatrix}\begin{pmatrix} 0 & \alpha \\ \alpha^{-1} & 0\end{pmatrix}\\
&\overset{\star}{=} \begin{pmatrix} 0 & \alpha \\ \alpha^{-1} & 0 \end{pmatrix}\begin{pmatrix} i\sinh(\ln Q - \ln 2) & \cosh(\ln Q - \ln 2) \\ \cosh(\ln Q - \ln 2) & -i\sinh(\ln Q - \ln 2)\end{pmatrix}\begin{pmatrix} 0 & \alpha \\ \alpha^{-1} & 0\end{pmatrix}\\
&= \begin{pmatrix} -i\sinh(-i\hbar^{-1}I - \ln 2) & \alpha^2\cosh(-i\hbar^{-1}I - \ln 2) \\ \alpha^{-2}\cosh(-i\hbar^{-1}I - \ln 2) & i\sinh(-i\hbar^{-1}I - \ln 2)\end{pmatrix},
\end{aligned} \tag{4.88}$$

where **A** and **B** are as in (2.56), $I := I^q_{-q}$, and for $\star$ we used

$$\begin{aligned}
Q^{-1} + Q/4 = \tfrac{1}{2}((Q/2)^{-1} + Q/2) = \tfrac{1}{2}(e^{\ln(Q/2)} + e^{-\ln(Q/2)}) &= \cosh(\ln(Q/2))\\
&= \cosh(\ln Q - \ln 2),
\end{aligned} \tag{4.89}$$

and similarly for the sinh terms. As such, employing (4.82), we find that

$$S(k) = \frac{\exp(-2ik\nu)}{\alpha^2\cosh(-i\hbar^{-1}I - \ln 2)} \tag{4.90}$$

is the general transmission amplitude for a WKB potential in the case of two turning points.

We would also like to consider the simplified case of $\mathcal{E} = E > 0$. Note that then $\mathcal{E} - V(x')$ becomes a negative real number inside of the interval $(-q, q)$, and so the integrand $\sqrt{\mathcal{E} - V(x')}$ becomes purely imaginary. We must be careful, though: as we have introduced before (subsection 3.1.1), the square root has two possible images, and these are not equivalent to each other!

As addressed in that same section, the right choice for us is that square root with image in the lower half plane. As such, the integrand is a negative imaginary number across the entire integration domain, yielding us that I is also negative imaginary. Thus, we justify the equality $-i\hbar^{-1}I = -\hbar^{-1}|I|$ for real $\mathcal{E} > 0$, and we can write down the transmission amplitude and coefficient for that case to be

$$S_{\mathcal{E}>0}(k) = \frac{\exp(-2ik\nu)}{\alpha^2 \cosh(\hbar^{-1}|I| + \ln 2)} \quad \text{and} \quad T_{\mathcal{E}>0}(k) = \cosh^{-2}\big(\hbar^{-1}|I| + \ln 2\big). \tag{4.91}$$

Notably, from this second formula we learn that we expect an upper limit to the transmission:

$$T_{\mathcal{E}>0} < \cosh^{-2}(\ln 2) = 16/25 = .64. \tag{4.92}$$

This means that with a barrier in place, based on the WKB approximation, we would not expect transparency for any energy. This is with the caveat that for $E \approx \max V$, the WKB approximation is no longer valid.

Under the additional assumption that $\hbar^{-1}|I| - \ln 2 \gg 1$, we may simplify $T_{\mathcal{E}>0}$ even further to read

$$T_{\mathcal{E}>0} \approx \exp\big(-2\hbar^{-1}|I|\big). \tag{4.93}$$

This formula for the transmission coefficient then agrees with established literature in, for instance, [7, (9.60)].

Example: a Gaussian potential

To illustrate the above, consider the Gaussian potential

$$V_{\text{gauss}}(x) = 30 \exp\big(-x^2\big), \tag{4.94}$$

where we do not bound x as the value of V gets small very quickly anyway. Since the maximum of this potential lies at 30, for any energy lower than this we will have two turning points, so the above formulae apply. The numerically computed and theoretical transmission coefficients, based on the above expression for $S_{\mathcal{E}>0}(k)$, are shown in Figure 4.5. We notice that we have a very good match between the theoretical prediction of (4.91) and the computed value, bolstered by the fact that the difference between the two (in dotted red), consistently lies about an order of magnitude below their respective values.

4.3.3 Four turning points; two hills, one valley

Let us move on to the situation of two hills with a valley inbetween, i.e. the situation with four turning points (e.g. the **dashed green** line in Figure 4.4). For this, notice that by symmetry we can lay our turning points at $-p$, $-q$, q, and p, with $0 < q < p < \nu$. Thus, $\pm p$ are the outer turning points, and $\pm q$ the inner ones.

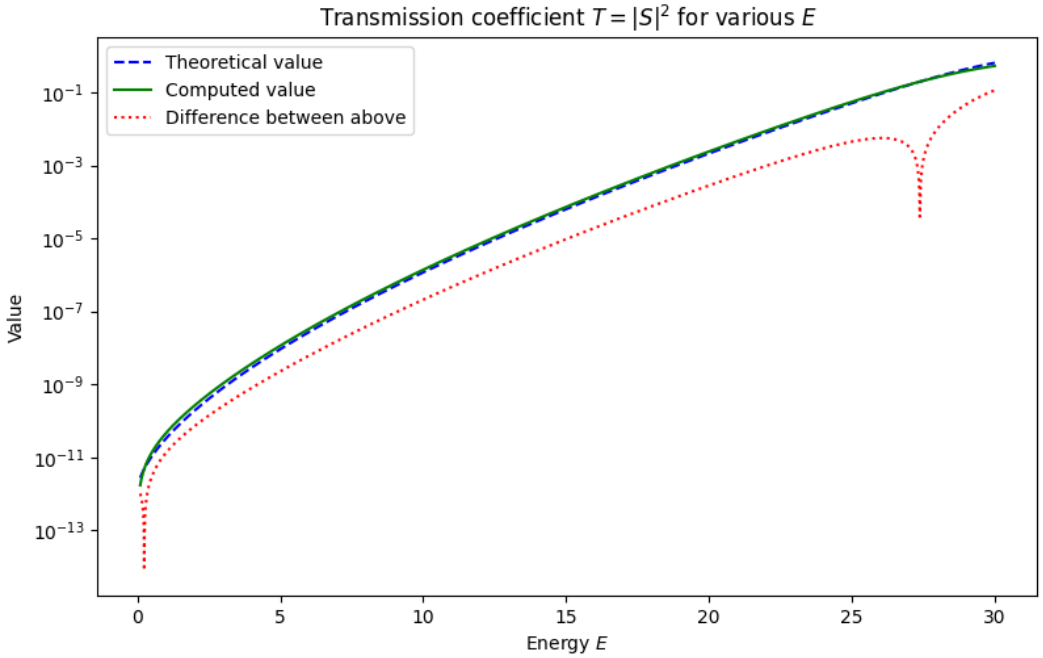


Figure 4.5: Transmission spectra for Gaussian potential of (4.94). All three curves contain 3 000 equispaced data points, and assume $\hbar \equiv 1$.

To calculate $\mathbf{P}$, we have to find

$$\mathbf{P} = \mathbf{F}(p \to \nu)\,\mathbf{B}\,\mathbf{F}(q \to p)\,\mathbf{A}\,\mathbf{F}(-q \to q)\,\mathbf{B}\,\mathbf{F}(-p \to -q)\,\mathbf{A}\,\mathbf{F}(-\nu \to -p). \tag{4.95}$$

The matrices $\mathbf{A}$ and $\mathbf{B}$ are as in (2.56), while the $\mathbf{F}$s can be written as

$$\begin{cases} \mathbf{F}(p \to \nu) = \mathbf{F} = (-\nu \to -p) = \begin{pmatrix} 0 & \alpha \\ \alpha^{-1} & 0 \end{pmatrix} \\ \mathbf{F}(q \to p) = \mathbf{F}(-p \to -q) = \begin{pmatrix} 0 & \beta \\ \beta^{-1} & 0 \end{pmatrix} \\ \mathbf{F}(-q \to q) = \begin{pmatrix} 0 & \gamma \\ \gamma^{-1} & 0 \end{pmatrix} \end{cases}, \tag{4.96}$$

for

$$\alpha = \exp\bigl(-i\hbar^{-1} I_{-\nu}^{-p}\bigr),\ \beta = \exp\bigl(-i\hbar^{-1} I_{-p}^{-q}\bigr),\ \text{and}\ \gamma = \exp\bigl(-i\hbar^{-1} I_{-q}^{q}\bigr). \tag{4.97}$$

With the help of Mathematica we can calculate $\mathbf{P}$ as in equation (4.95):

$$\begin{aligned} \mathbf{P} &= \frac{1+\gamma^2}{16\beta^2\gamma} \begin{pmatrix} -i(\beta^4 - 16) & \alpha^2(\beta^4 + 16 + 8\beta^2 \frac{\gamma^2-1}{\gamma^2+1}) \\ \alpha^{-2}(\beta^4 + 16 - 8\beta^2 \frac{\gamma^2-1}{\gamma^2+1}) & i(\beta^4 - 16) \end{pmatrix} \\ &= \frac{\cos\bigl(\hbar^{-1} I_{-q}^{q}\bigr)}{8} \begin{pmatrix} -i(\beta^2 - 16\beta^{-2}) & \alpha^2(\beta^2 + 16\beta^{-2} - 8i\tan\bigl(\hbar^{-1} I_{-q}^{q}\bigr)) \\ \alpha^{-2}(\beta^2 + 16\beta^{-2} + 8i\tan\bigl(\hbar^{-1} I_{-q}^{q}\bigr)) & i(\beta^2 - 16\beta^{-2}) \end{pmatrix} \end{aligned} \tag{4.98}$$

Therefore, once more employing (4.82), we have that $S(k)$ will be given by

$$S(k) = \alpha^{-2} \exp(-2ik\nu) \left[\tfrac{1}{8} \cos\bigl(\hbar^{-1} I_{-q}^{q}\bigr)(\beta^2 + 16\beta^{-2}) - i \sin\bigl(\hbar^{-1} I_{-q}^{q}\bigr)\right]^{-1}. \tag{4.99}$$

Notice that we have a stark difference as compared to the case of two turning points: here we have trigonometric functions involved as well, which suggest that the transmission amplitude exhibits some manner of oscillation and/or periodicity in $\mathcal{E}$. Since this expression is not trivial, it should be rewarding to calculate the transmission coefficient for this system. Assuming real $\mathcal{E} = E > 0$, we find that

$$\begin{aligned} T_{\mathcal{E}>0} &= \left[64^{-1}\cos^2\left(\hbar^{-1}I^q_{-q}\right)(\beta^2+16\beta^{-2})^2 + \sin^2\left(\hbar^{-1}I^q_{-q}\right)\right]^{-1} \\ &= \left[1+64^{-1}\cos^2\left(\hbar^{-1}I^q_{-q}\right)\{(\beta^2+16\beta^{-2})^2-64\}\right]^{-1} \\ &= \left[1+64^{-1}\cos^2\left(\hbar^{-1}I^q_{-q}\right)(\beta^2-16\beta^{-2})^2\right]^{-1} \\ &\overset{\star}{=} \left[1+\cos^2\left(\hbar^{-1}I^q_{-q}\right)\sinh^2(2\ln\beta-2\ln 2)\right]^{-1} \\ &= \left[1+\cos^2\left(\hbar^{-1}I^q_{-q}\right)\sinh^2\left(-2i\hbar^{-1}I^{-q}_{-p}-2\ln 2\right)\right]^{-1} \\ &\overset{\star\star}{=} \left[1+\cos^2\left(\hbar^{-1}I^q_{-q}\right)\sinh^2\left(2\hbar^{-1}|I^{-q}_{-p}|+2\ln 2\right)\right]^{-1} \end{aligned} \tag{4.100}$$

where in $\star$ we used a trick identical to (4.89), and for $\star\star$ we used the same reasoning as for the one turning point case to argue $-iI^{-q}_{-p} = -|I^{-q}_{-p}|$ (and noticed $\sinh^2$ is even so we can remove an overall minus sign). From this expression, notice foremost that $0 \leq T \leq 1$ due to the constant $+1$ in the denominator and the rest of the sum being positive. A welcome result, since this is the allowed range of T for real k, so this checks out on physicality on that front.

We can compare this formula to one in established literature, namely [7, (9.106)]:

$$T_{\text{WKB}} = \frac{\exp(-2(K_{\text{II}}+K_{\text{IV}}))}{4\cos^2 L_{\text{III}}}. \tag{4.101}$$

Here K_{II} and K_{IV} are the (absolute values of) the integrations over the hills, and L_{III} is the same for the valley inbetween. Comparing to our notation, this boils down to

$$K_{\text{II}} \equiv \hbar^{-1}|I^{-q}_{-p}|, \quad K_{\text{IV}} \equiv \hbar^{-1}|I^{p}_{q}|, \quad \text{and} \quad L_{\text{III}} = \hbar^{-1}|I^{q}_{-q}|. \tag{4.102}$$

This formula and (4.100) are asymptotically equal to each other under the assumption of $\hbar^{-1}|I^{-q}_{-p}| \gg 1$. However, the addition of $+1$ in the denominator of our formula makes it so that the the transmission coefficient can no longer explode, and instead reaches the expected maximum value of 1 for $\cos^2(\ldots) = 0$. Thus, the derived formula (4.100) represents an improvement over one found in the literature.

We moreover notice that the maximum transmission of 1 is not reached for only a single $\mathcal{E}$, but instead for potentially many such $\mathcal{E}$: whenever

$$k \in \mathbb{R} : \hbar^{-1}I^q_{-q} = \left(n+\tfrac{1}{2}\right)\pi \iff I^q_{-q} = \hbar\pi\left(n+\tfrac{1}{2}\right) \text{ for some } n \in \mathbb{N}, \tag{4.103}$$

we have a transparency energy. These are thus the energies at which *resonant tunneling* takes place: full transmission despite the energy being lower than the maximum of the potential.

Remark 4.15 (Bohr-Sommerfeld quantization II)**.** The condition (4.103) is a parallel of the *Bohr-Sommerfeld quantization condition* for quantized systems, a staple of the semiclassical treatment of QM. Since WKB is a semiclassical treatment of QM, it is not unsurprising that this appears "in the wild," and certainly a welcome result.

The $+1/2$ is derived from adding so-called *Morse indices* to this condition, which represent the fact that the potential slope is not infinite at the turning point. For more information/background we refer to [17, §4.2.2.5].

Normally the quantization is only applicable to bound state systems, but here it shows up where we explicitly do *not* have a bound state. This suggests that the particle views the potential valley in the middle as an unbounded harmonic potential $V_{\text{harm}}(x) = \alpha x^2 - V_0$.

Another feature that we can glance from (4.100) is a notion of the width of the peaks for the above $\mathcal{E}$. Upon using an expansion in orders of δE—à la Section 4.2.1—we find that around a transparency E_{trans} the transmission coefficient will read

$$\begin{aligned} T(E_{\text{trans}} + \delta E) &\approx \frac{1}{1 + \left(\frac{1}{2}\hbar^{-1} J^q_{-q}\right)^2 \sinh^2\!\left(2\hbar^{-1}|I^{-q}_{-p}| + 2\ln 2\right) \delta E^2} \\ &= \left(\frac{2\hbar}{J^q_{-q} \sinh\!\left(2\hbar^{-1}|I^{-q}_{-p}| + 2\ln 2\right)}\right)^2 \left[\delta E^2 + \left(\frac{2\hbar}{J^q_{-q} \sinh\!\left(2\hbar^{-1}|I^{-q}_{-p}| + 2\ln 2\right)}\right)^2\right]^{-1}, \end{aligned} \tag{4.104}$$

where

$$J^q_{-q} := \int_{-q}^{q} [E_{\text{trans}} - V(x')]^{-1/2}\, dx' \,. \tag{4.105}$$

That is to say, around transparencies the transmission coefficient follows an FBW-distribution with the width Γ given by

$$\Gamma = \frac{4\hbar}{J^q_{-q} \sinh\!\left(2\hbar^{-1}|I^{-q}_{-p}| + 2\ln 2\right)} \sim \frac{4\hbar\sqrt{E}}{\sinh\!\left(2\hbar^{-1}|I^{-q}_{-p}| + 2\ln 2\right)}, \tag{4.106}$$

and where we also used that $J^q_{-q} \sim E^{-1/2}$, very broadly speaking.

Analogously to the square well, as we decrease the energy, $|I^{-q}_{-p}|$ will increase, thus so will the sinh term, and so Γ will decrease. This translates itself to narrower peaks in a transmission spectrum. Contrary to the square well, though, here Γ in principle will decrease *exponentially* owing to the sinh, as opposed to sub-exponential.

To draw the comparison even further, the above suggests a remarkable similarity between the spectra qualitatively speaking. Namely, as long as $\Gamma/(\Delta E)$ remains sufficiently small, any two hill, one valley potential should permit an approximation by means of FBW-distributions around the transparency energies, just as was shown to be case for the square well.

Example: a sinc potential

As an example of the above situation, let us consider the sinc potential

$$V_{\text{sinc}}(x) = \begin{cases} -150\,\text{sinc}(\pi x/5) = \dfrac{-150\sin(\pi x/5)}{\pi x/5} & \text{if} \quad x \in [-10, 10] \\ 0 & \text{otherwise} \end{cases}. \tag{4.107}$$

A picture of this potential may be found in Figure 4.6. As can be seen, for any real

n	28	29	30	31	32	33	34	35	36	37
$E_n \pm 0.01$	0.96	4.98	8.87	12.63	16.25	19.71	23.01	26.10	28.94	31.45

Table 4.1: Values of transparency energy corresponding to n for the sinc potential, as determined from Figure 4.7.

energy lower than the peaks which values are ≈ 32.585, there will be four turning points, so we may apply the above formalism.

In particular, we may find the transparency energies E_n as solutions to the equation

$$\hbar^{-1} I^q_{-q}(E_n) = \hbar^{-1} \int_{-q}^{q} \sqrt{E_n + \frac{150 \sin(\pi x/5)}{\pi x/5}}\, dx = \pi \left(n + \tfrac{1}{2}\right) \text{ for some } n \in \mathbb{Z}, \quad (4.108)$$

cf. equation (4.103), and where the bounds of integration $\pm q$ depend on E as well (they must be chosen so that the integrand is positive real over the entire integration domain). An effective way to find the transparencies is to plot $\hbar^{-1} I^q_{-q}$ as a function of E, and then overlay $\pi(n + 1/2)$-gridlines to find the appropriate E_n. This has been done in Figure 4.7.

We should expect that these will be seen back in the transmission spectrum of the potential; in fact, we expect FBW-distributions precisely around these transparency energies, as based on the discussion above. In Figure 4.8, both the theoretical and computed transmission spectra for the sinc potential are shown. Firstly, observe that the peaks in (a) do not reach all the way up to 1, even though this is to be expected (at least from the theoretical value) for the transparency energies. This is due to our discretization not being fine enough. As a result, the energy which forms the peak in the Figure is not *the* local transparency, but a close "neighbor" thereof. If we were to make the discretization finer, these peaks should all bona fide reach $T = 1$.

Secondly, we notice that although the match in (a) seems to be quite well, the relative difference displayed in (b) is erratic with many spikes up and down. These can be explained, however.

Spikes up. These spikes are located around where the theoretical value has a peak, but the computed value does not—see Figure 4.9 for zoomed-in views around several peaks. As a result, the relative difference is effectively the ratio of the theoretical to the computed value, which is very high as the peak is very narrow (so the computed value is nowhere near 1).

Spikes down. These occur where the theoretical and computed values intersect each other: the relative difference will be almost zero, hence a spike down on the log-plot.

Optimistically discarding these spikes as "glitches," we would estimate that the relative difference is approximately $\pm 10\%$ over the entire energy interval. This is in agreement with Figure 4.5, where the difference is consistently about one order of magnitude below the computed/theoretical values.

Owing to the fact that T can be written as an FBW-distribution, we should also be expecting to find resonances at those real energies where a transparency occurs cf. Remark 4.11. In Figure 4.10, we have plotted the phase of $S(\mathcal{E})$ on a section of the

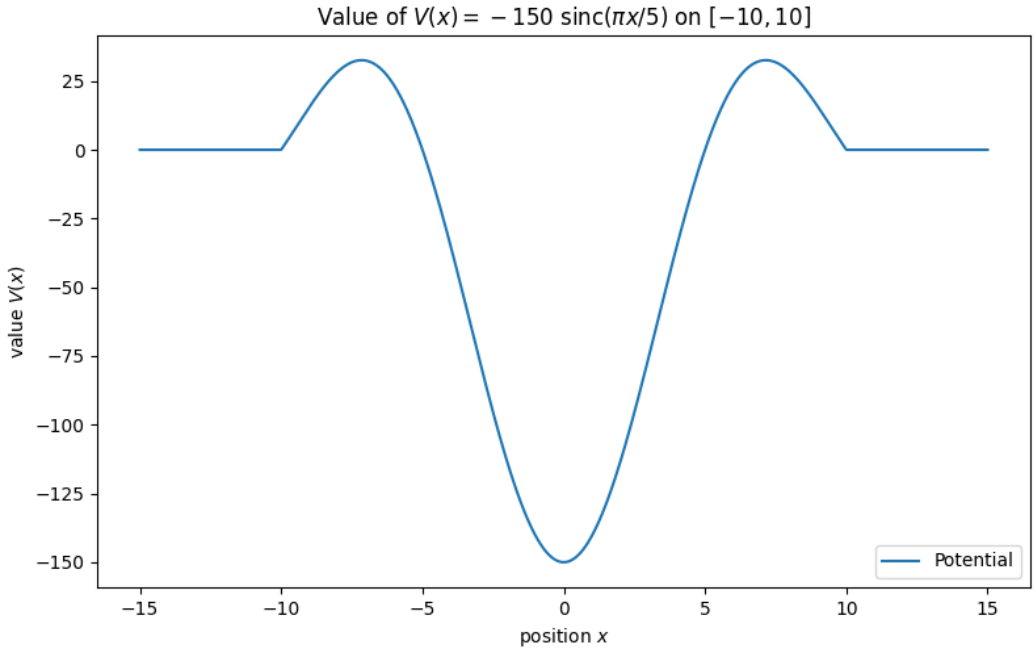


Figure 4.6: Illustration of the sinc-potential in (4.107).

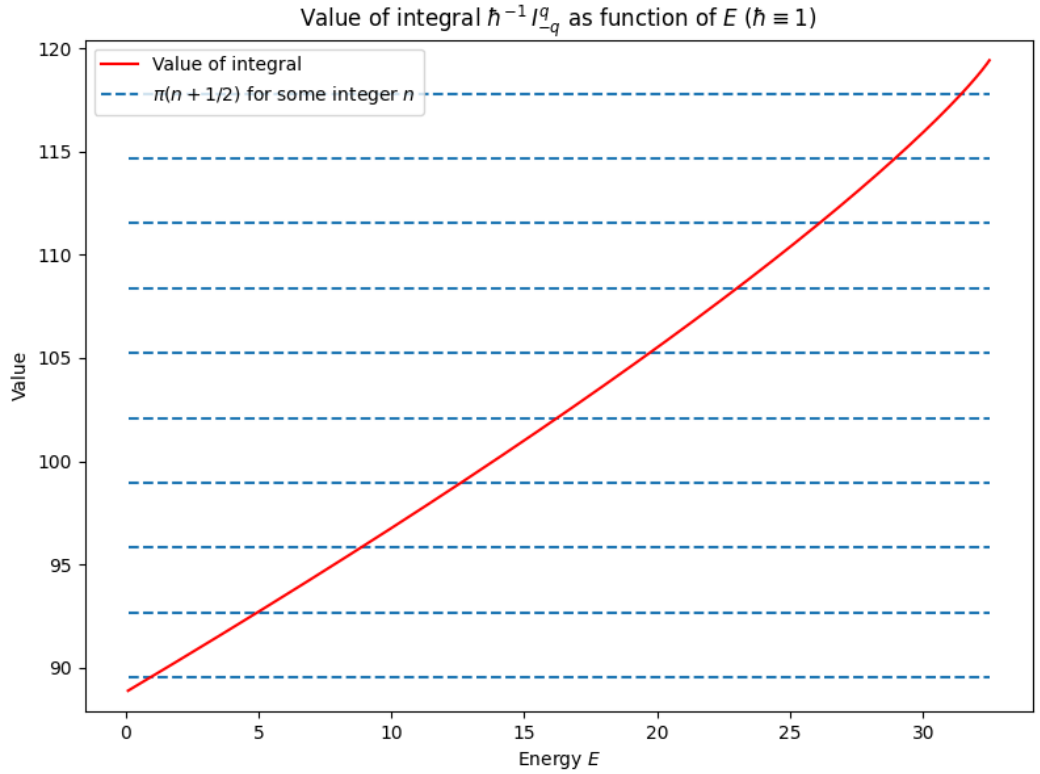
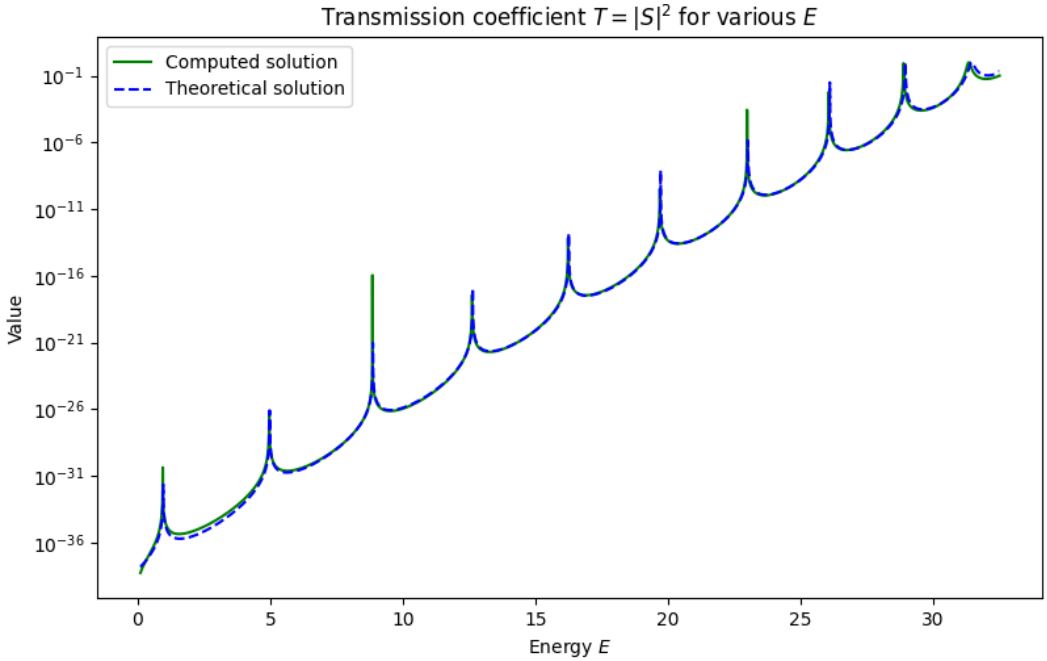
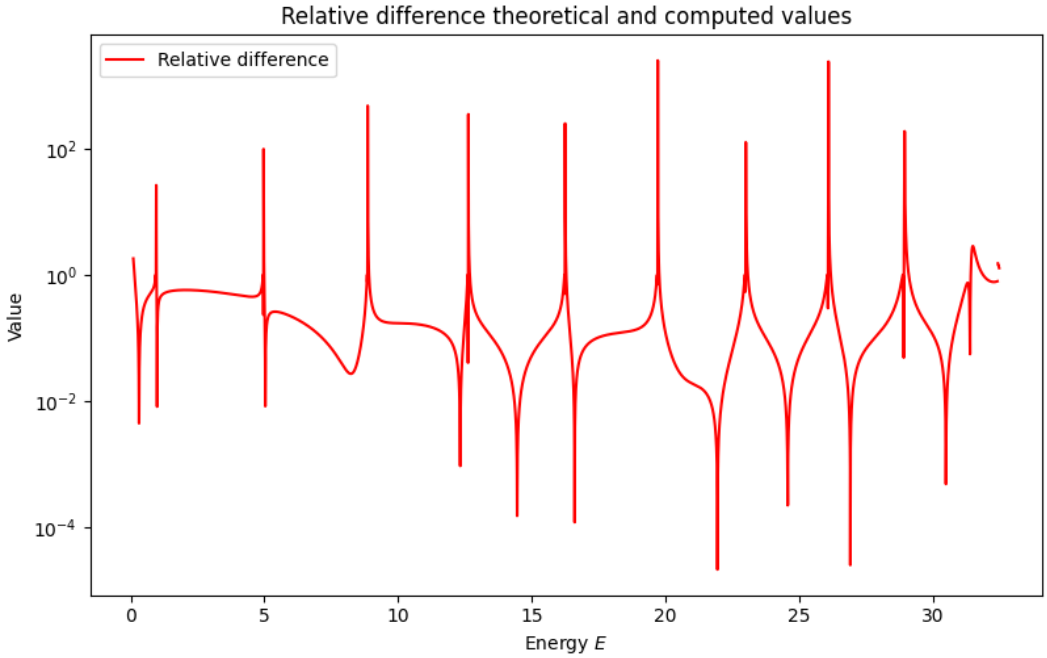


Figure 4.7: A plot of (4.108), comparing against values $\pi(n+1/2)$, $n \in \mathbb{Z}$. The integral does not resemble a square root as the bounds of integration also increase with varying E.

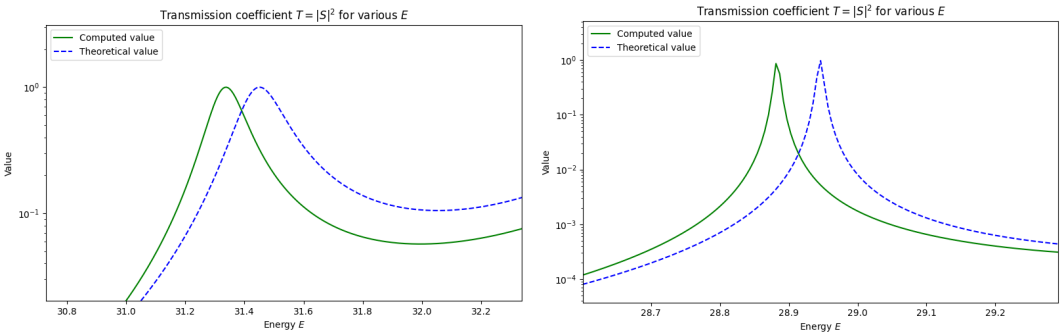


(a) Computed and theoretical values of T.



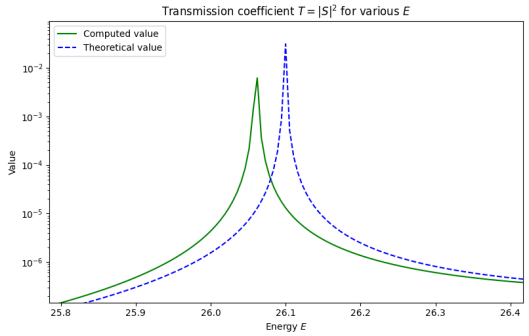
(b) Relative difference between the two values in (a) ($|\text{th.} - \text{comp.}|/\text{comp.}$).

Figure 4.8: Transmission spectra for the sinc potential of (4.107), where the theoretical value is based on applying (4.100) to this case. For both plots, 6 000 equispaced points were used, and we assume $\hbar \equiv 1$.

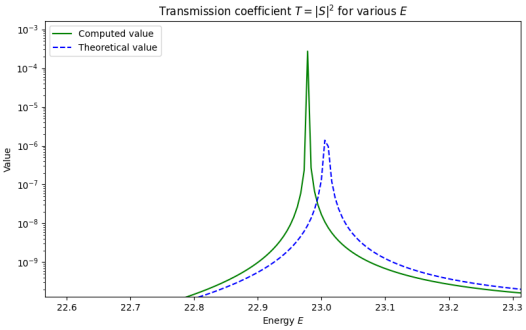


(a) Zoomed around 31.4 ($n = 37$)

(b) Zoomed around 29.0 ($n = 36$)



(c) Zoomed around 26.1 ($n = 35$)



(d) Zoomed around 23.0 ($n = 34$)

Figure 4.9: Zoomed-in views around four peaks in Figure 4.8.

second sheet in order to investigate this. Indeed, there are resonances located at those energies whose real parts constitute transparencies. We also see that these resonances rapidly near the real axis as we decrease in energy, as we would expect due to the rapid decreasing in Γ cf. (4.106).

On a final note: we can compare our result (4.100) to the one found in literature (4.101), to see whether a (significant) improvement was made. This has been done by calculating the relative difference between the two values, and it is shown in Figure 4.11. We see that our formula has the greatest impact on accuracy for larger energies, and that its improvement quickly drops off as we decrease. From around $E = 20$, the relative difference seems to stagnate at $\approx 10^{-15}$, although due to erratic behavior also found there this is more than likely to be a glitch.

To conclude

In this section we determined, for symmetric potentials, the general form of the transmission amplitude (4.14) in terms of the solution to the Schrödinger equation inside the potential, namely the parameters $\theta_{\mathrm{e,o}}$. We then proceeded to find closed expressions for these parameters for i) potentials composed of square barriers and wells, and ii) potentials where we would apply the WKB approximation, leading to formulae (4.27) and (4.82), respectively.

We also treated several examples, wherein using the derived relevant formulae for $S(k)$ we could explain features of the transmission spectrum, or determine algebraically where resonances would be located. One recurring observation is that transparency

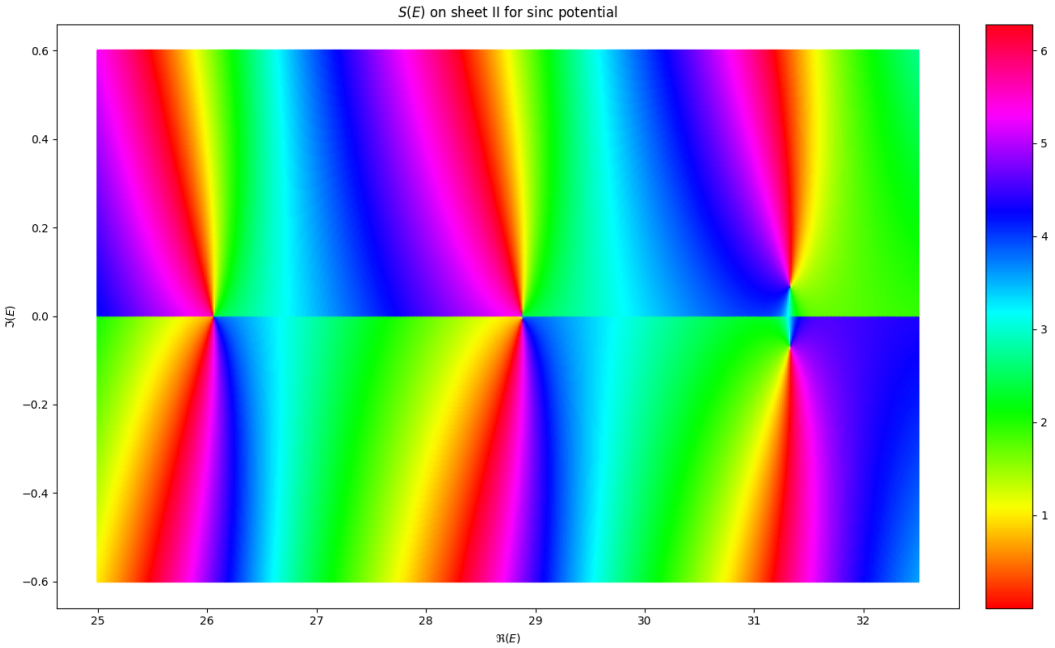


Figure 4.10: Phase of $S(\mathcal{E})$ for the potential V_{sinc} (4.107) ($\hbar \equiv 1$).

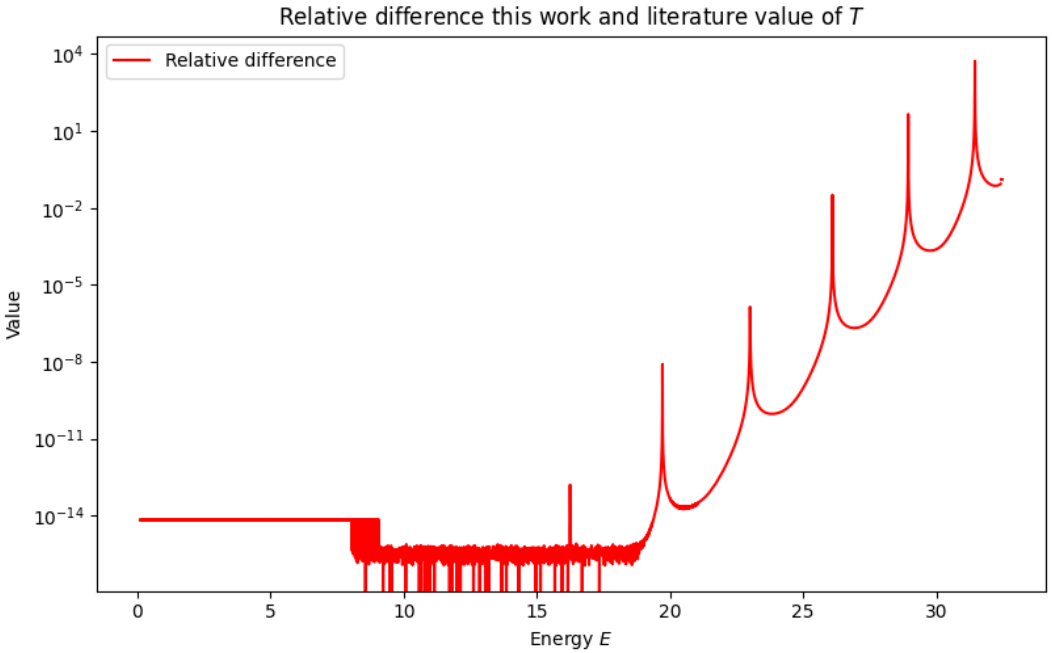


Figure 4.11: Relative difference between our approximation for T (4.100) and one found in the literature (4.101) for the case of the sinc potential V_{sinc} (4.107) ($\hbar \equiv 1$).

energies are related to the appropriate Bohr-Sommerfeld quantization condition for that potential, even though these energies do not represent bound states and lie in the continuous spectrum of the relevant Hamiltonian.

Moreover, in the example of the sinc potential, we saw that the transparency peaks could once more be written as FBW-distributions. This allowed us to locate resonances easily as was the case for the square well (see Remark 4.11), and also verify by evaluating $S(\mathcal{E})$ over (a section of) the second sheet.

This same example also allowed us to compare our derived formula for T (4.100) to one found in the literature (4.101), in order to gauge whether an improvement was made. The relative difference, plotted in Figure 4.11, shows that our formula is more accurate particularly for higher energies, and that for lower energies the two match quite well. (This was also to be expected, as our formula limits to the literature one for lower energies.)

What we carefully avoided in our analysis of WKB-applicable potentials, though, are those energy ranges over which the amount of turning points changes. This is not something that our analysis up to this points allows: the matrix $\mathbf{P}$ depends on the amount of turning points, and once that amount changes a new $\mathbf{P}$ would need to be constructed. In the following section we shall attempt to form a "bridge" between two energy ranges in which WKB is applicable, but between which the amount of turning points changes.

5 Quantum Normal Forms

Up to this point, we have sought to calculate the transmission amplitude either by assuming that our potential was square (i.e. consisting of square wells and barriers), or assuming that the WKB approximation was valid. Although some nice results were obtained by these methods for a large amount of energy & potential configurations, needless to say it does not cover all possibilities.

One such excluded kind of configuration is when the energy (closely) matches a local maximum in the potential, for instance in the case of a smooth barrier potential. Purely from considering the WKB approximation, we expect the transmission amplitudes in the regions above and below the threshold energy to look radically different from each other. Indeed, we lose two turning points, so $\mathbf{P}$ will obtain a very different form.

More crucially, the peak of the barrier cannot considered to be a turning point: the derivative of the potential there is zero, and a turning point *requires* a non-zero derivative of the potential (refer back to subsection 2.4.2). So, we could not even alter our construction of $\mathbf{P}$ in order to handle this (if we maintained its basis in WKB).

But when one door closes, another one opens. From the point of view of classical mechanics, such a peak would correspond to an equilibrium position: if we choose our energy to be the threshold energy, the total energy precisely at the peak is zero. This observation motivates us to consider methods from classical mechanics (e.g. for equilibrium analysis) in order to study the quantum problem.

One such way, which we will explore here, is by means of a *normal form* of the Hamiltonian around the equilibrium point (considered in phase space). The idea of the normal form is to find approximate, local constants of motion around the equilibrium point, which should provide insight into the motion in the neighborhood of said equilibrium point.

We first want to remind the reader that in the preliminaries we treated the classical Birkhoff Gustavson normal form (CNF), and that we build upon that knowledge in this section. We shall "translate" the methodology of CNF into quantum mechanics, discovering that the classical methodology still holds broadly and utilizing it to find the *quantum normal form* (QNF) of a barrier top potential (see Figure 5.1). Then we determine the scattering matrix for this potential in terms of a new variable I, which we subsequently link back to the energy $\mathcal{E}$ with the aim of finding resonances. In the final subsection we discuss some examples of the treated theory.

5.1 From classical to quantum

In the quantum realm, instead of talking about variables q and p living in state space, we have to interpret these as *operators* instead, together acting on a state in a Hilbert space. That is to say, we have to make the shift $q \to \mathrm{Op}[q] \equiv \hat{q}$ and similarly for p, by means of the transformation Op. The construction of this transformation is non-trivial, and the subject of [16, §3.1]. Importantly, however, we maintain the standard quantization relations

$$\hat{q} = q \quad \text{and} \quad \hat{p} = -i\hbar\frac{\partial}{\partial q} \tag{5.1a}$$

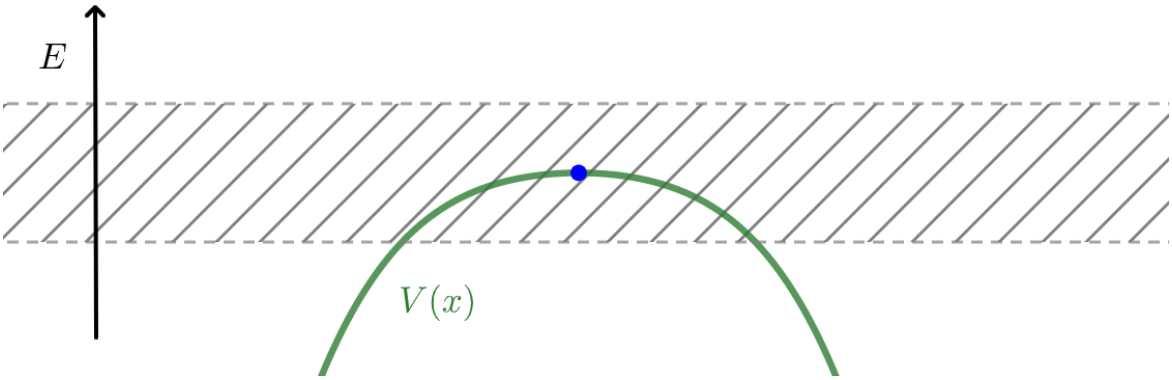


Figure 5.1: Illustration of the validity regions of WKB. The **dashed gray** region shows where WKB is *not* applicable, whilst it is valid above and below it (by assumption). The **blue** dot shows the peak of the barrier. The motivation for studying QNFs is to find the transmission amplitude and/or coefficient in the **dashed gray** region.

in the q-representation, and

$$\hat{q} = i\hbar\frac{\partial}{\partial p} \quad \text{and} \quad \hat{p} = p \tag{5.1b}$$

in the p-representation.

Let us now consider the relation between two "operatorfied" state space functions A and B. It turns out that there exists the *star product* $*$, given by

$$A * B := \sum_{j=0}^{\infty} \frac{1}{j!}\left(\frac{i\hbar}{2}\right)^j A\left[\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q}\right]^j B = AB + \tfrac{1}{2}i\hbar\{A,B\} + \mathcal{O}(\hbar^2), \tag{5.2}$$

so that we have the relation

$$\mathrm{Op}[A]\,\mathrm{Op}[B] = \mathrm{Op}[A * B]. \tag{5.3}$$

The arrows above the partials indicate in which direction the differential is operating. Also notice that here we started in the semiclassical spirit of quantum mechanics, in treating $\hbar$ as a small perturbative parameter in which we can make an expansion. The star product thus allows us to consider a single function in state space, $A * B$, instead of two "operatorfied" ones. The importance hereof lies in the fact that state space is easier to work with than operator space.

Developing this further, we can find for the commutator between two operators that

$$[\mathrm{Op}[A], \mathrm{Op}[B]] = \mathrm{Op}[A]\,\mathrm{Op}[B] - \mathrm{Op}[B]\,\mathrm{Op}[A] = \mathrm{Op}[A * B - B * A]. \tag{5.4}$$

Relation (5.4) allows us to translate commutators of operators (or rather, of "operatorfied" state space functions) to the operator form of a single state space relation, being the function $A*B-B*A$. Due to this nice property, $A*B-B*A$ should be the fundamental relation between state space variables if we have the intent of consider their quantum analogues. This motives the following definition.

j	Term	hom. order	Power of $\hbar$	qho
0	$\{A, B\}$	$ab-2$	0	$ab-2$
1	$\propto \hbar^2 A[\dots]^3 B$	$ab-6$	2	$ab-2$
2	$\propto \hbar^4 A[\dots]^5 B$	$ab-10$	4	$ab-2$
3	$\propto \hbar^6 A[\dots]^7 B$	$ab-14$	6	$ab-2$

Table 5.1: Determination of the qho of the various terms comprising the Moyal bracket expansion (5.5a) up to $j=3$, assuming A and B have qhos a and b, respectively. Here, hom. order is as defined in Definition 2.3, and the term $[\dots]$ indicates the relevant differential operator.

Definition 5.1 (Moyal bracket)**.** For state space functions A and B, we define

$$\{A,B\}_{\mathrm{M}} := -i\hbar^{-1}(A*B-B*A) = \sum_{j=0}^{\infty} \frac{(-1)^j(\frac{1}{2}\hbar)^{2j}}{(2j+1)!} A\left[\overleftarrow{\partial}_q\overrightarrow{\partial}_p - \overleftarrow{\partial}_p\overrightarrow{\partial}_q\right]^{2j+1} B \tag{5.5a}$$

$$= \{A,B\} + \mathcal{O}\big(\hbar^2\big) \tag{5.5b}$$

to be their *Moyal bracket*.[3] In analogy to (2.10), we define $\mathrm{Mad}_A\, B := \{A,B\}_{\mathrm{M}}$ as the *Moyal adjoint*. Note that in (5.5b), the higher order terms disappear when either A or B is of hom. order 2 cf. Definition 2.3.

The Moyal bracket essentially takes the role of the Poisson bracket for quantum considerations. This is exemplified in particular by the appearance of $\hbar$ in what is otherwise still a function in state space. Also note that if we set $\hbar \equiv 0$—i.e. we turn QM "off"—the Moyal bracket reduces to the Poisson bracket identically.

From this starting point, we can develop the theory of QNFs along much the same vein as for CNFs in the preliminaries, but with some key alterations. The first concerns the analogue of the spaces $\mathcal{W}^n$, which quantum doppelgänger we define next.

Definition 5.2 (Quantum homogeneous orders, qho)**.** We define

$$\mathcal{W}^n_{\mathrm{QM}} := \mathrm{span}\{\hbar^\gamma q^\alpha p^\beta : \alpha,\beta,\gamma \in \mathbb{N} \text{ and } \alpha+\beta+2\gamma = n\} \text{ over } \mathbb{C} \tag{5.6}$$

as the space of functions of *quantum homogeneous order* (qho) n. Notice that it is equal to the hom. order of the term plus twice the exponent of $\hbar$.

That here we need to consider additionally the (double counted!) powers of $\hbar$ comes from the Moyal bracket. Referring back to (5.5a), as the powers of q and p decrease due to differentiation, we pick up powers of $\hbar$—two for each iteration. To illustrate, we refer to Table 5.1, wherein we take stock of the orders of the various terms in the expansion. Since the qho spaces $\mathcal{W}_{\mathrm{QM}}$ are closed under addition, this means that the Moyal bracket lies within $\mathcal{W}^{ab-2}_{\mathrm{QM}}$. If we did not count the factors of $\hbar$, i.e. if we considered hom. order spaces instead of the qho ones, the Moyal bracket of A

[3] This object should more accurately be named the *Groenewold-Moyal* bracket, in honor of Groningen professor Dr. H.J. Groenewold's contributions to its development. For further background, see this webpage.

and B with qho a and b, respectively, would not lie within any hom. order space $\mathcal{W}$, as each term is of a different hom. order.

We can now present the definition of the QNF, which has a stark resemblance to that of the CNF in Definition 2.4.

Definition 5.3 (Quantum Normal Form)**.** Let H have an equilibrium point at the origin $(q,p)=(0,0)$, and H_2 be its Taylor expansion up to qho 2. Then we say that H is in *quantum normal form (QNF) up to order N* if

$$\{H_2, H\}_{\mathrm{M}} = 0 + \mathcal{O}_{\mathrm{qho}}(N+1). \tag{5.7}$$

Mirroring the procedure to putting a Hamiltonian into CNF, we want to find a series of transformations $W_m \in \mathcal{W}^m_{\mathrm{QM}}$ to furnish

$$H \xrightarrow{W_3} H^{(3)} \xrightarrow{W_4} H^{(4)} \xrightarrow{W_5} \cdots \xrightarrow{W_N} H^{(N)}, \tag{5.8}$$

where we wish for $H^{(N)}$ to be in QNF up to order N. However, now W_m acts as

$$H^{(m)} = \sum_{j=0}^{\infty} (j!)^{-1} (\mathrm{Mad}_{W_m})^j H^{(m-1)}, \tag{5.9}$$

exhibiting the Moyal adjoint instead of Poisson. Note that W_m may comprise terms of lower order in q and p, compensated by powers of $\hbar$ cf. the definition of qho. For this reason, together with the Moyal adjoint, $\hbar$ will "sneak into" our calculations, which are otherwise based entirely in CM. This also means that we get a revised version of Lemma 2.5:

$$\boxed{H^{(m)}_h = \sum_{j=0}^{\lfloor h/(m-2)\rfloor} (j!)^{-1} (\mathrm{Mad}_{W_m})^j H^{(m-1)}_{h-j(m-2)}.} \tag{5.10}$$

We posit this equation without proof, instead referring to [16].

It turns out the homological equation, derived in Proposition 2.6, carries over to the case of QNFs almost identically:

Proposition 5.4 (Quantum homological equation)**.** *Assume that $H^{(N-1)}$ is in QNF up to order $N-1$. In order to guarantee that $H^{(N)}$ is in QNF up to order N, we need that $W_N \in \mathcal{W}^N_{\mathrm{QM}}$ satisfies*

$$\boxed{H^{(N-1)}_N - \mathcal{D}W_N \in \ker \mathcal{D},} \tag{5.11}$$

where $\mathcal{D} = \{H_2, \cdot\} : \mathcal{W}^N_{\mathrm{QM}} \to \mathcal{W}^N_{\mathrm{QM}}$.

Proof. The proof is analogous to the one for Proposition 2.6, and as such omitted. □

With the homological equation in hand, the theory for putting some Hamiltonian into QNF is complete. We can then proceed with applying this theory to our situation of interest, being that of a potential barrier in 1D. This shall be content of the following subsection.

5.2 1D Potential barrier

Let us now apply the above theory on QNFs to the setting of interest, i.e. around the top of a potential barrier. Firstly, we shall put the relevant Hamiltonian—with a potential V s.t. $V'(0) = 0 > V''(0)$—into QNF up to order 4. We will then deduce how, utilizing it, an expression may be found for the transmission amplitude and coefficient—in terms of a yet to be determined quantity I. Finally, we will express I in terms of the energy E., which is ultimately our input variable.

Corresponding to the standard Hamiltonian *operator* $\mathcal{H}$ we have the Hamiltonian *function* H:

$$\mathcal{H} = -\hbar^2 \frac{d^2}{dx^2} + V(x) \quad \longleftrightarrow \quad H = p^2 + V(q), \tag{5.12}$$

cf. the quantization rule (5.1a). Assume that we have an equilibrium at $(0, 0)$, i.e. $V'(0) = 0$, and that it is a local maximum, i.e. $V''(0) < 0$. We make the Maclaurin expansion

$$H = p^2 + V_0 - \tfrac{1}{4}\lambda^2 q^2 + \sum_{j=3}^{\infty} \frac{V^{(j)}(0)}{j!} q^j, \tag{5.13}$$

where we introduce $\lambda := \sqrt{-2V''(0)}$. Before we start the QNF procedure, we first wish to rewrite so that we have 1 term at qho 2; at this moment we have both p^2 and $-\frac{1}{4}\lambda^2 q^2$, which is not desired. Notice that

$$\begin{aligned} p^2 - \tfrac{1}{4}\lambda^2 q^2 &= (p + \tfrac{1}{2}\lambda q)(p - \tfrac{1}{2}\lambda q) \\ &= \lambda \underbrace{(\lambda^{-1/2} p + \tfrac{1}{2}\lambda^{1/2} q)}_{=:\tilde{q}} \underbrace{(\lambda^{-1/2} p - \tfrac{1}{2}\lambda^{1/2} q)}_{=:\tilde{p}}. \end{aligned} \tag{5.14}$$

As such, we make the symplectic coordinate transformation $(q, p) \mapsto (\tilde{q}, \tilde{p})$, where the tilde variables are as indicated above. Therefore, in the new tilde coordinates, our expansion becomes

$$H = V_0 + \lambda \tilde{q}\tilde{p} + \sum_{j=3}^{\infty} \frac{V^{(j)}(0)}{j!} \lambda^{-j/2} (\tilde{q} - \tilde{p})^j = V_0 + \lambda \tilde{q}\tilde{p} + \sum_{j=0}^{\infty} \sum_{\ell=0}^{j} C_{j,\ell} \tilde{q}^{\ell} \tilde{p}^{j-\ell}, \tag{5.15}$$

featuring

$$C_{j,\ell} := \frac{(-1)^{j-\ell} V^{(j)}(0)}{(j-\ell)!\, \ell!\, \lambda^{j/2}}. \tag{5.16}$$

We also note that for various ℓ, the constants $C_{j,\ell}$ should be related to each other for the common factor of the jth derivative.

Lemma 5.5 (Relations $C_{j,\ell}$)**.** *We have that*

$$C_{j,\ell} = (-1)^{\ell} \binom{j}{\ell} C_{j,0}. \tag{5.17}$$

Proof. Observe that

$$\frac{C_{j,\ell}}{C_{j,0}} = \frac{(-1)^{-\ell}\, j!}{(j-\ell)!\, \ell!} = (-1)^{\ell} \binom{j}{\ell}, \tag{5.18}$$

from which the query follows. □

We can now bona fide start putting the Hamiltonian (5.15) into QNF. Since the rest of this construction will feature only the tilde variables, let us drop the tildes on q and p from now on. Furthermore, we note that $H \equiv H^{(2)}$, since H is already in QNF up to qho 2.

5.2.1 Its QNF

Step 1: to order 3

We start with the QNF procedure. Notice that on $\mathcal{W}^3_{\mathrm{QM}}$, the homological operator is given by

$$\mathcal{D} = \{\lambda pq, \cdot\} = \lambda p\frac{\partial}{\partial p} - \lambda q\frac{\partial}{\partial q} \equiv \lambda\,\mathrm{diag}(-3,-1,1,3,-1,1), \tag{5.19}$$

where the matrix is written in the basis $\{q^3, q^2p, qp^2, p^3, \hbar q, \hbar p\}$. Since the matrix is diagonal without zero entries, the inverse exists and we can simply find $\mathcal{W}^3_{\mathrm{QM}} \ni W_3 = \mathcal{D}^{-1}H^{(2)}_3$. In the basis above, $H^{(2)}_3 \equiv (C_{3,3}\,, C_{3,2}\,, C_{3,1}\,, C_{3,0}\,, 0\,, 0)^\intercal$, so we obtain

$$W_3 = \mathcal{D}^{-1}H^{(2)}_3 = \lambda^{-1}\left[-\tfrac{1}{3}C_{3,3}q^3 - C_{3,2}q^2p + C_{3,1}qp^2 + 3C_{3,0}p^3\right]. \tag{5.20}$$

Then the next order terms to be obtained are utilizing (5.10):

$$\begin{aligned} H^{(3)}_3 &= H^{(2)}_3 + \mathrm{Mad}_{W_3} H^{(2)}_2 + \cancel{\tfrac{1}{2}(\mathrm{Mad}_{W_3})^2 H^{(2)}_1} + \cancel{\tfrac{1}{6}(\mathrm{Mad}_{W_3})^3 H^{(2)}_0} \\ &= H^{(2)}_3 - \mathcal{D}W_3 \\ &= 0. \end{aligned} \tag{5.21}$$

Notably, the third order of the normal is equal to zero. This means that

$$\begin{aligned} H^{(3)}_4 &= H^{(2)}_4 + \mathrm{Mad}_{W_3} H^{(2)}_3 + \tfrac{1}{2}(\mathrm{Mad}_{W_3})^2 H^{(2)}_2 + \cancel{\tfrac{1}{6}(\mathrm{Mad}_{W_3})^3 H^{(2)}_1} + \cancel{\tfrac{1}{24}(\mathrm{Mad}_{W_3})^4 H^{(2)}_0} \\ &= H^{(2)}_4 + \mathrm{Mad}_{W_3} H^{(2)}_3 + \tfrac{1}{2}\,\mathrm{Mad}_{W_3} \underbrace{\mathrm{Mad}_{W_3} H^{(2)}_2}_{=-H^{(2)}_3} \\ &= H^{(2)}_4 + \tfrac{1}{2}\,\mathrm{Mad}_{W_3} H^{(2)}_3 \\ &\overset{\star}{=} C_{4,0}\left[q^4 - 4q^3p + 6q^2p^2 - 4qp^3 + p^4\right] \\ &\quad - C^2_{3,0}\lambda^{-1}\left[3q^4 + 12q^3p - 30q^2p^2 + 12qp^3 + 3p^4 - 4\hbar^2\right]. \end{aligned} \tag{5.22}$$

The first half of $\star$ is plugging in $H^{(2)}_4$ as we know it, and using Lemma 5.5 to rewrite in terms of $C_{4,0}$; the second half is the Moyal adjoint, which calculation we have relegated to Appendix B.

Notice that we have the occurence of $\hbar^2$, even though it did not appear in the original Hamiltonian. As mentioned earlier, this is due to the Moyal bracket at higher orders being expanded in powers of $\hbar$, and the fact we reach these higher orders due to Moyal bracket-ing two functions of qho larger than 2.

In a similar manner as the above, we could continue with finding $H^{(3)}_5$, $H^{(3)}_6$, et cetera. However, as one can glance from the above, the calculations become longer as we consider terms of higher qho, especially given the involvement of the Moyal adjoint. We thus elect to stop calculating $H^{(3)}$ here, so that we have obtained

$$\boxed{H^{(3)} = V_0 + \lambda pq + H^{(3)}_4 + \mathcal{O}_{\mathrm{qho}}(5),} \tag{5.23}$$

where $H^{(3)}_4$ is as obtained in (5.22).

Step 2: to order 4

To find W_4, we need first to recalculate the homological operator on $\mathcal{W}^4_{\mathrm{QM}}$. In the basis $\{q^4, q^3p, q^2p^2, qp^3, p^4, \hbar q^2, \hbar qp, \hbar p^2, \hbar^2\}$, it will be given by

$$\mathcal{D} \equiv \lambda \,\mathrm{diag}(-4, -2, 0, 2, 4, -2, 0, 2, 0). \tag{5.24}$$

We notice that $\mathcal{D}$ is still diagonal, but also that due to its zero entries it is no longer invertible. Does this mean that the homological equation is not solvable? Not necessarily: the quantum homological equation merely says that $H^{(3)}_4 - \mathcal{D}W_4$ needs to be in the kernel of $\mathcal{D}$, but does not force it to be 0. This means that we can still hope to find W_4 that can satisfy the homological equation.

Making our hope more concrete, we observe that for our specific homological operator the following holds:

$$\mathcal{W}^4_{\mathrm{QM}} = \mathrm{Im}\,\mathcal{D} \oplus \ker \mathcal{D}. \tag{5.25}$$

As a consequence, we may make the splitting $H^{(3)}_4 = H^{(3)}_{4;\mathrm{Im}} + H^{(3)}_{4;\ker}$, where the additional subscripts indicate that these parts live in the image or kernel of $\mathcal{D}$, respectively. Then,

$$H^{(3)}_4 - \mathcal{D}W_4 = H^{(3)}_{4;\ker} + H^{(3)}_{4;\mathrm{Im}} - \mathcal{D}W_4 \overset{!}{\in} \ker \mathcal{D} \implies H^{(3)}_{4;\mathrm{Im}} - \mathcal{D}W_4 = 0. \tag{5.26}$$

Thus, to complete the next step of the QNF, we will have to find W_4 that satisfies this rightmost equation, and with it find $H^{(4)}$.

Remark 5.6 (Splitting (5.25); Fredholm alternative)**.** The splitting introduced in (5.25) is very specific to our case, and cannot generally be made for arbitrary $\mathcal{D}$. As an example, if we let the full space be $\mathbb{C}^2$, then for

$$\mathcal{D} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{5.27}$$

we find $\ker \mathcal{D} = \mathrm{Im}\,\mathcal{D} = \mathrm{span}\begin{pmatrix} 1 & 0 \end{pmatrix}^{\mathsf{T}}$, so $\mathbb{C}^2 \neq \ker \mathcal{D} \oplus \mathrm{Im}\,\mathcal{D}$.

However, there exists a splitting of the full space that will always work, given by the *Fredholm alternative*. Let $\mathcal{L} : V \to V$ be linear on a finite-dimensional complex vector space V with inner product $\langle \cdot, \cdot \rangle$. Then, we have that

$$V = \mathrm{Im}\,\mathcal{L} \oplus \ker \mathcal{L}^*, \tag{5.28}$$

with additionally that $\mathrm{Im}\,\mathcal{L} \perp \ker \mathcal{L}^*$. For a proof (and further context) of this fact, we refer to [14, Thm. 2.2.1]. Since the operators $\mathcal{D}$ in our case are self-adjoint, this statement reduces to the splitting (5.25) and the QNF can bona fide be found.

Observe that we have

$$H^{(3)}_{4;\ker} = [6C_{4,0} + 30C^2_{3,0}\lambda^{-1}]q^2p^2 + 4C^2_{3,0}\lambda^{-1}\hbar^2 \tag{5.29a}$$

and

$$\begin{aligned} H^{(3)}_{4;\mathrm{Im}} = {} & [C_{4,0} - 3C^2_{3,0}\lambda^{-1}]q^4 - [4C_{4,0} + 12C^2_{3,0}\lambda^{-1}]q^3p \\ & - [4C_{4,0} + 12C^2_{3,0}\lambda^{-1}]qp^3 + [C_{4,0} - 3C^2_{3,0}\lambda^{-1}]p^4. \end{aligned} \tag{5.29b}$$

Taking (5.24) to heart, it is not hard to see that W_4 should thus be chosen as

$$\begin{aligned} W_4 = &-\tfrac{1}{4}[C_{4,0}\lambda^{-1} - 3C_{3,0}^2\lambda^{-2}]q^4 + \tfrac{1}{2}[4C_{4,0}\lambda^{-1} + 12C_{3,0}^2\lambda^{-2}]q^3p \\ &- \tfrac{1}{2}[4C_{4,0}\lambda^{-1} + 12C_{3,0}^2\lambda^{-2}]qp^3 + \tfrac{1}{4}[C_{4,0}\lambda^{-1} - 3C_{3,0}^2\lambda^{-2}]p^4. \end{aligned} \tag{5.30}$$

Therefore,

$$H_4^{(4)} = H_{4;\mathrm{ker}}^{(3)} = [6C_{4,0} + 30C_{3,0}^2\lambda^{-1}]q^2p^2 + 4C_{3,0}^2\lambda^{-1}\hbar^2. \tag{5.31}$$

With W_4 in hand, we could proceed with obtaining $H_5^{(4)}$, $H_6^{(4)}$, and so on by the procedure that we have demonstrated above. This would increase the accuracy of the QNF of H we are building. However, for the sake of brevity we elect to stop the procedure here. Thus, the fourth order QNF of the 1D potential barrier is as follows:

$$\boxed{H^{(4)} = V_0 + \lambda pq + [6C_{4,0} + 30C_{3,0}^2\lambda^{-1}]q^2p^2 + 4C_{3,0}^2\lambda^{-1}\hbar^2 + \mathcal{O}_{\mathrm{qho}}(5).} \tag{5.32}$$

Unlike for $H^{(3)}$, the term $\hbar^2$ is now here to stay: it is at qho 4, and the next steps in the QNF algorithm will only change the terms at qho 5 and higher. The term $4C_{3,0}^2\lambda^{-1}\hbar^2$ can thus be seen as the "quantum correction" to the classical normal form of the 1D potential barrier.

It is here that we notice that $H^{(4)}$ only features terms with equal powers of q and p. If this is a pattern that continues, then we could rightfully consider $H^{(m)}$ to be a function solely of qp, i.e. $H^{(m)}(q,p,\hbar) = H^{(N)}(qp,\hbar)$. As luck would have it, this is a pattern that does hold, as we will show in the next Theorem.

Theorem 5.7 (Equal occurence powers of q and p)**.** *For the 1D potential barrier, we have that the Nth order QNF of the Hamiltonian can be written as*

$$H^{(N)} = \sum_{j=0}^{\lfloor N/2\rfloor} \alpha_j I^j + \mathcal{O}_{\mathrm{qho}}(N+1), \tag{5.33}$$

for $I := pq$ and constants $\alpha_j = \alpha_j(\hbar)$. Cf. [16, Thm. 3].

Proof. Let us prove by induction on N. By the above, we already know that this holds for $N = 4$, which is our base case.

Now assume the statement holds for some $b-1 \in \mathbb{N}$. We shall need the homological operator,

$$\begin{aligned} \mathcal{D} &= \lambda p\frac{\partial}{\partial p} - \lambda q\frac{\partial}{\partial q} \\ &\equiv \lambda\,\mathrm{diag}(-b, -b+2, \cdots, b, -b+2, -b+4, \cdots, b-2, -b+4, \cdots), \end{aligned} \tag{5.34}$$

operating on $\mathcal{W}_{\mathrm{QM}}^b$, where the matrix is written in the basis

$$\{q^b, q^{b-1}p, \cdots, p^b, \hbar q^{b-2}, \hbar q^{b-3}p, \cdots, \hbar p^{b-2}, \hbar^2 q^{b-4}, \cdots\}. \tag{5.35}$$

That this operator will indeed be diagonal for all b and has the form it does we assume as evident. Now we need to distinguish cases between even and odd b.

- **Odd** $b-1$. Then b will be even, and so the homological operator will have zeros on the diagonal. This means there is a non-trivial kernel, and it is given by

$$\begin{aligned}\ker\mathcal{D} &= \mathrm{span}\{\hbar^k q^{b/2-k}p^{b/2-k} : k = 0, 1, \cdots, b/2\}\\ &= \mathrm{span}\{\hbar^k I^{b/2-k} : k = 0, 1, \cdots, b/2\}.\end{aligned} \tag{5.36}$$

  Since the other basis elements of $\mathcal{W}^b_{\mathrm{QM}}$ (of the basis in (5.35)) are mapped onto themselves, they comprise the image of $\mathcal{D}$, and so we have the relation $\mathcal{W}^b_{\mathrm{QM}} = \ker\mathcal{D} \oplus \mathrm{Im}\,\mathcal{D}$. We can thus make the split $H^{(b-1)}_b = H^{(b-1)}_{b;\mathrm{ker}} + H^{(b-1)}_{b;\mathrm{Im}}$, where the subscripts indicate that the relevant term lives in either the kernel or image of $\mathcal{D}$, respectively. We can now choose $W_b \in \mathcal{W}^b_{\mathrm{QM}}$ so that $H^{(b-1)}_{b;\mathrm{Im}} = \mathcal{D}W_b$, and thus we obtain

$$H^{(b)}_b = H^{(b-1)}_b - \mathcal{D}W_b = H^{(b-1)}_{b;\mathrm{ker}} + \cancel{H^{(b-1)}_{b;\mathrm{Im}}} - \cancel{\mathcal{D}W_b} = H^{(b-1)}_{b;\mathrm{ker}}. \tag{5.37}$$

  As such, the qho b term in $H^{(b)}$ will belong to the kernel of $\mathcal{D}$, which as we established is spanned by $\hbar^k I^{b/2-k}$, $k = 0, 1, \cdots, b/2$. The QNF $H^{(b)}$ will thus remain a power series in I, except that now the highest order in I will be $b/2$ instead of $b/2-1$. That is to say, we have shown

$$H^{(b-1)} = \sum_{j=0}^{b/2-1}\alpha_j I^j + \mathcal{O}_{\mathrm{qho}}(b) \longrightarrow H^{(b)} = \sum_{j=0}^{b/2}\widetilde{\alpha}_j I^j + \mathcal{O}_{\mathrm{qho}}(b+1). \tag{5.38}$$

  where the tildes indicate that the α_js may have been altered in this procedure.

- **Even** $b-1$. Then b will be odd, and we observe that $\mathcal{D}$ will be diagonal without zero entries. As such, $\mathcal{D}^{-1}$ exists and we can choose $\mathcal{W}^b_{\mathrm{QM}} \ni W_b := \mathcal{D}^{-1}H^{(b-1)}_b$ so that

$$H^{(b)}_b = \cancel{H^{(b-1)}_b} - \cancel{\mathcal{D}W_b} = 0. \tag{5.39}$$

  Thus,

$$H^{(b-1)} = \sum_{j=0}^{(b-1)/2}\alpha_j I^j + \mathcal{O}_{\mathrm{qho}}(b-1) \longrightarrow H^{(b)} = \sum_{j=0}^{(b-1)/2}\alpha_j I^j + \mathcal{O}_{\mathrm{qho}}(b+1). \tag{5.40}$$

  Here too the form we want to maintain has been shown.

Since both cases for b have been shown to yield the correct result, the induction step—and by extension the entire proof—has been completed. □

To recap, with some labor we have found that we can rewrite our 1D Hamiltonian into QNF (which we have done up to fourth order, see (5.32)), and that the QNF is a power series in $I = pq$. In the next subsection we will delve further into the quantity I and associated operator $\mathcal{I} = \mathrm{Op}[I]$, with the aim of finding the scattering matrix in terms of it.

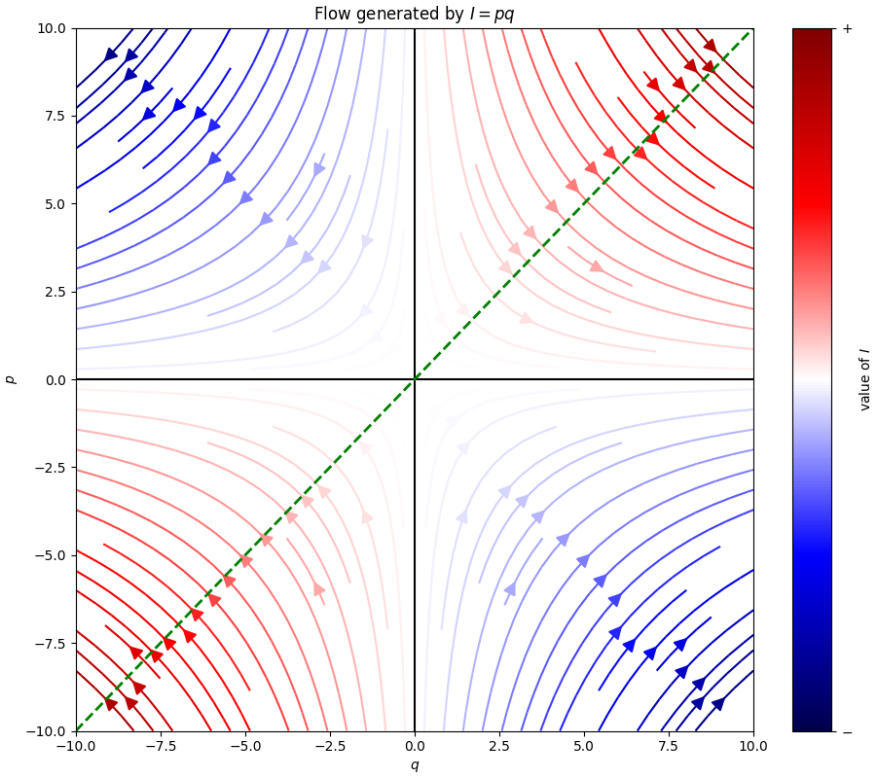


Figure 5.2: Curves (hyperbolae) of constant $I = pq$ in the q-p-plane. The vector field generated by I is $q\partial_q - p\partial_p$. The **dashed green** line indicates the boundary between the "reactant" (upper left) and "product" (lower right) regions of the phase portrait.

5.2.2 Transmission amplitude and coefficient

In order to construct from the Hamiltonian (5.32) the scattering matrix (and associated transmission amplitude and coefficient), we shall need to consider its eigenstates as well. That is to say, we need to find a description/expression for states incoming into and outgoing from the barrier, and relate these to each other.

Considering that our Hamiltonian is now expanded in I, it is natural to consider the incoming and outgoing states as eigenstates of $\mathcal{I} = \mathrm{Op}[I]$. Hence, we need to study the eigenvalue equation

$$\mathcal{I}\phi = I\phi, \tag{5.41}$$

which states ϕ will simultaneously be eigenstates of the Hamiltonian $\mathcal{H}$—up to a certain qho.

Since $I = pq$ is supposed to be constant for the motion of the eigenstate ϕ, if we interpret ϕ classically we can determine its behavior by looking at the phase portraits of I. That is to say, since for a given I, ϕ is constrained to that curve on which I is conserved, that curve determines completely the behavior of ϕ—see Figure 5.2. From here we can also determine the long-term behavior of states, for any given initial condition, which is indicated by the arrows in the aforementioned Figure. That is to say, whether the states originated from and/or will end up in the "reactant" (r) or "product" (p) region of this phase portrait. This we have recorded in Table 5.2. In particular, we see from the table that for any I, the eigenstates ϕ, when represented in q-space, are *outgoing* towards (positive/negative) infinity, and in p-space are *incoming*

Eigenvalue I		$I>0$		$I<0$	
Initial conditions		$q>0, p>0$	$q<0, p<0$	$q>0, p<0$	$q<0, p>0$
Forward	q-space	$+\infty$	$-\infty$	$+\infty$	$-\infty$
	p-space	0^+	0^-	0^-	0^+
	Region	prod.	reac.	prod.	reac.
Backward	q-space	0^+	0^-	0^+	0^-
	p-space	$+\infty$	$-\infty$	$-\infty$	$+\infty$
	Region	reac.	prod.	prod.	reac.
Symbol	q-rep.	$\psi_{\mathrm{o;p}}$	$\psi_{\mathrm{o;r}}$	$\psi_{\mathrm{o;p}}$	$\psi_{\mathrm{o;r}}$
	p-rep.	$\overline{\psi}_{\mathrm{i;r}}$	$\overline{\psi}_{\mathrm{i;p}}$	$\overline{\psi}_{\mathrm{i;p}}$	$\overline{\psi}_{\mathrm{i;r}}$

Table 5.2: Behavior of states as determined by their initial conditions in Figure 5.2. "Forward" and "Backward" refer to the evolution in time.

towards the origin.

Now that we have made sense of the "directionality" of the eigenstates of $\mathcal{I}$, let us find these explicitly so we can make a quantitative analysis. We calculate that

$$\mathcal{I} = \tfrac{1}{2}(\hat{q}\hat{p} + \hat{p}\hat{q}) = \begin{cases} -i\hbar\left(q\partial_q + \tfrac{1}{2}\right) & \text{in } q\text{-representation} \\ i\hbar\left(p\partial_p + \tfrac{1}{2}\right) & \text{in } p\text{-representation} \end{cases}, \tag{5.42}$$

where we also utilized the quantization relation $[\hat{q}, \hat{p}] = i\hbar$. If we now let ψ and $\overline{\psi}$ denote solutions to the differential equation $\mathcal{I}\phi = I\phi$ in q- and p-representation, respectively, we will find that these are given by

$$\psi_{\mathrm{o;p,r}}(q) = \Theta(\pm q)|q|^{-1/2+i\hbar^{-1}I} = \Theta(\pm q)\exp\!\left(-\tfrac{1}{2}\ln|q| + i\hbar^{-1}I\ln|q|\right) \tag{5.43a}$$

and

$$\overline{\psi}_{\mathrm{i;p,r}}(p) = \Theta(\mp p)|p|^{-1/2-i\hbar^{-1}I} = \Theta(\mp p)\exp\!\left(-\tfrac{1}{2}\ln|p| - i\hbar^{-1}I\ln|p|\right), \tag{5.43b}$$

where Θ denotes the Heaviside step function. Tying back to the roles in terms of ϕ, the above notation thus implies that $\psi_{\mathrm{o;p,r}}$ are outgoing states, whilst $\overline{\psi}_{\mathrm{i;p,r}}$ are incoming (hence the subscripts "o" and "i"). We also refer to the "Symbol" column in Table 5.2. Moreover, we notice a mathematical relationship between the incoming and outgoing states, being

$$\boxed{\overline{\psi}_{\mathrm{i;p}}(p) = \psi^*_{\mathrm{o;r}}(p) \quad \text{and} \quad \overline{\psi}_{\mathrm{i;r}}(p) = \psi^*_{\mathrm{o;p}}(p),} \tag{5.44}$$

where $*$ indicates the complex conjugate.

We now have incoming states in the p-, and outgoing states in the q-representation, and a relation between them. However, we ideally want to have *both* directions of states in one of the two variables, which would allow us to learn the scattering behavior most

easily. This we can do by changing from p- to q-representation for the incoming states $\overline{\psi}_{\mathrm{i;p,r}}$. Namely, we do a Fourier-esque transformation, with which we obtain

$$\begin{aligned}\psi_{\mathrm{i;p,r}}(q) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\overline{\psi}_{\mathrm{i;p,r}}(p)\exp\bigl(i\hbar^{-1}qp\bigr)\,dp \\ &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi^{*}_{\mathrm{o;r,p}}(p)\exp\bigl(i\hbar^{-1}qp\bigr)\,dp \\ &= \begin{cases}\mathrm{p}: & \dfrac{1}{\sqrt{2\pi\hbar}}\displaystyle\int_{-\infty}^{0}(-p)^{-1/2-i\hbar^{-1}I}\exp\bigl(i\hbar^{-1}qp\bigr)\,dp \\ \mathrm{r}: & \dfrac{1}{\sqrt{2\pi\hbar}}\displaystyle\int_{0}^{\infty}p^{-1/2-i\hbar^{-1}I}\exp\bigl(i\hbar^{-1}qp\bigr)\,dp\end{cases}.\end{aligned} \tag{5.45}$$

These integrals can then be evaluated by means of an adaptation of the formula for the gamma function:

$$\int_{0}^{\infty}y^{z-1}e^{-ty}\,dy = \exp(-z\ln t)\Gamma(z), \tag{5.46}$$

where $z,t\in\mathbb{C}$. The integral on the lhs (and with it the entire equation) is only defined for $t_{\mathrm{R}}>0$, but we may use an analytic continuation to define this equation for $t_{\mathrm{R}}=0$ as well. For the "r" case in (5.45) we determine $t=-i\hbar^{-1}q$ and $z=1/2-i\hbar^{-1}I$, so that

$$\psi_{\mathrm{i;r}}(q) = \frac{g}{\sqrt{2\pi\hbar}}\exp\bigl(-(1/2-i\hbar^{-1}I)\ln\bigl(-i\hbar^{-1}q\bigr)\bigr), \tag{5.47a}$$

where for brevity we made the definition $g:=\Gamma(1/2-i\hbar^{-1}I)$. For the "p" case we preface the above with the substitution $p'=-p$, so that we obtain an integral compatible with (5.46) featuring $z=1/2-i\hbar^{-1}I$ and $t=i\hbar^{-1}q$, which means that

$$\psi_{\mathrm{i;p}}(q) = \frac{g}{\sqrt{2\pi\hbar}}\exp\bigl(-(1/2-i\hbar^{-1}I)\ln\bigl(i\hbar^{-1}q\bigr)\bigr) \tag{5.47b}$$

In order to further simplify this, we need to distinguish between positive and negative q. Using log rules for complex numbers, we determine that

$$\ln\bigl(\pm i\hbar^{-1}q\bigr) = -\ln\hbar + \begin{cases}\ln(\pm i)+\ln q = \ln q \pm i\pi/2 & \text{if}\quad q>0 \\ \ln(\mp i)+\ln(-q) = \ln(-q)\mp i\pi/2 & \text{if}\quad q<0\end{cases}. \tag{5.48}$$

With this in mind simplification is possible, leading to the expressions.

$$\psi_{\mathrm{i;r}} = \frac{g\exp(-i\hbar^{-1}I\ln\hbar)}{\sqrt{2\pi}}\times\begin{cases}e^{i\pi/4}\exp(\hbar^{-1}\pi I/2)q^{-1/2+i\hbar^{-1}I} & \text{if}\quad q>0 \\ e^{-i\pi/4}\exp(-\hbar^{-1}\pi I/2)(-q)^{-1/2+i\hbar^{-1}I} & \text{if}\quad q<0\end{cases} \tag{5.49a}$$

and

$$\psi_{\mathrm{i;p}} = \frac{g\exp(-i\hbar^{-1}I\ln\hbar)}{\sqrt{2\pi}}\times\begin{cases}e^{-i\pi/4}\exp(-\hbar^{-1}\pi I/2)q^{-1/2+i\hbar^{-1}I} & \text{if}\quad q>0 \\ e^{i\pi/4}\exp(\hbar^{-1}\pi I/2)(-q)^{-1/2+i\hbar^{-1}I} & \text{if}\quad q<0\end{cases}. \tag{5.49b}$$

Thanks to the step function in the definition of $\psi_{\mathrm{o;p,r}}$, we can get rid of the case distinction in (5.49). After all, that step function will regulate for us which case we

are targeting. This means that (5.49) is equivalent to the equations

$$\psi_{\mathrm{i;r}} = \frac{g\exp(-i\hbar^{-1}I\ln\hbar)}{\sqrt{2\pi}}\left[e^{i\pi/4}\exp\big(\hbar^{-1}\pi I/2\big)\psi_{\mathrm{o;p}} + e^{-i\pi/4}\exp\big(-\hbar^{-1}\pi I/2\big)\psi_{\mathrm{o;r}}\right] \tag{5.50a}$$

and

$$\psi_{\mathrm{i;p}} = \frac{g\exp(-i\hbar^{-1}I\ln\hbar)}{\sqrt{2\pi}}\left[e^{-i\pi/4}\exp\big(-\hbar^{-1}\pi I/2\big)\psi_{\mathrm{o;p}} + e^{i\pi/4}\exp\big(\hbar^{-1}\pi I/2\big)\psi_{\mathrm{o;r}}\right]. \tag{5.50b}$$

The above equations are the relationships between the incoming and outgoing states, both in the q-representation, which we intended to find.

Glancing at these equations, we notice that they have the structure of a linear transformation, which means that the incoming states are connected to the outgoing states by means of a matrix transformation in suitable bases. This matrix is in fact the scattering matrix, and by means of the above equations we can construct it. In the bases $\{\psi_{\mathrm{i;r}}, \psi_{\mathrm{i;p}}\}$ and $\{\psi_{\mathrm{o;r}}, \psi_{\mathrm{o;p}}\}$ for the incoming and outgoing states, we see that

$$\begin{pmatrix}1\\0\end{pmatrix} \overset{\mathbf{S}}{\longmapsto} \frac{g\exp(-i\hbar^{-1}I\ln\hbar)}{\sqrt{2\pi}}\begin{pmatrix}e^{-i\pi/4}\exp(-\hbar^{-1}\pi I/2)\\ e^{i\pi/4}\exp(\hbar^{-1}\pi I/2)\end{pmatrix} \tag{5.51a}$$

and

$$\begin{pmatrix}0\\1\end{pmatrix} \overset{\mathbf{S}}{\longmapsto} \frac{g\exp(-i\hbar^{-1}I\ln\hbar)}{\sqrt{2\pi}}\begin{pmatrix}e^{i\pi/4}\exp(\hbar^{-1}\pi I/2)\\ e^{-i\pi/4}\exp(-\hbar^{-1}\pi I/2)\end{pmatrix}, \tag{5.51b}$$

which means that the scattering matrix is given by

$$\boxed{\mathbf{S} = \frac{g\exp(-i\hbar^{-1}I\ln\hbar)}{\sqrt{2\pi}}\begin{pmatrix}e^{-i\pi/4}\exp(-\hbar^{-1}\pi I/2) & e^{i\pi/4}\exp(\hbar^{-1}\pi I/2)\\ e^{i\pi/4}\exp(\hbar^{-1}\pi I/2) & e^{-i\pi/4}\exp(-\hbar^{-1}\pi I/2)\end{pmatrix}.} \tag{5.52}$$

From here, then, we determine the transmission amplitude as

$$S = \mathbf{S}_{21} = \frac{ge^{i\pi/4}}{\sqrt{2\pi}}\exp\big(\hbar^{-1}I[\pi/2 - i\ln\hbar]\big), \tag{5.53}$$

and the associated transmission coefficient (assuming real I)

$$T = |\mathbf{S}_{21}|^2 = \frac{|g|^2\exp(\hbar^{-1}\pi I)}{2\pi} \overset{\star}{=} \frac{1}{1+\exp(-2\pi\hbar^{-1}I)}, \tag{5.54}$$

where in $\star$ we used a reflection formula for the gamma function in order to derive its absolute value (for full justification, see Appendix B).

5.2.3 It's all coming together ...

We have now achieved what we wanted to do for the potential barrier, but which WKB did not allow: to find expressions for the transmission amplitude and coefficient which are valid around a classically unstable equilibrium. However, there is a problem with the obtained expressions (5.53) and (5.54): they are written in terms of the quantity I instead of the desired E. As such, we will need to make a relation between I and E in order to fully complete our wish for expressions.

This is done by realizing that we have an expression for H in terms of I, meaning there should be an analogous expression for $\mathcal{H}$ in terms of $\mathcal{I}$. Due to this form, $\mathcal{H}$ will on the one hand act as a scalar E on an eigenstate $\psi_{\mathrm{i,o;r,p}}$, and also as its expanded form in terms of I. This should then yield a relation between the two quantities—a relation that we find in the following Proposition.

Proposition 5.8 (Relation $I \leftrightarrow E$)**.** *We have that I and E, the eigenvalues of $\mathcal{I}$ and $\mathcal{H}$, respectively, are related as follows:*

$$\boxed{E = V_0 + \lambda I + [6C_{4,0} + 30C_{3,0}^2\lambda^{-1}]I^2 - \hbar^2\left[\tfrac{3}{2}C_{4,0} + \tfrac{7}{2}C_{3,0}^2\lambda^{-1}\right].} \tag{5.55}$$

Proof. From the QNF calculation, we have that to fourth order in qho $\mathcal{H}$ is given in terms of $\mathcal{I}$ by

$$\begin{aligned}\mathcal{H} = \mathrm{Op}[H] &= \mathrm{Op}\big[V_0 + \lambda I + [6C_{4,0} + 30C_{3,0}^2\lambda^{-1}]I^2 + 4C_{3,0}^2\lambda^{-1}\hbar^2\big] \\ &= V_0 + 4C_{3,0}^2\lambda^{-1}\hbar^2 + \lambda\,\mathrm{Op}[I] + [6C_{4,0} + 30C_{3,0}^2\lambda^{-1}]\,\mathrm{Op}[I^2].\end{aligned} \tag{5.56}$$

By definition, $\mathrm{Op}[I] = \mathcal{I}$. However, for $\mathrm{Op}[I^2]$ we need to be more careful. Observe that using the definition of the star product (5.2), we can determine

$$\begin{aligned}I * I &= I^2 + \cancel{\tfrac{1}{2}i\hbar\{I,I\}} + \frac{1}{2}\left(\frac{i\hbar}{2}\right)^2 \underbrace{I\left[\overleftarrow{\partial_q^2}\overrightarrow{\partial_p^2} + \overleftarrow{\partial_p^2}\overrightarrow{\partial_q^2} - 2\,\overleftarrow{\partial_q}\overleftarrow{\partial_p}\overrightarrow{\partial_q}\overrightarrow{\partial_p}\right] I}_{-2} \\ &= I^2 + \tfrac{1}{4}\hbar^2.\end{aligned} \tag{5.57}$$

Then,

$$\mathrm{Op}[I^2] = \mathrm{Op}\left[I * I - \tfrac{1}{4}\hbar^2\right] = \mathrm{Op}[I]^2 - \tfrac{1}{4}\hbar^2 = \mathcal{I}^2 - \tfrac{1}{4}\hbar^2. \tag{5.58}$$

We plug this into (5.56) to obtain

$$\begin{aligned}\mathcal{H} &= V_0 + 4C_{3,0}^2\lambda^{-1}\hbar^2 + \lambda\mathcal{I} + [6C_{4,0} + 30C_{3,0}^2\lambda^{-1}]\left(\mathcal{I}^2 - \tfrac{1}{4}\hbar^2\right) \\ &= V_0 - \hbar^2\left[\tfrac{3}{2}C_{4,0} + \tfrac{7}{2}C_{3,0}^2\lambda^{-1}\right] + \lambda\mathcal{I} + [6C_{4,0} + 30C_{3,0}^2\lambda^{-1}]\mathcal{I}^2.\end{aligned} \tag{5.59}$$

Finally, since we take $\mathcal{I}$ and $\mathcal{H}$ to act on eigenstates only, we must have that that the respective eigenvalues are equal to each other. We then directly obtain what was to be shown. □

From this Proposition, we see the contribution of quantum mechanics to our analysis, being the final term involving $\hbar^2$. The ramification of this addition is that we disconnect $E = V_0 \leftrightarrow I = 0$, which would necessarily be true in a purely classical treatment (where $\hbar \equiv 0$). Indeed, if we consider the expression for the transmission coefficient (5.54), we see that if $E = V_0 \leftrightarrow I = 0$, then precisely at the threshold energy the particle would have a probability of $1/2$ to make it over, as we would expect classically. The fact that $E = V_0 \not\leftrightarrow I = 0$ may be true (supposing V is not precisely so that the final term cancels) shows that, depending on the geometry of the potential, we can have $T > 1/2$ or $T < 1/2$ at the threshold energy. Therefore, QM can act as a "boost" or a "drag" on the transmission w.r.t. to the classical case.

One more issue arising from this is the choice of I with which to relate a given E. Disregarding the case of there being no solutions for now, there will generally be

precisely two I corresponding to a single E, so if we want to determine I from E, we need to make a choice. From a physical perspective, we would expect that as we increase E, T increases as well. After all, barring exceptions, adding more energy should just make our particle more likely to go through. Thus,

$$0 \overset{!}{<} \frac{dT}{dE} = \frac{dT}{dI}\frac{dI}{dE} = \underbrace{\frac{2\pi\hbar^{-1}\exp(-2\pi\hbar^{-1}I)}{(1+\exp(-2\pi\hbar^{-1}I))^2}}_{>0}\frac{dI}{dE} \implies \frac{dI}{dE} > 0. \tag{5.60}$$

Thus, to each E we choose that I so that $dI/dE > 0$.

The final step is then to write the transmission amplitude and coefficient (5.53) and (5.54) in terms of E instead of I. That is to say, we write $I = I(E)$. We could solve exactly for I in terms of E utilizing the quadratic formula, however i) the quadratic formula is cumbersome and quite dense, and ii) the form $I(E)$ is more general, for instance for the case where more orders of QNF are desired and hence a larger order polynomial is obtained. We thus find the expressions

$$S(E) = \frac{e^{i\pi/4}}{\sqrt{2\pi}}\Gamma\left(\tfrac{1}{2} - i\hbar^{-1}I(E)\right)\exp\left(\hbar^{-1}I(E)[\pi/2 + i\ln\hbar]\right) \tag{5.61a}$$

and

$$T(E) = \left[1+\exp\left(-2\pi\hbar^{-1}I(E)\right)\right]^{-1}. \tag{5.61b}$$

These expressions then also allow us to find resonances, by allowing the energy to be complex and finding for which energies a pole occurs. Considering the transmission amplitude, a pole may only arise due to the gamma function, which has poles at zero and the negative integers. We will thus have resonances whenever

$$\tfrac{1}{2} - i\hbar^{-1}I(\mathcal{E}) = -n \iff I(\mathcal{E}) = -i\hbar\left(n+\tfrac{1}{2}\right) \quad \text{for} \quad n \in \mathbb{N}. \tag{5.62}$$

This may be substituted back into the relation (5.55) to find the resonance energies as

$$\begin{aligned}\mathcal{E}_n = V_0 - \hbar^2\left[\left\{6C_{4,0} + 30C_{3,0}^2\lambda^{-1}\right\}\left(n+\tfrac{1}{2}\right)^2 + \tfrac{3}{2}C_{4,0} + \tfrac{7}{2}C_{3,0}^2\lambda^{-1}\right] \\ - i\hbar\lambda\left(n+\tfrac{1}{2}\right).\end{aligned} \tag{5.63}$$

We remark, however, that this formula should only be valid for a finite amount of n: for large enough n, the real part will deviate substantially from equilibrium energy V_0, making the approximation by QNF invalid.

Notice that for small enough $\hbar$, we may drop the $\hbar^2$ term and so be left with a simpler expression for the resonances of the system. These resonances, moreover, will lie on a vertical line in the complex plane, directly below the threshold energy V_0, at regular intervals. Their constant distance of separation is modulated by λ, which depends on the curvature of the barrier top.

5.3 Examples

Gaussian potential

We recall the gaussian potential we also utilized earlier:

$$V_{\text{gauss}}(x) = 30\exp\left(-x^2\right). \tag{5.64}$$

n	Energy $\mathcal{E}_n$		Wavenumber k_n
	Exact	Decimal	
0	$30 - 3\hbar^2/8 - i \cdot \hbar\sqrt{30}$	$29.6250 - i \cdot 5.4772$	$5.4659 - i \cdot 0.5010$
1	$30 - 15\hbar^2/8 - i \cdot 3\hbar\sqrt{30}$	$28.1250 - i \cdot 16.4317$	$5.5090 - i \cdot 1.4913$
2	$30 - 39\hbar^2/8 - i \cdot 5\hbar\sqrt{30}$	$25.1250 - i \cdot 27.3861$	$5.5808 - i \cdot 2.4536$
3	$30 - 75\hbar^2/8 - i \cdot 7\hbar\sqrt{30}$	$20.6250 - i \cdot 38.3406$	$5.6640 - i \cdot 3.3846$
4	$30 - 123\hbar^2/8 - i \cdot 9\hbar\sqrt{30}$	$14.6250 - i \cdot 49.2950$	$5.7465 - i \cdot 4.2892$

Table 5.3: Resonance energies for the gaussian potential V_{gauss} (5.64), obtained using QNF. Columns k_n and $\mathcal{E}_n$/decimal assume $\hbar \equiv 1$.

Evidently $V_{\text{gauss}}(0) = 30$ is a local maximum, so that we may apply the QNF methodology around that energy. It can be verified that $V''(0) = -60$ and $V^{(4)}(0) = 360$, so that

$$\lambda = \sqrt{-2V''(0)} = 2\sqrt{30} \quad \text{and} \quad C_{4,0} = \frac{V^{(4)}(0)}{4! \times \lambda^2} = \frac{1}{8}. \tag{5.65}$$

Notably, $C_{3,0} = 0$. This is because the gaussian is a symmetric function, and $C_{3,0}$—which is proportional to $V^{(3)}(0)$—is a measure of the asymmetry of the barrier top under consideration. We utilize (5.63) by plugging in these numbers, and we find that the resonance energies are given by:

$$\mathcal{E}_n = 30 - \tfrac{3}{4}\hbar^2 \left[\left(n + \tfrac{1}{2}\right)^2 + \tfrac{1}{4}\right] - i \cdot 2\hbar\sqrt{30}\left(n + \tfrac{1}{2}\right). \tag{5.66}$$

We are also interested in the associated wavenumber resonance $k_n = \hbar^{-1}\sqrt{\mathcal{E}_n}$. Eyeing the expression above, it would be rather cumbersome and unintuitive to attempt to obtain the exact expression for k_n. However, it turns out that we can make the approximation

$$k_n \approx k_{n,\text{app}} = \hbar^{-1}\sqrt{30} - i \cdot \left(n + \tfrac{1}{2}\right), \tag{5.67}$$

for which it holds

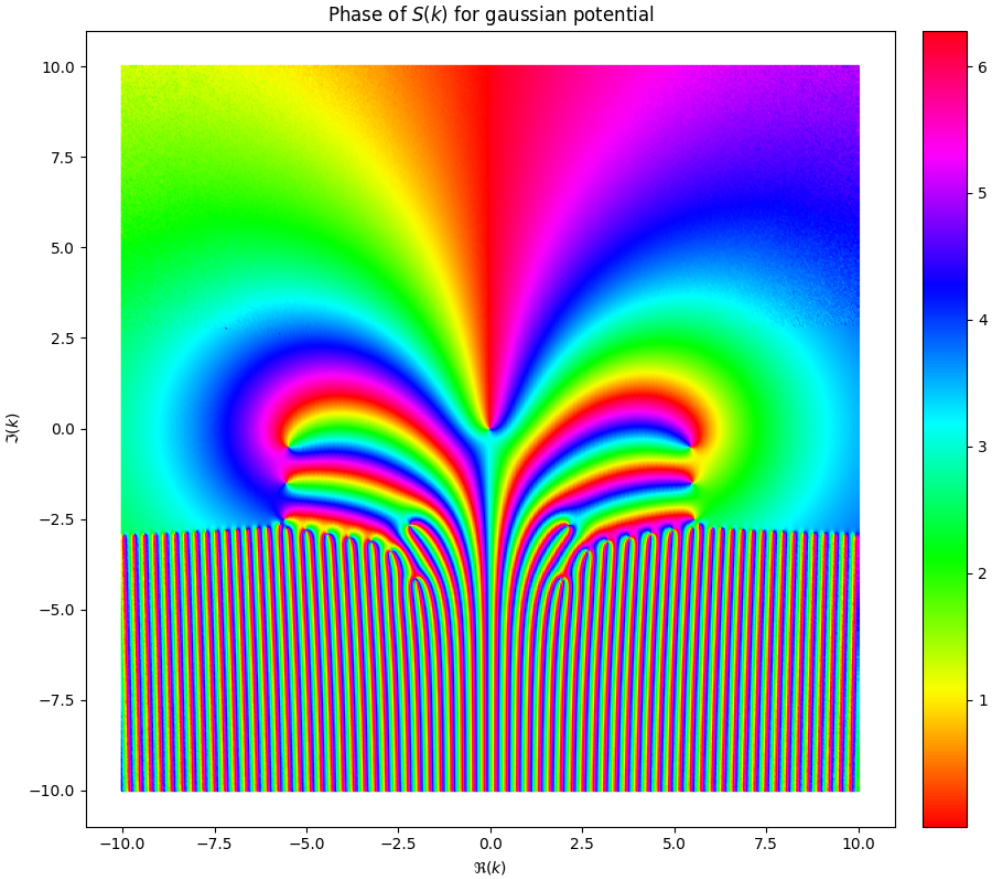
$$|\mathcal{E}_n - \hbar^2 k_{n,\text{app}}^2| = \tfrac{1}{4}\hbar^2 \left|\left(n + \tfrac{1}{2}\right)^2 - \tfrac{3}{4}\right|. \tag{5.68}$$

The reason for the accuracy of this approximation is that the real part of $\mathcal{E}_n$ has downward opening quadratic behavior as function of n, whilst the imaginary part has linear behavior. This lends itself particularly well to approximation by k_n with constant real part and linear imaginary part, as may be seen from the decomposition (3.8). As a result, we expect $\operatorname{Re} k_n$ to be roughly constant, and $\operatorname{Im} k_n$ to increase roughly linearly.

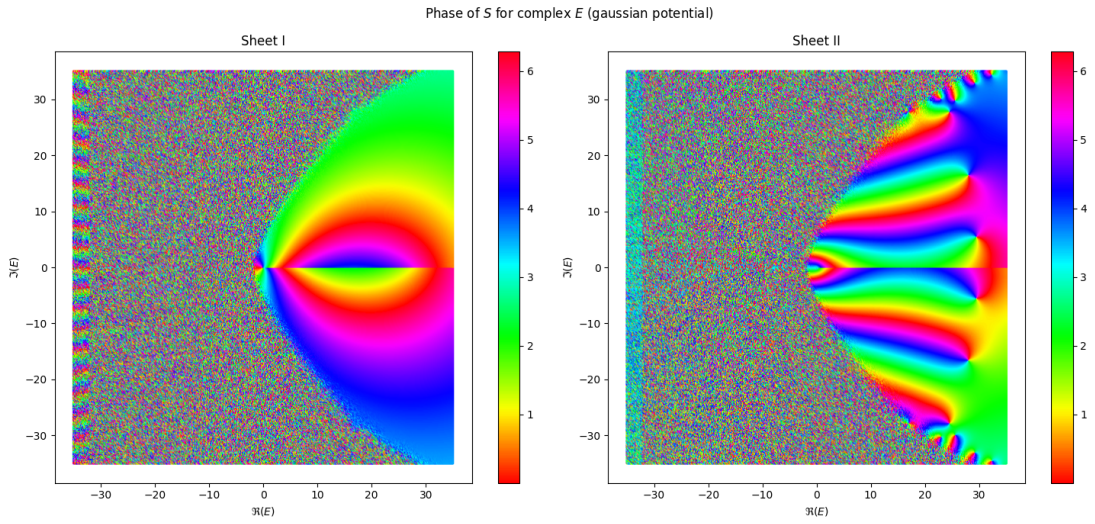
In Table 5.3, the first few resonances as obtained using the above formula may be found. We see that indeed the real part of k_n stays roughly constant, whilst we have roughly linear behavior in the imaginary part.

We should be able to locate these resonances on a plot of S as function of $\mathcal{E}$ or k. We have calculated the relevant values of S, and the plot may be found in Figure 5.3. Indeed, we find that there are resonances located roughly there where we expect them to be based on the calculation. We can locate the resonances $\mathcal{E}_{0,1,2}$ and $k_{0,1,2}$.

More interestingly, though, in Figure 5.3a we find the appearance of a "wall" of resonances around $k_{\text{I}} = -3$, obfuscating the resonances $k_{n>2}$. (The start of this "wall" is also visible in Figure 5.3b, in the lower right corner.) These resonances are



(a) Phase of $S(k)$.



(b) Phase of $S(\mathcal{E})$. The noise on the left of both sheets is a glitch in the calculations.

Figure 5.3: Phase of S as function of k (a) and $\mathcal{E}$ (b) for the gaussian potential V_{gauss} (5.64) ($\hbar \equiv 1$).

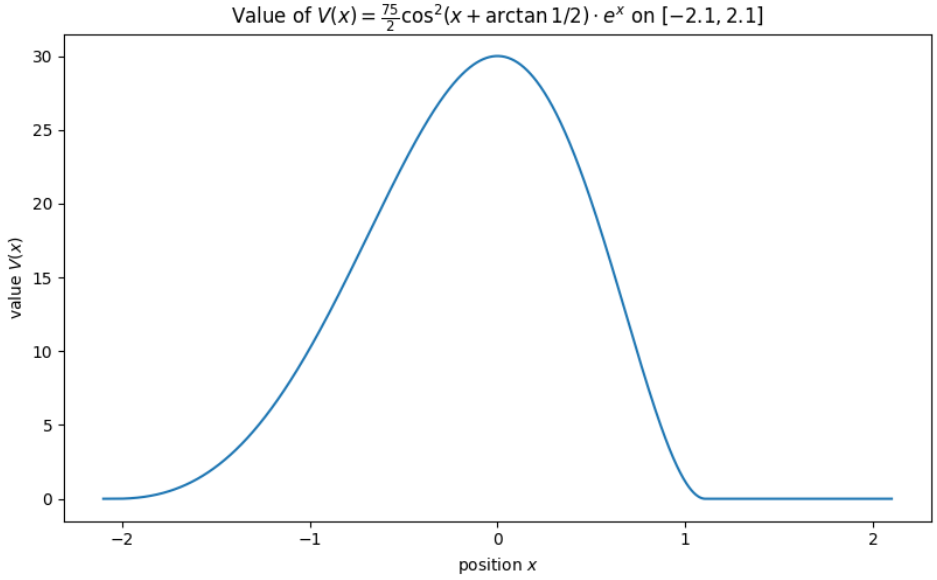


Figure 5.4: Illustration of the asymmetric potential V_{asym} in (5.69).

known as *Regge resonances*, and they appear due to the discontinuity in the potential landscape that was used to generate these pictures [1]. (This type of resonance was also featured in Figure 3.5.) Concretely, the bounds used for generation of the images in Figure 5.3 were $(-5.5, 5.5)$, and so there was a discontinuity at the start and end of $V_{\text{gauss}}(\mp 5.5) = 2.2 \times 10^{-12}$.

We also note the similarity between Figure 5.3a and the transmission amplitude for the square well in Figure 4.1. Since for square well it is precisely the discontinuity that creates these wavefronts on the lower half of the k-plane, this bolsters our confidence in characterizing these as Regge resonances. Moreover, in Figure 5.3a we count that for small k_{I}, there are ≈ 21 wavefronts between $k_{\text{R}} = 0$ and $k_{\text{R}} = 2\pi$. This means that the frequency of this wave is $\omega \approx 21 \approx 4 \times 5.5 = 4\nu$, matching the behavior of the square well $S(k)$ (Proposition 4.8).

Asymmetric potential

To illustrate QNFs for asymmetric potential barriers, consider

$$V_{\text{asym}}(x) = \begin{cases} \frac{75}{2}\cos^2(x+a)\exp(x) & \text{if} \quad x \in [-(\pi/2+a), \pi/2-a] \approx [-2.03, 1.11] \\ 0 & \text{otherwise} \end{cases}, \tag{5.69}$$

where we set $a \equiv \operatorname{atan} 1/2$. A sketch of this potential may be found in Figure 5.4. It may be checked that we have a local maximum at $x = 0$. Thus, we can apply the QNF methodology to find the resonances around $x = 0$.

Using Mathematica we obtain the following Maclaurin expansion of V_{asym}:

$$V_{\text{asym}}(x) = 30 - \frac{75}{2}x^2 - \frac{25}{2}x^3 + \frac{25}{2}x^4 + \frac{35}{2}x^5 + \mathcal{O}\big(x^6\big), \tag{5.70}$$

so we can read off $V(0) = 30$, $V''(0) = -75$, $V^{(3)}(0) = -75$, and $V^{(4)}(0) = 300$. Thus

n	Energy $\mathcal{E}_n$	Wavenumber k_n
0	$29.6736 - i \cdot 6.1237$	$5.4760 - i \cdot 0.5591$
1	$28.2569 - i \cdot 18.3712$	$5.5660 - i \cdot 1.6503$
2	$25.4236 - i \cdot 30.6186$	$5.7106 - i \cdot 2.6809$
3	$21.1736 - i \cdot 42.8661$	$5.8730 - i \cdot 3.6494$
4	$15.5069 - i \cdot 55.1135$	$6.0316 - i \cdot 4.5687$

Table 5.4: Resonances energies for the asymmetric potential V_{asym} (5.69), obtained using QNF ($\hbar \equiv 1$).

the relevant coefficients may be calculated to be

$$\lambda = 5\sqrt{6}, \quad C_{3,0} = \frac{5}{2\sqrt{30}\sqrt[4]{6}}, \quad \text{and} \quad C_{4,0} = \frac{1}{12}. \tag{5.71}$$

We fill these into the resonance equation (5.63) and simplify to obtain

$$\mathcal{E}_n = 30 - \hbar^2 \left[\tfrac{17}{24} \left(n + \tfrac{1}{2} \right)^2 + \tfrac{43}{288} \right] - i \cdot 5\hbar\sqrt{6} \left(n + \tfrac{1}{2} \right). \tag{5.72}$$

The first five resonances calculated using this formula—as well as the relevant wavenumbers k_n—may be found in Table 5.4.

To check that these reflect reality, we may calculate S for sections of k- and $\mathcal{E}$-space, and check that we indeed find resonances. This has been done in Figure 5.5. We find only one resonance as predicted by QNF; the others are (presumably) obfuscated by the Regge resonances, which start at a k_{I} considerably larger than they did for the gaussian potential.

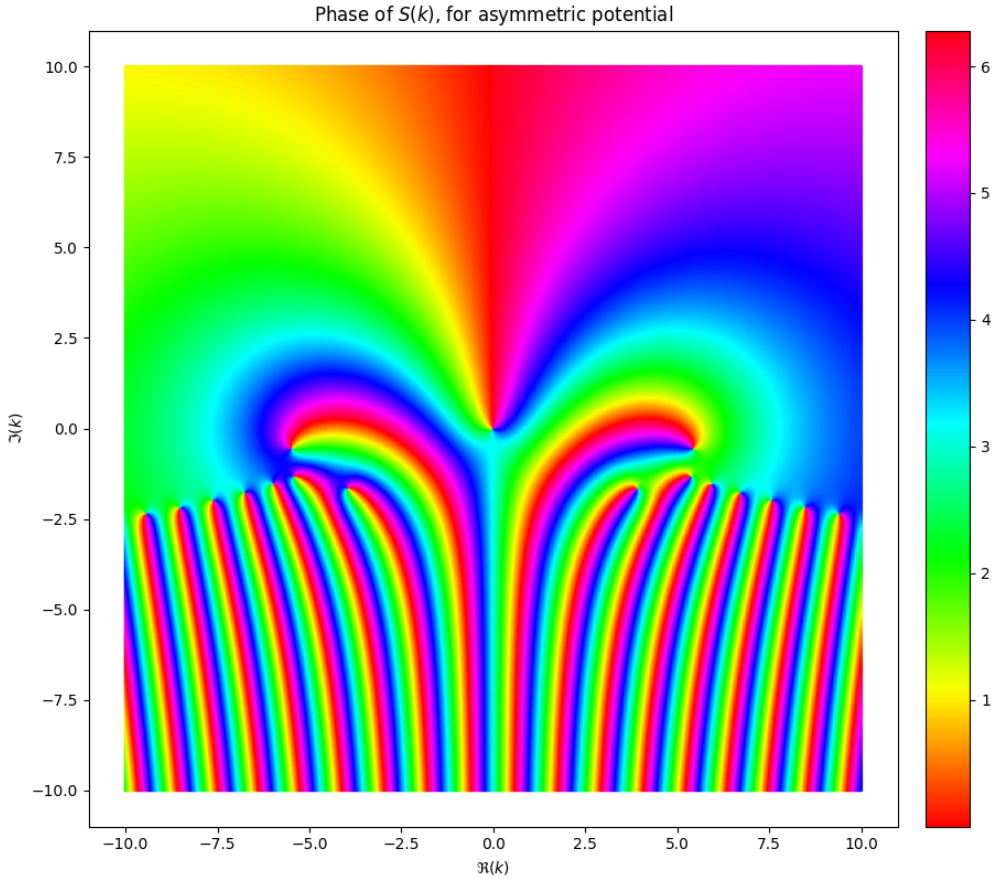
Furthermore, doing as we did for the gaussian potential, if we count the waves in the lower half-plane we find that the frequency is given by $\omega \approx 5.5$. Though this is not approximately equal to $4 \times 2.1 = 8.4 = 4\nu$, it is approximately equal to $2 \times (2 + 1.1) = 6.2$. Since ν is supposed to represent half of the total length of the potential's support, we argue that the comparison with 6.2 (which is twice the total length) is more fitting.

Since now the discontinuity is not in V itself ($V_{\text{asym}}(\mp 2.1) \equiv 0$), we suspect that discontinuity at higher order derivatives plays a role as well. Namely, at the negative "interface" $x \approx -2.03$, $V_{\text{asym}}(-2.03) = V'_{\text{asym}}(-2.03) = 0$, but $V''_{\text{asym}}(-2.03) \approx 9.8 \neq 0$.

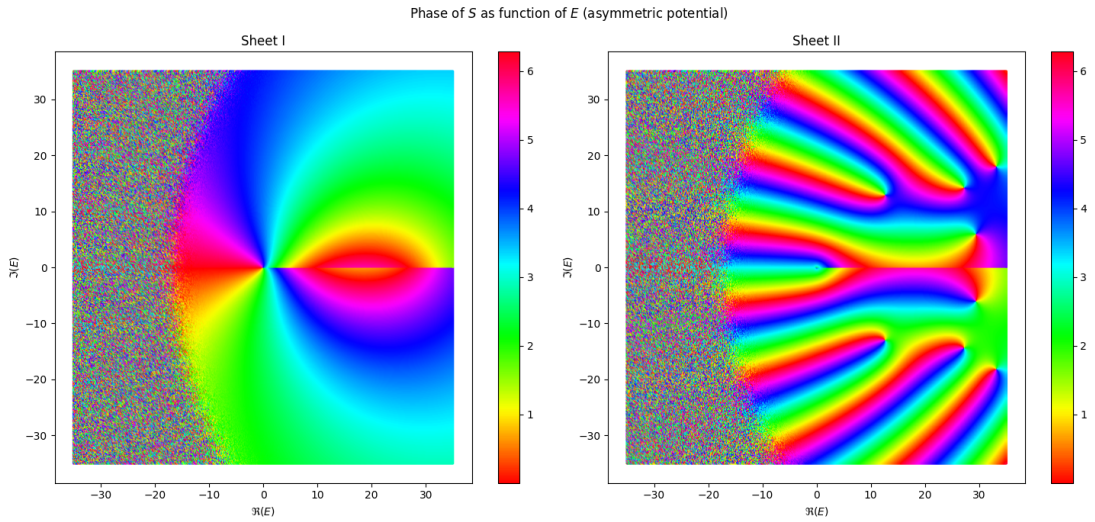
To conclude

We started this section by adapting the classical algorithm for rewriting a Hamiltonian into CNF to our quantum case. This yielded us a way to transform a Hamiltonian into QNF, up to any desired order. Then we applied this to the case of the 1D potential barrier, and derived explicit formulae for the transmission amplitude and coefficient in the form of (5.53) and (5.54), written in terms of the variable I. We finally related E to I, obtaining a description of both in terms of the energy. Finally, we noticed for particular choices of I resonances should occur, and thus we were able to find a general formula for resonance energies, namely (5.63).

We also applied the QNF theory to two examples—that of the gaussian potential V_{gauss} (5.64) and an asymmetric potential (5.69)—with the aim of finding resonances.



(a) Phase of $S(k)$.



(b) Phase of $S(\mathcal{E})$. As in Figure 5.3, the noise on the left sides are glitches from the calculation.

Figure 5.5: Phase of S as a function of k (a) and $\mathcal{E}$ (b) for the asymmetric potential V_{asym} (5.69) ($\hbar \equiv 1$).

In the former case, QNF gave a good match with the numerically computed results featured in Figure 5.3. We were also able to classify the non-predicted resonances as Regge resonances, for instance by means of comparison to the square well (Figure 4.1. In the example of the asymmetric potential much the same was observed. Unfortunately, here we only found one resonance before the Regge resonances appeared.

The motivation for studying QNFs was to find a "bridge" between energy regions for which the WKB approximation is valid, and in this we have succeeded—for the case of one barrier top. In the case of multiple barriers (e.g. the sinc potential V_{sinc} (4.107) with energy $E \approx 32.585$), what we are still missing is a description that evolves the wavefunction from one of the peaks to the other peak à la the matrix $\mathbf{F}$ of (2.4.3). We elaborate more on this in the Conclusion.

6 Conclusion

In this thesis, we strove to get a broad overview of the meaning and effect of resonances in 1D quantum systems. In this way, we aimed to get a better understanding of some of the prototypical "quantum weirdness" that sets QM apart from classical mechanics.

The preliminaries saw us discuss some introductory QM and Hamiltonian mechanics, as well as theory on CNFs, scattering, and the WKB approximation. Considering this final item, upon rewriting the connection formulae and adding a "forward" propagating operator, we were able to derive the matrix $\mathbf{P}$ which describes the propagation of the wavefunction through the entire potential.

In the first section we saw how complex (eigen)energies carry with them an interpretation of decay, wherein the imaginary part is the inverse lifetime of the associated (eigen)state:

$$\mathcal{E} = E - i\Gamma/2 \implies |\langle\psi|\mathcal{U}(t)|\psi\rangle|^2 \propto \exp(-\Gamma t), \quad \text{for} \quad \Gamma > 0. \tag{6.1}$$

Furthermore, we discussed how complex energy lives on a two-sheeted Riemann surface, in order to allow for two distinct wavenumbers $k := \hbar^{-1}\sqrt{\mathcal{E}}$.

We then used the resolvent operator to define resonances of quantum systems, and tied this definition to the transmission amplitude $S(k)$ by means of linear independence of the solutions to the Schrödinger equation. Finally we showed that $S(k)$ is a meromorphic function, and that the model also remains valid when we consider $V \in L^1_1$, instead of as having bounded support.

We started the next section by deriving a general expression for $S(k)$ under the assumption that the potential V was even. This expression depended on two parameters $\theta_{\text{e,o}}$ (the logarithmic derivatives of the even and odd solutions inside the potential), and the rest of the section was dedicated to finding these for specific potential classes.

For the case of piecewise constant potentials (i.e. consisting of square barriers and wells), we were able to obtain an *exact* expression for $S(k)$, and we used this to analyze the case of the square well. The result was that the Bohr-Sommerfeld quantization condition determined the transparency energies (energies at which $T = 1$), and so that, generally, $T \neq 1$ for $E > 0$. Furthermore, when expanding T around such transparencies, we found that T had the shape of an FBW-distribution, which allowed us an easy avenue to finding resonances (Remark 4.11).

For the case of a potential-energy combination for which a WKB approximation was admissible, we found a concise expression for $S(k)$ in terms of the matrix $\mathbf{P}$,

$$S(k) = \frac{\exp(-2ik\nu)}{\mathbf{P}_{12}(k)}. \tag{6.2}$$

This expression made no further approximations, other than what was already necessary to derive $\mathbf{P}$ (which utilizes the WKB approximation).

This allowed us to mathematically analyze the case of the sinc-potential, in which we were able to explain the experimentally found transparencies in the transmission spectrum at energies smaller than the threshold energy. These turned out to be intimately related to i) resonances which lay off-axis on the second Riemann sheet, and ii) the Bohr-Sommerfeld quantization condition—similarly to the case of the square well. Especially this latter point is intriguing, as this condition is normally only utilized

when finding bound states, which these are not (the energies under consideration were all larger than zero).

The final section concerned itself with the topic of quantum normal forms (QNFs). These are applicable in situations where the energy is approximately equal to the maximum height of a potential barrier—precisely a situation in which WKB breaks down. In this way, QNF may "bridge" between two regions in which WKB is applicable (for suitable potentials), so as to obtain a more full understanding of the overall transmission spectrum, amplitude, and/or coefficient.

By drawing heavily on the interplay quantum $\leftrightarrow$ classical, we derived approximate quantum "constants of motion," which then informed the transmission amplitude. In turn, this determined the transmission coefficient, and where the resonances are located. We compared our resonance predictions with simulations for two 1D potential barriers (a gaussian and an asymmetric), and found good agreement between the predictions of the QNF and the numerically obtained data.

Additionally, in the simulations we encountered so-called Regge resonances, which appear due to discontinuities in the potential landscape. This appearance formed a connection between the two treated examples for QNF and the that of the square well, where resonances also appear due to a discontinuity.

The structure of the findings in this thesis may be summarized in a flowchart, which shows under which conditions what methodology applies. This flowchart is found in Figure 6.1.

Suggestions for further research

As a result of this research, there are some unanswered questions still that may/should be investigated.

- **Transmission amplitudes for non-even potentials.** In section 4, we immediately require that the potential is even in order to derive the general expression for $S(k)$. However, this should not be a *requirement* for finding a closed expression for $S(k)$ in the case of square and WKB potentials; merely a convenience to simplify the expression. For instance, Fernández-García also notes that the generalization to odd potentials is immediate [4, §5.1], and expressions found in Galindo & Pascual hold without symmetry requirements [7, §9].

  In particular, it would be interesting to see whether the demonstrated appearance of the Bohr-Sommerfeld quantization condition still occurs when two or more non-identical valleys are considered.

- **Conditions for resonances to effect transparencies.** For the case of transparencies in the square well and sinc potentials, we saw that these are linked to the appearance of transparencies in the transmission spectrum. However, we also saw resonances appear in the case of gaussian and asymmetric potentials barriers when treated with QNF, but these do not lead to transparencies in the transmission spectrum. Intuitively it is clear that transparencies should not occur, but mathematically no explanation was found/articulated in this thesis.

- **Multiple barrier-top scattering.** In the QNF treatment we specifically only addressed the case of scattering by *one* barrier top, leaving out the possibility

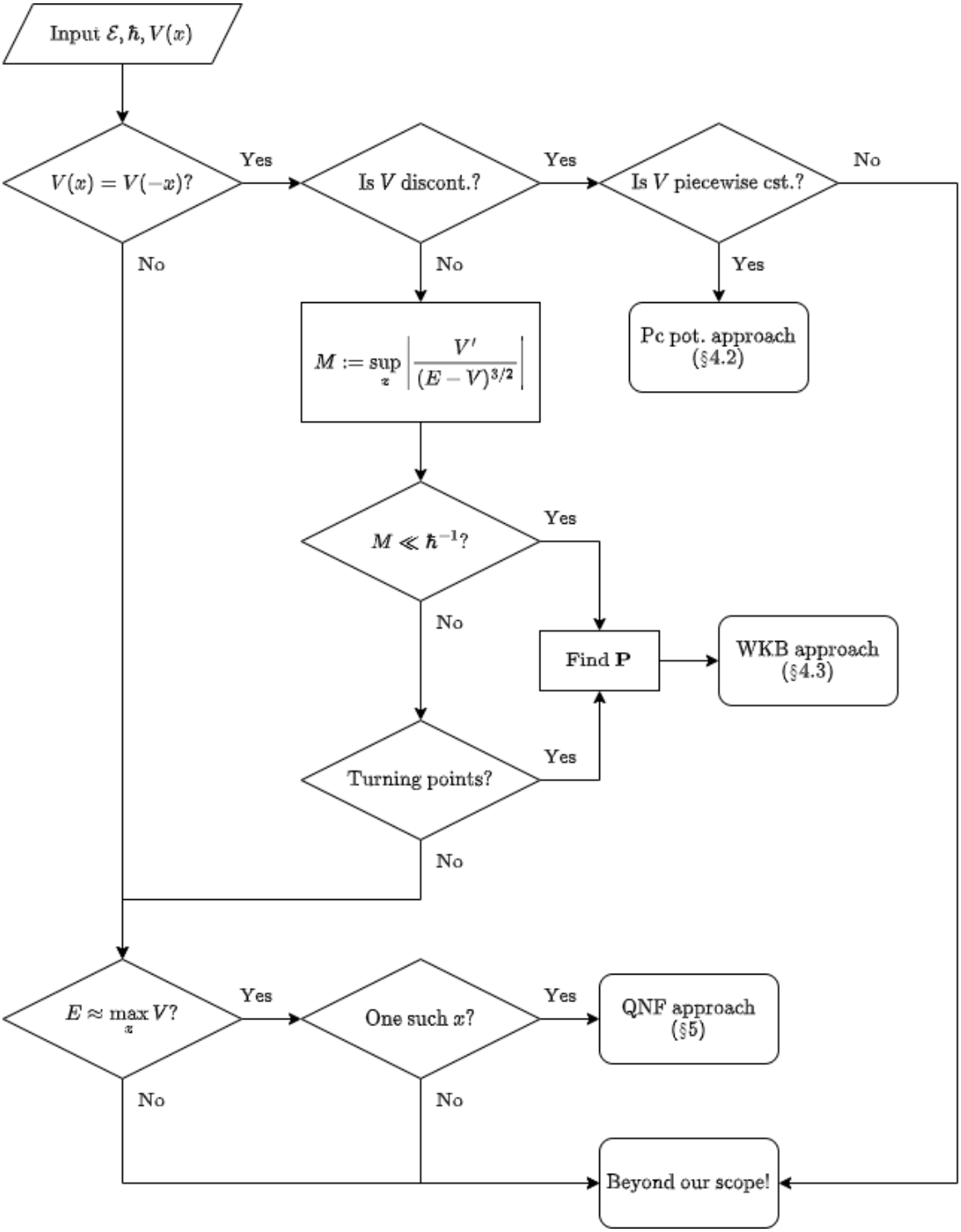


Figure 6.1: Flowchart to identify the right approach for finding the transmission amplitude S (from the ones that we treated in this thesis).

of multiple. This is because, à la the WKB treatment, one should propagate the wavefunction from one barrier top to the next in order to obtain a bona fide description of this type of scattering.

This description is hindered by the fact that the basis of the scattering matrix found in (5.52) is valid only in a neighborhood around the barrier peak, and it is not immediately clear how it relates to "standard" wavefunction forms. Once such a conversion transformation is found, though (perhaps to a WKB-style basis), multiple barrier scattering should be describable.

It is also briefly touched upon in [16, §5.6].

- **Find more resonances predicted by QNF.** With particular reference to Figures 5.3 and 5.5, it would be insightful to attempt to try and get rid of the Regge resonances, in order to find more resonances predicted by QNF. In the case of the gaussian potential, this could be achieved by choosing larger boundaries over which to integrate, which should decrease the size of the discontinuity. (When this was attempted for this work, glitches appeared à la the left sides of Figure 5.3b.) In the case of the asymmetric potential V_{asym} (5.69), this might be more difficult as the discontinuity in higher order derivatives does not disappear with choosing larger bounds.

  In addition to this, one might attempt to use the equation for $S(k)^{-1}$ (3.47) for a potential with known solution (e.g. the Pöschl-Teller potential), and examine whether Regge resonances still occur. If not, then this bolsters the confidence that their appearance is indeed due to various encountered discontinuities in the (derivatives of) the potentials.

Acknowledgments

One does not create a thesis alone, especially one that has been in the making for 10 or so months.

I wish to express gratitude to my supervisors Profs. Boer and Waalkens not only for the guidance in understanding the material, but also for letting me wind and turn the thesis in the ways that I saw fit. This helped me in getting a taste for how to build a research project, and how the various encountered paths may connect up in the end.

Adding to this, I also want to thank Gianni van Marion, who, as PhD student, was my unofficial third supervisor. I could always ask a question or initiate a discussion on something I didn't (quite) understand, and he would enthusiastically aid me. If not walking away with an understanding, I definitely had found another avenue by which to acquire it. Also his enthusiasm for this topic has proven quite contagious!

I also want to thank Dr. Fernández-García for sending me (the Spanish version of) his thesis, which proved a great asset.

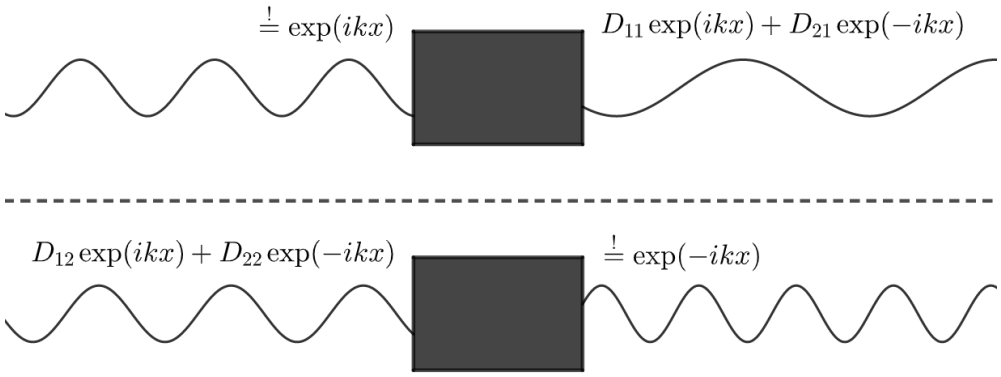


Figure A.1: Implicit definition of the constants D_{ij}, $1 \leq i, j \leq 2$.

A Computation of S-matrices

To verify theoretical calculations done in this thesis, there is a need to compute transmission amplitudes and/or coefficients for the potentials under investigation. This can be done by calculating the S-matrix $\mathbf{S}$ for said given situation.

Finding it is not a trivial task in most cases, though: since there is a definite temporal ordering, the S-matrix would have to be computed over both space *and* time—a PDE calculation. This is despite the fact that we only need to solve the ODE that is the Schrödinger equation in order to get the full solution of the system. So, calculating $\mathbf{S}$ directly would be doing double work.

The issue is that an ODE solver would solve the differential equation in *one* pass only. This means that it would need to be able to calculate, say, the wave outgoing to the left before it has even considered the potential or the wave incoming from the right. Evidently this is impossible, and so we cannot use an ODE solver to find $\mathbf{S}$—at least not directly.

Declare initial conditions on one side of the potential, and then consider which wave corresponds to it on the other side. Specifically, when written in the basis on that side of the target, there must exist unique constants (in x) $D_{ij} \in \mathbb{C}$, $1 \leq i, j \leq 2$, so that

$$\psi|_{\text{left}} \stackrel{!}{=} \exp(ikx) \implies \psi|_{\text{right}} = D_{11}\exp(ikx) + D_{21}\exp(-ikx) \tag{A.1a}$$

and

$$\psi|_{\text{right}} \stackrel{!}{=} \exp(-ikx) \implies \psi|_{\text{left}} = D_{12}\exp(ikx) + D_{22}\exp(-ikx). \tag{A.1b}$$

To connect the introduction of the numbers D_{ij} to $\mathbf{S}$, notice that the statements in (A.1) can be written involving $\mathbf{S}$ as

$$\begin{pmatrix} 1 \\ D_{21} \end{pmatrix} \stackrel{\mathbf{S}}{\longmapsto} \begin{pmatrix} 0 \\ D_{11} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} D_{12} \\ 1 \end{pmatrix} \stackrel{\mathbf{S}}{\longmapsto} \begin{pmatrix} D_{22} \\ 0 \end{pmatrix}, \tag{A.2}$$

since the solution should be unique. As such,

$$\mathbf{S}\begin{pmatrix} 1 & D_{12} \\ D_{21} & 1 \end{pmatrix} = \begin{pmatrix} 0 & D_{22} \\ D_{11} & 0 \end{pmatrix} \implies \mathbf{S} = \begin{pmatrix} 0 & D_{22} \\ D_{11} & 0 \end{pmatrix}\begin{pmatrix} 1 & D_{12} \\ D_{21} & 1 \end{pmatrix}^{-1}, \tag{A.3}$$

which is to say that

$$\boxed{\mathbf{S} = \frac{1}{1 - D_{12}D_{21}} \begin{pmatrix} -D_{21}D_{22} & D_{22} \\ D_{11} & -D_{11}D_{12} \end{pmatrix}.} \tag{A.4}$$

As such, if we can find D_{ij}, $1 \leq i, j \leq 2$, then we can find $\mathbf{S}$.

To determine these numbers we have to use the derivative of the solution. Let us take the first item in (A.1) as an example. We evaluate the solution and its derivative at some point x_0 right of the potential, and substitute in the expressions for the basis functions. Then we arrive at the two equations

$$\begin{cases} \psi|_{\text{right}}(x_0) = D_{11}\exp(ikx_0) + D_{21}\exp(-ikx_0) \\ \psi'|_{\text{right}}(x_0) = ik \cdot [D_{11}\exp(ikx_0) - D_{21}\exp(-ikx_0)] \end{cases}, \tag{A.5}$$

in which we know everything but D_{11} and D_{21}. Rewriting as a matrix and solving for these, we find

$$\begin{pmatrix} D_{11} \\ D_{21} \end{pmatrix} = \begin{pmatrix} \exp(ikx_0) & \exp(-ikx_0) \\ ik\exp(ikx_0) & -ik\exp(-ikx_0) \end{pmatrix}^{-1} \begin{pmatrix} \psi|_{\text{right}}(x_0) \\ \psi'|_{\text{right}}(x_0) \end{pmatrix}, \tag{A.6a}$$

so we have found D_{11} and D_{21} in terms of the solution to the Schrödinger equation. In an analogous way, we have that

$$\begin{pmatrix} D_{12} \\ D_{22} \end{pmatrix} = \begin{pmatrix} \exp(iky_0) & \exp(-ikx_0) \\ ik\exp(iky_0) & -ik\exp(-iky_0) \end{pmatrix}^{-1} \begin{pmatrix} \psi|_{\text{left}}(y_0) \\ \psi'|_{\text{left}}(y_0) \end{pmatrix}, \tag{A.6b}$$

where here y_0 is some point to the left of the target.

With all the above in mind, we can now present the algorithm to calculate the scattering matrix used for this thesis.

Algorithm A.1 (Finding scattering matrix $\mathbf{S}$)**.** In order to find $\mathbf{S}$ at a specific k, we take the following steps.

1. With initial condition $\psi|_{\text{left}} = \exp(ikx)$, calculate $\psi|_{\text{right}}$ and $\psi'|_{\text{right}}$.
2. Evaluate these in a point x_0, and use (A.6a) to find D_{11} and D_{21}.
3. Repeat steps 1 & 2, now with initial condition $\psi|_{\text{right}} = \exp(-ikx)$ and applying (A.6b).
4. Arrange D_{ij}, $1 \leq i, j \leq 2$, in the manner of (A.4) to obtain $\mathbf{S}$.

This algorithm has been implemented in `Python`, using the in-built ODE solver `solve_ivp` from `scipy`, and assuming $\hbar \equiv 1$. (Note that there is also no way to choose a different/smaller $\hbar$ in the code.) The code can be admired in Listing 1.

Listing 1: Python code implementing Algorithm A.1

```
import numpy as np
from scipy.integrate import solve_ivp
import potentials as pots

def f(x, u, k, V):

  # Matrix form of Schroedinger equation
  E = k[0]**2 - k[1]**2 + 2j * k[0] * k[1]  # E = k^2
  A = np.array([[0, 1], [V(x) - E, 0]], dtype = complex)
  return A @ u

def scatmat(k_coord, V, step = 0.05, bounds = (-21, 21), return_E =
    False):

  # Preliminary definitions
  k = k_coord[0] + 1j * k_coord[1]
  minus_k = (-k_coord[0], -k_coord[1])
  lb, ub = bounds

  # Calculate e^(ikx) ~ D_11 * e^(ikx) + D_21 * e^(-ikx)
  phs_lb1, phs_ub1 = np.exp(1j * k * lb), np.exp(1j * k * ub)
  ini_cond1 = np.array([phs_lb1, 1j * k * phs_lb1], dtype = complex)
  sol1 = solve_ivp(f, [lb, ub], ini_cond1, max_step = step, args = (
      k_coord, V), method = 'DOP853')
  U1, U_deriv1 = sol1.y

  A = np.array([[phs_ub1, 1 / phs_ub1], [1j * k * phs_ub1, -1j * k /
      phs_ub1]])
  b = np.array([U1[-1], U_deriv1[-1]])
  D_11, D_21 = np.linalg.solve(A, b)

  # Calculate D_12 * e^(ikx) + D_22 * e^(-ikx) ~ e^(-ikx)
  phs_lb2, phs_ub2 = np.exp(-1j * k * lb), np.exp(-1j * k * ub)
  ini_cond2 = np.array([phs_ub2, -1j * k * phs_ub2], dtype = complex)
  sol2 = solve_ivp(f, [ub, lb], ini_cond2, max_step = step, args = (
      minus_k, V), method = 'DOP853')
  U2, U_deriv2 = sol2.y

  C = np.array([[1 / phs_lb2, phs_lb2], [1j * k / phs_lb2, -1j * k *
      phs_lb2]])
  d = np.array([U2[-1], U_deriv2[-1]])
  D_12, D_22 = np.linalg.solve(C, d)

  # Determine the scattering matrix S from D
  S_11, S_12 = -D_22 * D_21, D_22
  S_21, S_22 = D_11, -D_11 * D_12
  scatmat = np.array([[S_11, S_12], [S_21, S_22]]) / (1 - D_21 * D_12
      )

  # Which coordinate to return?
  if return_E:
    ret_x = k_coord[0]**2 - k_coord[1]**2
    ret_y = 2 * k_coord[0] * k_coord[1]
  else:
    ret_x, ret_y = k_coord

  # Return the coordinate and assoc. S matrix
  return ret_x, ret_y, tuple(scatmat.flatten())
```

B Omitted proofs & justifications

Equation 3.9

Justification. We know that for $x > \nu$, the wavefunction takes the form $\psi_{\text{full}}(x) = S\exp(ikx)$. Then, multiplying with the time dependence $\exp(-i\hbar^{-1}\mathcal{E}t)$, we so find that

$$\begin{aligned}
\rho(x,t) &= |\exp\big(-i\hbar^{-1}\mathcal{E}t\big)\psi_{\text{full}}(x)|^2 \\
&= |S|^2|\exp\big(ikx - i\hbar^{-1}\mathcal{E}t\big)|^2 \\
&= |S|^2|\exp\big(i[k_{\text{R}}x - \hbar^{-1}\mathcal{E}_{\text{R}}t]\big)|^2 \times |\exp\big(-k_{\text{I}}x + \hbar^{-1}\mathcal{E}_{\text{I}}t\big)|^2 \qquad (\to 1) \\
&\overset{\star}{=} |S|^2\exp\left(\frac{2\mathcal{E}_{\text{I}}}{\hbar}\left[t - \frac{x}{2\hbar k_{\text{R}}}\right]\right) \\
&\overset{\star\star}{=} |S|^2\exp\left(-\Gamma\left[t - \frac{x}{2\hbar k_{\text{R}}}\right]\right),
\end{aligned} \tag{B.1}$$

wherein $\star$ we utilized $\mathcal{E}_{\text{I}} = 2\hbar^2 k_{\text{R}}k_{\text{I}}$, and in $\star\star$ $\Gamma := -2\hbar^{-1}\mathcal{E}_{\text{I}}$ (Definition 3.2). □

Equation 3.10

Justification. For $x < -\nu$, the wavefunction takes the form $\psi_{\text{full}}(x) = \exp(ikx) + L\exp(-ikx)$. Multiplying with the time dependence $\exp(i\hbar^{-1}\mathcal{E}t)$, we find that

$$\begin{aligned}
\rho(x,t) &= |\exp\big(-i\hbar^{-1}\mathcal{E}t\big)\psi_{\text{full}}(x)|^2 \\
&= |\exp\big(ikx - i\hbar^{-1}\mathcal{E}t\big) + L\exp\big(-ikx - i\hbar^{-1}\mathcal{E}t\big)|^2 \\
&= \exp\big(2\mathcal{E}_{\text{I}}\hbar^{-1}t\big)|\exp(ikx) + L\exp(-ikx)|^2 \\
&\overset{\star}{=} \exp(-\Gamma t)|\exp(ik_{\text{R}}x)\exp(-k_{\text{I}}x) + L\exp(-ik_{\text{R}}x)\exp(k_{\text{I}}x)|^2 \\
&= \exp(-\Gamma t)\left[\exp(-2k_{\text{I}}x) + |L|^2\exp(2k_{\text{I}}x) + 2\,\text{Re}(L\exp(2ik_{\text{R}}x))\right] \\
&= \exp\left(-\Gamma\left[t - \frac{x}{2\hbar k_{\text{R}}}\right]\right) + |L|^2\exp\left(-\Gamma\left[t + \frac{x}{2\hbar k_{\text{R}}}\right]\right) + 2L_{\text{R}}\cos(2k_{\text{R}}x),
\end{aligned} \tag{B.2}$$

where in $\star$ we used Definition 3.2 for $\Gamma = -2\hbar^{-1}\mathcal{E}_{\text{I}}$. In the final line, the term $2L_{\text{R}}\cos(2k_{\text{R}}x)$ is comparatively unimportant and so we designate it simply as "oscillation" (or osc. for short). □

Lemma 3.18

Proof. We shall prove by induction on n. For the base case $n = 1$, the integral reduces to one dimension, which trivially satisfies the given relation.

Assume the statement to hold for some $b \in \mathbb{N}$. Then, we consider the lhs for the

case of $b+1$:

$$\begin{aligned}\int_x^\infty \int_{x_1}^\infty \cdots \int_{x_{b-1}}^\infty \int_{x_b}^\infty |q(x_1)| \cdots |q(x_{b+1})|\, dx_{b+1} \cdots dx_1 \\ = \int_x^\infty |q(x_1)| \times \left\{ \int_{x_1}^\infty \cdots \int_{x_b}^\infty |q(x_2)| \cdots |q(x_{b+1})|\, dx_{b+1} \cdots dx_2 \right\} dx_1 \\ = \frac{1}{b!} \int_x^\infty |q(x_1)| \left(\int_{x_1}^\infty |q(t)|\, dt \right)^b dx_1 \,. \end{aligned} \tag{B.3}$$

We now make the substitution

$$y := \int_{x_1}^\infty |q(t)|\, dt \implies -dy = |q(x_1)|\, dx_1 \,, \tag{B.4}$$

with the bounds becoming

$$x_1 \to \infty \longleftrightarrow y = 0 \quad \text{and} \quad x_1 = x \longleftrightarrow y = \int_x^\infty |q(t)|\, dt =: \ell. \tag{B.5}$$

Filling this into the expression (B.3), we so get that

$$\begin{aligned}\frac{1}{b!} \int_x^\infty |q(x_1)| \left(\int_{x_1}^\infty |q(t)|\, dt \right)^b dx_1 = -\frac{1}{b!} \int_\ell^0 y^b\, dy = \frac{\ell^{b+1}}{(b+1)!} \\ = \frac{1}{(b+1)!} \left(\int_x^\infty |q(t)|\, dt \right)^{b+1} . \end{aligned} \tag{B.6}$$

As such, the induction step has also been completed.

Both the base case an induction steps have been shown. Therefore, the proof is now completed. □

Lemma 4.4

Proof. Observe that for $A \neq 0$ we can diagonalize the exponent as

$$\begin{pmatrix} & \ell \\ \ell A & \end{pmatrix} = \frac{-1}{2\sqrt{A}} \begin{pmatrix} 1 & 1 \\ \sqrt{A} & -\sqrt{A} \end{pmatrix} \begin{pmatrix} \ell\sqrt{A} & \\ & -\ell\sqrt{A} \end{pmatrix} \begin{pmatrix} -\sqrt{A} & -1 \\ -\sqrt{A} & 1 \end{pmatrix} . \tag{B.7}$$

The exponentiation hereof becomes

$$\begin{aligned}\exp\left[\begin{pmatrix} & \ell \\ \ell A & \end{pmatrix} \right] &= \frac{-1}{2\sqrt{A}} \begin{pmatrix} 1 & 1 \\ \sqrt{A} & -\sqrt{A} \end{pmatrix} \begin{pmatrix} e^{\ell\sqrt{A}} & \\ & e^{-\ell\sqrt{A}} \end{pmatrix} \begin{pmatrix} -\sqrt{A} & -1 \\ -\sqrt{A} & 1 \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2}(e^{\ell\sqrt{A}} + e^{-\ell\sqrt{A}}) & A^{-1/2}\, \frac{1}{2}(e^{\ell\sqrt{A}} - e^{-\ell\sqrt{A}}) \\ A^{1/2}\, \frac{1}{2}(e^{\ell\sqrt{A}} - e^{-\ell\sqrt{A}}) & \frac{1}{2}(e^{\ell\sqrt{A}} + e^{-\ell\sqrt{A}}) \end{pmatrix} \\ &= \begin{pmatrix} \cosh\big(\ell A^{1/2}\big) & A^{-1/2} \sinh\big(\ell A^{1/2}\big) \\ A^{1/2} \sinh\big(\ell A^{1/2}\big) & \cosh\big(\ell A^{1/2}\big) \end{pmatrix} , \end{aligned} \tag{B.8}$$

as we wanted to show. □

Equation (5.22)

Justification. We start with the quantities

$$\begin{cases} W_3 = \lambda^{-1}\left(-\frac{1}{3}C_{3,3}q^3 - C_{3,2}q^2p + C_{3,1}qp^2 + \frac{1}{3}C_{3,0}p^3\right) \\ H_3^{(2)} = C_{3,3}q^3 + C_{3,2}q^2p + C_{3,1}qp^2 + C_{3,0}p^3 \end{cases}. \tag{B.9}$$

Then, adapting from the definition of the Moyal bracket we see that

$$\mathrm{Mad}_{W_3} H_3^{(2)} = \{W_3, H_3^{(2)}\} - \frac{\hbar^2}{24} W_3 \left[\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q}\right]^3 H_3^{(2)}, \tag{B.10}$$

with higher order terms neglected as both W_3 and $H_3^{(2)}$ are of qho 3. The first term becomes

$$\begin{aligned} \{W_3, H_3^{(2)}\} &= \partial_q W_3 \partial_p H_3^{(2)} - \partial_p W_3 \partial_q H_3^{(2)} \\ &= 2\lambda^{-1}C_{3,2}C_{3,3}q^4 - 8\lambda^{-1}C_{3,1}C_{3,3}q^3p - 6\lambda^{-1}(C_{3,1}C_{3,2} + C_{3,0}C_{3,3})q^2p^2 \\ &\quad - 8\lambda^{-1}C_{3,2}C_{3,0}qp^3 + 2\lambda^{-1}C_{3,1}C_{3,0}p^4. \end{aligned} \tag{B.11}$$

Then for the second term first expand the third-order differential operator as

$$\left[\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q}\right]^3 = \overleftarrow{\partial_q^3}\overrightarrow{\partial_p^3} - \overleftarrow{\partial_p^3}\overrightarrow{\partial_q^3} - 3\,\overleftarrow{\partial_q^2}\overleftarrow{\partial_p}\overrightarrow{\partial_q}\overrightarrow{\partial_p^2} + 3\,\overleftarrow{\partial_q}\overleftarrow{\partial_p^2}\overrightarrow{\partial_q^2}\overrightarrow{\partial_p}, \tag{B.12}$$

from where we then apply it to W_3 and $H_3^{(2)}$:

$$W_3\left[\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q}\right]^3 H_3^{(2)} = 24\lambda^{-1}(C_{3,1}C_{3,2} - C_{3,0}C_{3,3}). \tag{B.13}$$

Thus, collecting (B.11) and (B.13), we find that

$$\begin{aligned} \mathrm{Mad}_{W_3} H_3^{(2)} &= \lambda^{-1}\left[2C_{3,3}C_{3,2}q^4 - 8C_{3,3}C_{3,1} - 6(C_{3,1}C_{3,2} + C_{3,0}C_{3,3})q^2p^2\right. \\ &\qquad \left. + -8C_{3,2}C_{3,0}p^3 + 2C_{3,1}C_{3,0}p^4 - \hbar^2(C_{3,1}C_{3,2} - C_{3,3}C_{3,0})\right] \\ &= -C_{3,0}^2\lambda^{-1}\left[6q^4 + 24q^3p - 60q^2p^2 + 24qp^3 + 6p^4 - 8\hbar^2\right], \end{aligned} \tag{B.14}$$

where in the last line we also utilized Lemma 5.5 in order to rewrite in terms of $C_{3,0}$. □

Equation (5.54)

Justification. Recall that $g := \Gamma(1/2 - i\hbar^{-1}I)$. Utilizing the property $\Gamma(z)^* = \Gamma(z^*)$, valid for complex z, we find that

$$|g|^2 = \Gamma(1/2 - i\hbar^{-1}I)\Gamma(1/2 + i\hbar^{-1}I). \tag{B.15}$$

Then we invoke Euler's reflection formula, given by

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)}, \tag{B.16}$$

wherein we substitute $z = 1/2 - i\hbar^{-1}I$:

$$\begin{aligned}\Gamma(1/2 - i\hbar^{-1}I)\Gamma(1/2 + i\hbar^{-1}I) &= \pi \left[\sin\big(\pi(1/2 - i\hbar^{-1}I)\big)\right]^{-1} \\ &= \pi \left[\cos\big(i\pi\hbar^{-1}I\big)\right]^{-1} \\ &= \pi \left[\cosh\big(\pi\hbar^{-1}I\big)\right]^{-1} \\ &= 2\pi \left[\exp\big(\pi\hbar^{-1}I\big) + \exp\big(-\pi\hbar^{-1}I\big)\right]^{-1}. \qquad \text{(B.17)}\end{aligned}$$

The final step is to multiply with $\exp(\hbar^{-1}\pi I)/(2\pi)$, which then yields the desired expression. □

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