Chapter 2: Resonances

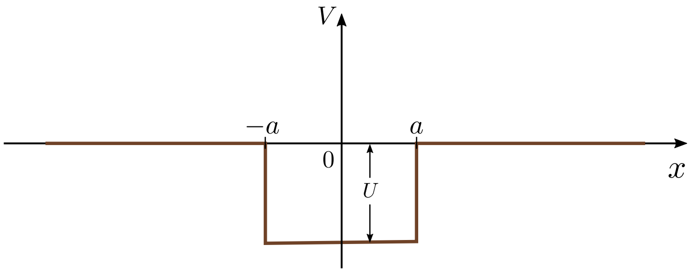
I. BOUND STATES AND FREE STATES

A curious feature of wavefunctions in infinite space is that they come in two distinct varieties: (i) **bound states** that are localized to one region of space, like the ground state of a harmonic oscillator, and (ii) **free states** that extend over the whole space, like plane waves. In fact, both kinds of states can co-exist in a single system.

A simple model exhibiting this is the **1D finite square well**. Consider the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} - U\,\Theta(a - |\hat{x}|), \tag{2.1}$$

where $\hat{x}$ and $\hat{p}$ are 1D position and momentum operators, m is the particle mass, U and a are positive real parameters governing the potential function, and Θ denotes the Heaviside step function (i.e., 1 if the input is positive, and 0 otherwise). As shown below, the potential forms a well of depth U and width $2a$, and vanishes elsewhere.



For such a Hamiltonian, the time-independent Schrödinger wave equation can be solved efficiently using a technique called the **transfer matrix method**. Here, we will describe a few key aspects of the calculation, bypassing most of the details. For a more detailed discussion of the transfer matrix method, refer to Appendix B.

We begin by noting that deriving solutions to the Schrödinger wave equation, like any other differential equation, requires us to specify boundary conditions.

If we are interested in bound state solutions, we look for wavefunctions that diminish exponentially as $x \to \pm\infty$. For $|x| > a$, the Schrödinger wave equation reduces to

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi(x), \tag{2.2}$$

subject to the boundary conditions

$$\psi(x) \sim e^{\mp\kappa x} \;\;\text{as}\;\; x \to \pm\infty \tag{2.3}$$

for some real κ. The functions satisfying Eqs. (2.2) and (2.3) are

$$\psi(x) = c_\pm\, e^{\mp\kappa x}, \;\;\text{where}\;\; -\frac{\hbar^2\kappa^2}{2m} = E, \;\; c_\pm \in \mathbb{C}. \tag{2.4}$$

Evidently, such a solution requires $E < 0$. Moreover, the variational principle implies that $E \geq -U$, so the bound state energies are restricted to the range $-U \leq E < 0$.

It is also possible to show that the bound state energies are *discrete*, and that each bound state wavefunction can always be normalized:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx \;=\; 1. \tag{2.5}$$

The normalization integral is finite since $|\psi(x)|^2$ vanishes exponentially for $x \to \pm\infty$. These two properties follow from the analysis of the general class of "Sturm-Liouville-type" differential equations; for details, refer to textbooks such as Courant and Hilbert [3].

For a free state, the situation is quite different. In this case, the wavefunction does not vanish exponentially at infinity, but instead takes the form

$$\psi(x) = \begin{cases} \alpha_- \, e^{ikx} + \beta_- \, e^{-ikx}, & x < -a \\ \text{(something)}, & -a < x < a \\ \alpha_+ \, e^{ikx} + \beta_+ \, e^{-ikx}, & x > a \end{cases} \tag{2.6}$$

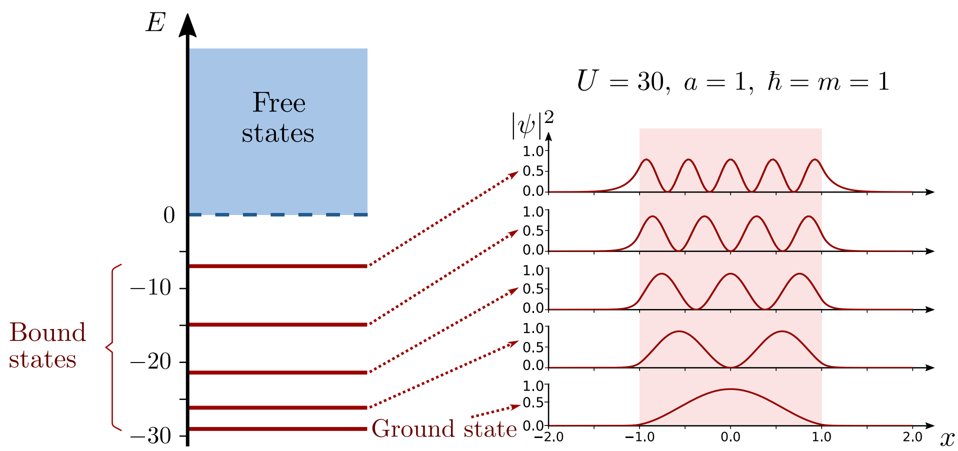
for some real k. Right now, we are not concerned about how $\psi(x)$ behaves in the well region $-a < x < a$. We focus on the outside region, where $\psi(x)$ consists of superpositions of left-moving and right-moving plane waves. To satisfy Schrödinger's equation here, we need

$$\frac{\hbar^2 k^2}{2m} = E, \tag{2.7}$$

which implies that $E \geq 0$. For each E, the coefficients $\alpha_\pm$ and $\beta_\pm$ are not independent, but are linked by a linear relation (see Appendix B). Unlike the bound states, the free states are not discrete; there exist free states for *every* $E \geq 0$.

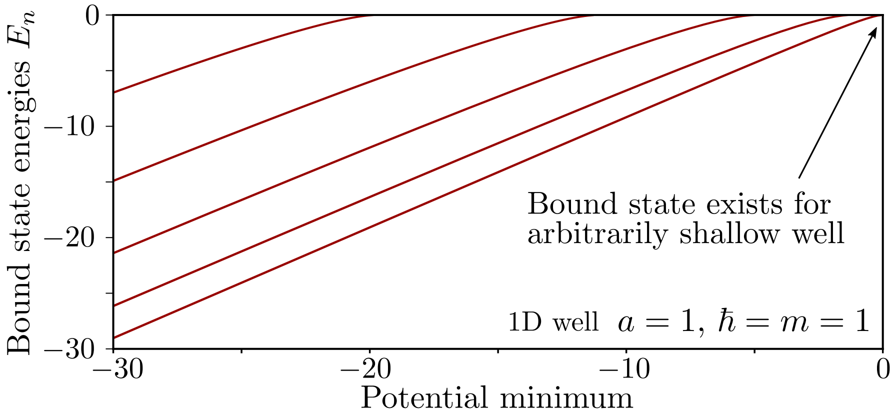
Moreover, since $|\psi(x)|^2$ does not diminish at infinity, the integral $\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx$ is divergent, so these wavefunctions cannot be normalized to unity.

The following figure shows numerically-obtained results for a square well with $U = 30$ and $a = 1$ (in units where $\hbar = m = 1$). The energy spectrum is shown on the left side. There exist five bound states; their plots of $|\psi|^2$ versus x are shown on the right side. These results were computed using the transfer matrix method described in Appendix B.



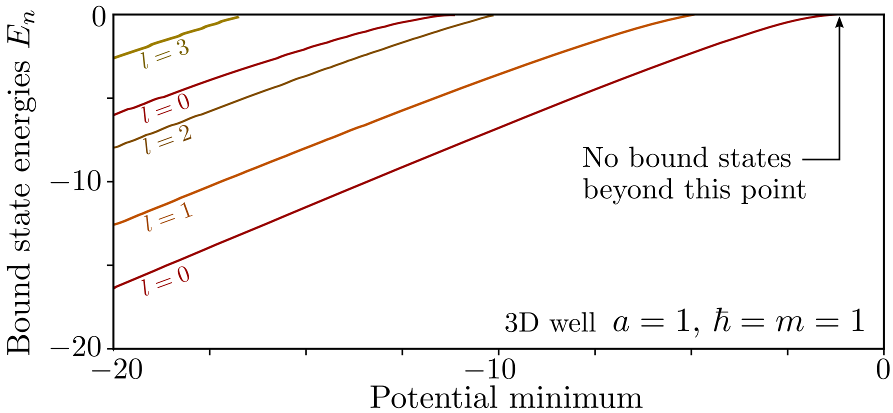
Many of the lessons drawn from the square well model can be generalized to more complicated potentials. In cases where the potential at infinity is V_{ext} rather than zero, free states occur for $E \geq V_{\text{ext}}$ and bound states occur for $\min(V) < E < V_{\text{ext}}$.

There is an important proviso to bear in mind. If we vary the potential, the number of bound states can change: i.e., bound state solutions can either appear or disappear. A numerical example is given below, showing the bound state energies for the square well model with fixed $a = 1$, as we vary the potential minimum $-U$:



For $U = 30$, there are five bound states, which disappear one by one as we make the potential well shallower. Note that one bound state survives in the limit $U \to 0$. There is a theorem stating that any 1D attractive potential, no matter how weak, always supports at least one bound state. For details, see Exercise 1.

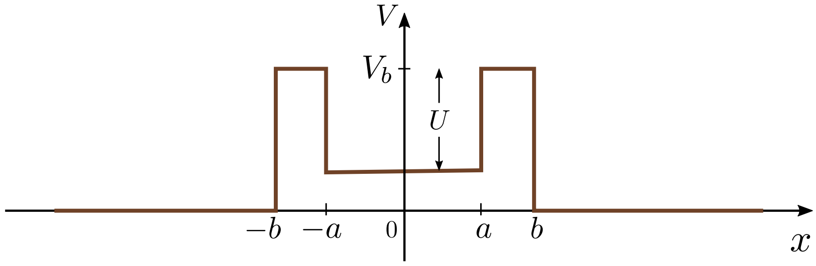
In 3D, it is possible for an attractive potential to be too weak to support a bound state. Intuitively, this happens when the zero-point energy of a prospective ground state exceeds the well depth. The figure below shows a numerical example, calculated for a uniform 3D spherically symmetric well (the l's labeling the various curves are angular momentum quantum numbers). To learn more about this phenomenon, refer to Exercise 2.



II. QUASI-BOUND STATES AND RESONANCES

For the 1D finite square well, there is a clear distinction between bound and free states. Certain potentials, however, can host special states called "**quasi-bound states**". Like a bound state, a quasi-bound state is strongly concentrated in one region of space, yet it lies within the energy range of the free states continuum. As we shall see, quasi-bound states play an important important role in scattering experiments.

The figure below shows an example of a potential function that gives rise to quasi-bound states. In the exterior region, $|x| > b$, the potential is zero. Between $x = -b$ and $x = b$, there is a "barrier" of positive potential V_b. Embedded in the middle of this barrier is a central well of depth U and width $2a$, such that $0 < V_b - U < V_b$.



The potential is purely repulsive (i.e., $V \geq 0$ everywhere), so there are no true bound states. All the exact eigenstates of the Hamiltonian must be free states.

However, there is something intriguing about the central well. Consider an alternative scenario where the potential in the exterior region is V_b rather than 0, so that

$$V_{\mathrm{alt}}(x) = \begin{cases} V_b - U, & |x| < a, \\ V_b, & \text{otherwise.} \end{cases} \tag{2.8}$$

This describes a finite square well, which should have one or more bound states in the energy range $V_b - U < E < V_b$. For each of these bound states, the wavefunction $\psi(x)$ diminishes exponentially away from the well, so $\psi(x) \approx 0$ for $|x| > b$. But $V(x)$ and $V_{\mathrm{alt}}(x)$ differ only in the region $|x| > b$, which implies that $\psi(x)$ is a good *approximate* solution to the Schrödinger equation for the original potential $V(x)$, in spite of the fact that $V(x)$ does not support true bound states! We call such an approximate solution a quasi-bound state.

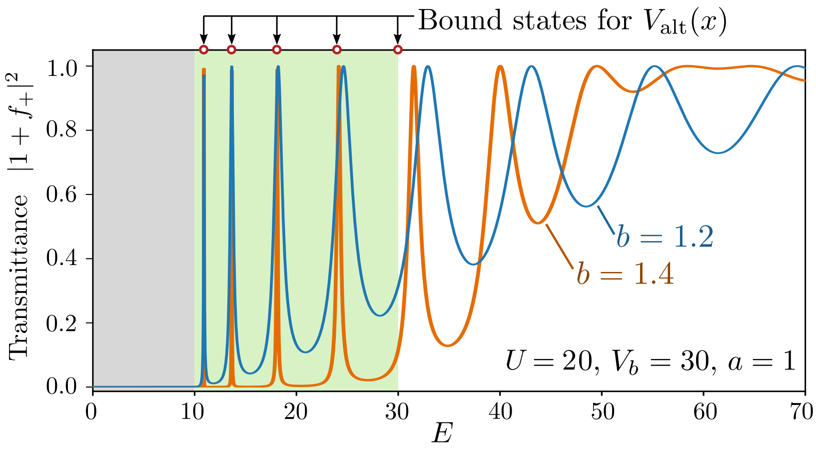
We can also analyze the situation using the scattering framework from the previous chapter. Consider an incident particle of energy $E > 0$ whose wavefunction is

$$\psi_i(x) = \Psi_i \, e^{ik_i x}. \tag{2.9}$$

This produces a scattered wavefunction, which takes the following form in the exterior region:

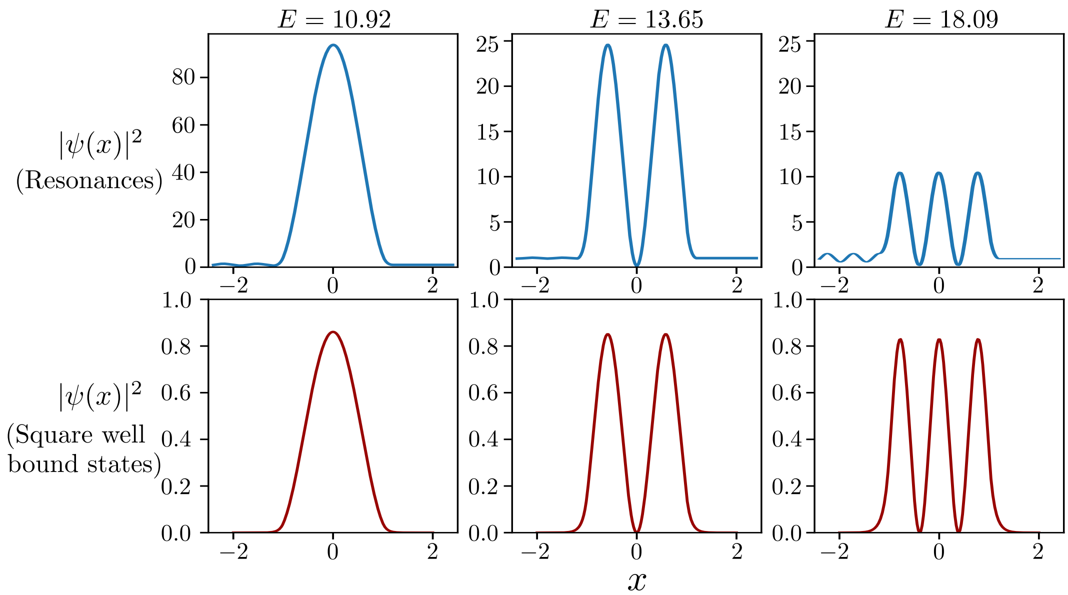
$$\psi_s(x) = \Psi_i \times \begin{cases} f_- \, e^{-ik_i x}, & x \leq -b \\ f_+ \, e^{ik_i x}, & x \geq b. \end{cases} \tag{2.10}$$

The scattering amplitudes f_+ and f_- can be found by solving the Schrödinger wave equation using the transfer matrix method (see Appendix B). The figure below shows numerical results obtained for $U = 20$, $V_b = 30$, $a = 1$, and $b \in \{1.2, 1.4\}$, with $\hbar = m = 1$.



The vertical axis shows the **transmittance** $|1+f_+|^2$, which is the probability for the particle to pass through the scatterer. The horizontal axis is the particle energy E. Unsurprisingly, for $E < V_b - U$ the transmittance approaches zero, and for $E \gtrsim V_b$ it approaches unity. For $V_b - U < E \lesssim V_b$, the transmittance forms a series of narrow peaks; for larger b (i.e., when the central well is more isolated from the exterior space), the peaks are narrower. At the top of the figure, we have also plotted the bound state energies for the square well potential $V_{\text{alt}}(x)$. These energies closely match the locations of the transmittance peaks!

If we look at the total wavefunction $\psi(x)$, we find other interesting features. Below, we plot $|\psi(x)|^2$ versus x at the energies of the first three transmittance peaks, along with the corresponding bound state wavefunctions for V_{alt}. At each transmittance peak, $|\psi(x)|^2$ is very large in the potential region, and its shape is very similar to a bound state of V_{alt}.



The enhancement of $|\psi(x)|^2$ is called a **resonance**. Roughly speaking, the incident particle enters the scatterer, and spends a long time trapped in the quasi-bound state, before eventually leaking out and escaping to infinity.

This is analogous to the phenomenon of resonance in a classical harmonic oscillator. When a damped harmonic oscillator is subjected to a periodic driving force, it settles into a steady-state oscillatory motion at the driving frequency. If the driving frequency matches the oscillator's natural frequency (i.e., the frequency of free oscillation in the absence of a drive), the oscillation amplitude becomes large, and the system is said to be "resonant". In our case, the incident wavefunction plays the role of a driving force, the energy of the incident particle is like the driving frequency, and the energy of the quasi-bound state is like the ocillator's natural frequency.

Resonances play a critical role throughout experimental physics. Experiments are often conducted for the express purpose of locating and studying resonances. When a resonance peak is found, its location and shape can be used to deduce various features of the quasi-bound state, which in turn supplies important information about the underlying system.

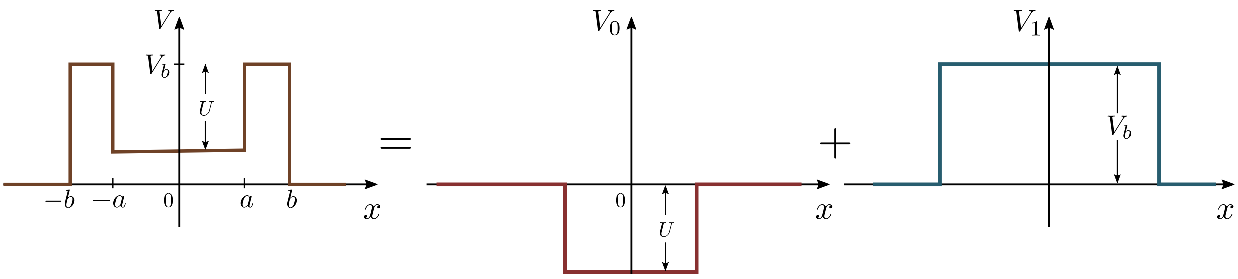
III. GREEN'S FUNCTION ANALYSIS OF SCATTERING RESONANCES

Quasi-bound states and resonances are not limited to 1D, but are also important in 2D and 3D. A convenient way to analyze them, in a general context, is to use the quantum Green's function formalism from the previous chapter.

Let $\hat{H} = \hat{T} + \hat{V}$ be the Hamiltonian of a system supporting resonances, where $\hat{T}$ is the kinetic energy operator and $\hat{V}$ is the potential operator. We decompose the potential into

$$\hat{V} = \hat{V}_0 + \hat{V}_1, \tag{2.11}$$

where $\hat{V}_0$ is a "confining potential" that supports a bound state, and $\hat{V}_1$ is a "deconfining potential" that turns the bound state into a quasi-bound state. For example, the figure below shows the potential functions for the 1D model discussed in the previous section:



When the potential is just $\hat{V}_0$, let there be a bound state $|\varphi\rangle$ with energy E_0. Furthermore, let us assume that the potential supports a continuum of free states $\{|\psi_k\rangle\}$ with energies $\{E_k\}$, where k is some continuous index for labelling the free states (we will discuss what this index might represent later). The states satisfy the Schrödinger equation

$$\big(\hat{T} + \hat{V}_0\big)|\varphi\rangle = E_0|\varphi\rangle \tag{2.12}$$

$$\big(\hat{T} + \hat{V}_0\big)|\psi_k\rangle = E_k|\psi_k\rangle, \tag{2.13}$$

along with the orthogonality and completeness relations

$$\langle\varphi|\psi_k\rangle = 0, \qquad |\varphi\rangle\langle\varphi| + \sum_k |\psi_k\rangle\langle\psi_k| = \hat{I}. \tag{2.14}$$

Here, $\sum_k$ represents a sum over all free states. Since the free states form a continuum, this sum will have to be expressed as an integral by re-normalizing the free states (e.g., delta normalization), as discussed in Section II of the previous chapter. For the moment, however, we will leave it as a discrete sum, with the free states normalized to unity.

As described in Section VII of the previous chapter, the causal Green's function is

$$\hat{G}_0(E) = \lim_{\varepsilon\to 0^+} \left(E - \hat{T} - \hat{V}_0 + i\varepsilon\right)^{-1}. \tag{2.15}$$

Now introduce the deconfining potential $\hat{V}_1$. According to Dyson's equations (from Section VI of the previous chapter), the Green's function for the full system is

$$\hat{G} = \hat{G}_0 + \hat{G}\hat{V}_1\hat{G}_0. \tag{2.16}$$

Note that this is exact, not an approximation. From $\hat{G}(E)$, the scattering amplitudes can be determined. We will calculate the matrix elements of $\hat{G}(E)$ by using $|\varphi\rangle$ and $\{|\psi_k\rangle\}$ as a convenient basis (note, however, that this is *not* the energy eigenbasis of $\hat{H}$).

As usual when dealing with Dyson's equations, we must note that $\hat{G}$ appears on both the left and right hand sides. Let us judiciously insert a resolution of the identity, as follows:

$$\begin{aligned} \hat{G} &= \hat{G}_0 + \hat{G}\hat{I}\hat{V}_1\hat{G}_0 \\ &= \hat{G}_0 + \hat{G}\left(|\varphi\rangle\langle\varphi| + \sum_k |\psi_k\rangle\langle\psi_k|\right)\hat{V}_1\hat{G}_0. \end{aligned} \tag{2.17}$$

We now compute the matrix element $\langle\varphi|\cdots|\varphi\rangle$ for both sides of the equation:

$$\begin{aligned} \langle\varphi|\hat{G}|\varphi\rangle &= \langle\varphi|\hat{G}_0|\varphi\rangle + \langle\varphi|\hat{G}|\varphi\rangle\,\langle\varphi|\hat{V}_1\hat{G}_0|\varphi\rangle + \sum_k \langle\varphi|\hat{G}|\psi_k\rangle\,\langle\psi_k|\hat{V}_1\hat{G}_0|\varphi\rangle \\ \langle\varphi|\hat{G}|\varphi\rangle\left(1 - \langle\varphi|\hat{V}_1\hat{G}_0|\varphi\rangle\right) &= \langle\varphi|\hat{G}_0|\varphi\rangle + \sum_k \langle\varphi|\hat{G}|\psi_k\rangle\,\langle\psi_k|\hat{V}_1\hat{G}_0|\varphi\rangle \\ \lim_{\varepsilon\to 0^+}\langle\varphi|\hat{G}|\varphi\rangle\left(1 - \frac{\langle\varphi|\hat{V}_1|\varphi\rangle}{E-E_0+i\varepsilon}\right) &= \lim_{\varepsilon\to 0^+}\frac{1}{E-E_0+i\varepsilon}\left(1 + \sum_k \langle\varphi|\hat{G}|\psi_k\rangle\,\langle\psi_k|\hat{V}_1|\varphi\rangle\right) \\ \lim_{\varepsilon\to 0^+}\langle\varphi|\hat{G}|\varphi\rangle\Big(E - E_0 - \langle\varphi|\hat{V}_1|\varphi\rangle + i\varepsilon\Big) &- \sum_k \langle\varphi|\hat{G}|\psi_k\rangle\,\langle\psi_k|\hat{V}_1|\varphi\rangle = 1. \end{aligned} \tag{2.18}$$

Similarly, computing the matrix element $\langle\varphi|\cdots|\psi_k\rangle$ gives:

$$\begin{aligned} \langle\varphi|\hat{G}|\psi_k\rangle &= \langle\varphi|\hat{G}_0|\psi_k\rangle + \langle\varphi|\hat{G}|\varphi\rangle\,\langle\varphi|\hat{V}_1\hat{G}_0|\psi_k\rangle + \sum_{k'} \langle\varphi|\hat{G}|\psi_{k'}\rangle\,\langle\psi_{k'}|\hat{V}_1\hat{G}_0|\psi_k\rangle \\ &= \lim_{\varepsilon\to 0^+}(E-E_k+i\varepsilon)^{-1}\left(\langle\varphi|\hat{G}|\varphi\rangle\,\langle\varphi|\hat{V}_1|\psi_k\rangle + \sum_{k'}\langle\varphi|\hat{G}|\psi_{k'}\rangle\,\langle\psi_{k'}|\hat{V}_1|\psi_k\rangle\right). \end{aligned}$$

So far, the equations have been exact, but now we apply an approximation: in the last line of the above equation, let the factor of $\langle\varphi|G|\varphi\rangle$ be large, so that the first term in the sum becomes dominant. It will be shown below that $\langle\varphi|G|\varphi\rangle$ being large is precisely the resonance condition, so this approximation will be self-consistent. With this, we obtain

$$\langle\varphi|\hat{G}|\psi_k\rangle \approx \lim_{\varepsilon\rightarrow 0^+} \frac{\langle\varphi|\hat{G}|\varphi\rangle\,\langle\varphi|\hat{V}_1|\psi_k\rangle}{E - E_k + i\varepsilon}. \tag{2.19}$$

Combining this with Eq. (2.18) gives

$$\lim_{\varepsilon\rightarrow 0^+}\left[\langle\varphi|\hat{G}|\varphi\rangle\left(E - E_0 - \langle\varphi|\hat{V}_1|\varphi\rangle + i\varepsilon\right) - \sum_k \frac{\langle\varphi|\hat{G}|\varphi\rangle\langle\varphi|\hat{V}_1|\psi_k\rangle}{E - E_k + i\varepsilon}\,\langle\psi_k|\hat{V}_1|\varphi\rangle\right] \approx 1.$$

Hence,

$$\langle\varphi|\,\hat{G}(E)\,|\varphi\rangle \approx \frac{1}{E - E_0 - \langle\varphi|V_1|\varphi\rangle - \Sigma(E)} \tag{2.20}$$

$$\text{where}\quad \Sigma(E) \equiv \lim_{\varepsilon\rightarrow 0^+}\sum_k \frac{|\langle\psi_k|\hat{V}_1|\varphi\rangle|^2}{E - E_k + i\varepsilon}. \tag{2.21}$$

The complex quantity $\Sigma(E)$ defined in Eq. (2.21) is called the **self-energy**. We will show later that $\text{Im}[\Sigma] < 0$, and discuss its physical meaning. Although Σ is E-dependent, we assume for now that the dependence is weak, so that it can be treated like a constant.

From Eq. (2.20), we see that $\langle\varphi|\hat{G}(E)|\varphi\rangle$ is large when the denominator is close to zero, which is consistent with the earlier approximation that led to Eq. (2.19). This "**resonance condition**" is satisfied when

$$E \;\approx\; E_0 + \langle\varphi|\hat{V}_1|\varphi\rangle + \text{Re}\big[\,\Sigma\,\big] \;\equiv\; E_{\text{res}}. \tag{2.22}$$

The real quantity E_{res} is called the **resonance energy**. It is the sum of three terms: the energy of the original bound state (in the absence of $\hat{V}_1$), the energy shift induced by $\hat{V}_1$, and the real part of the self-energy Σ. Based on Eq. (2.21), we can interpret this last term as being induced by the presence of the free states $\{|\psi_k\rangle\}$.

In Section VIII of the previous chapter, we derived the following relationship between the Green's function and the scattering amplitude f:

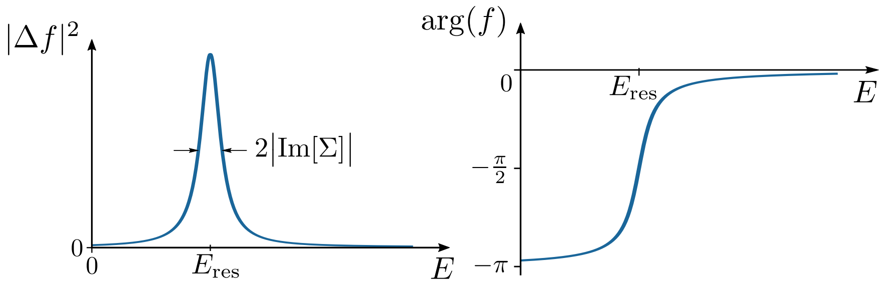
$$f(\mathbf{k}\rightarrow\mathbf{k}') \;\propto\; \langle\mathbf{k}'|\hat{V}|\mathbf{k}\rangle + \langle\mathbf{k}'|\hat{V}\hat{G}\hat{V}|\mathbf{k}\rangle. \tag{2.23}$$

Here, $|\mathbf{k}\rangle$ and $|\mathbf{k}'\rangle$ are incident and scattered plane wave states satisfying $|\mathbf{k}| = |\mathbf{k}'|$. The first term describes the lowest-order scattering process (the first Born approximation). The second term contains all second- and higher-order scattering processes. By inserting resolutions of the identity between each $\hat{V}$ and $\hat{G}$ operator in the second term, we find that f contains a contribution of the form

$$\Delta f(\mathbf{k}\rightarrow\mathbf{k}') \;\propto\; \langle\mathbf{k}'|\hat{V}|\varphi\rangle\langle\varphi|\hat{G}|\varphi\rangle\langle\varphi|\hat{V}|\mathbf{k}\rangle \;=\; \frac{\langle\mathbf{k}'|\hat{V}|\varphi\rangle\,\langle\varphi|\hat{V}|\mathbf{k}\rangle}{E - E_{\text{res}} - i\text{Im}[\,\Sigma\,]}. \tag{2.24}$$

At resonance, the denominator is small and hence Δf is the dominant contribution to f. It is worth emphasizing that Δf has contributions from *all* terms in the Born series, not just low-order terms. The particle bounces around inside the scatterer many times before it escapes, so high orders in the Born series contribute to the outcome.

The figure below shows the energy dependence of Δf, according to Eq. (2.24):



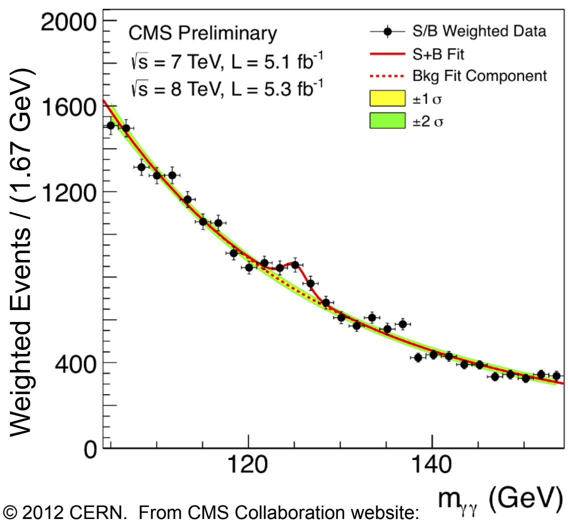
The shape of the graph of $|\Delta f|^2$ versus E is called a **Lorentzian**. It forms a peak centered at E_{res}. The width of the peak can be characterized by the **full-width at half-maximum** (FWHM), the spacing between the two energies where $|\Delta f|^2$ has half its maximum value. It can be shown that

$$\delta E^{(\text{FWHM})} = 2\,\Big|\text{Im}[\Sigma]\Big|. \tag{2.25}$$

Thus, the closer Σ gets to being a real quantity, the sharper the peak.

The phase $\arg[\Delta f]$ also contains useful information. As E crosses E_{res} from below, the phase increases by π. The energy range over which this phase shift occurs is $\sim |\text{Im}[\Sigma]|$.

These two signatures—peaks and phase shifts—are sought after in numerous real-world scattering experiments. In actual experiments, the peaks and phase shifts are often overlaid on a "background" caused by non-resonant processes. For example, the plot below was released by the CMS experiment at the Large Hadron Collider (LHC), showing a resonance peak on a large background. This was part of the evidence for the discovery of a new particle, the Higgs boson, in 2012.



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http://cms.web.cern.ch/news/observation-new-particle-mass-125-gev

IV. FERMI'S GOLDEN RULE

We have seen that the width of a resonance is determined by Im[Σ], the imaginary part of the self-energy. In this section, we will show that Im[Σ] represents the decay rate of a quasi-bound state, and that it can often be approximated using a simple formula called **Fermi's Golden Rule**.

Suppose we set the state of a particle to a quasi-bound state $|\varphi\rangle$ at time $t = 0$. Since $|\varphi\rangle$ is not an exact eigenstate of the Hamiltonian, the particle will not remain in that state for $t > 0$. Over time, the wavefunction will leak out of the potential well, corresponding to the "decay" of the quasi-bound state into the free state continuum.

The decay process can be described by

$$P(t) = \left|\langle\varphi|\exp\left(-i\hat{H}t/\hbar\right)|\varphi\rangle\right|^2, \tag{2.26}$$

which is the probability for the system to continue occupying state $|\varphi\rangle$ after time t. To calculate $P(t)$, let us define the function

$$f(t) = \begin{cases}\langle\varphi|\exp\left(-i\hat{H}t/\hbar\right)|\varphi\rangle\, e^{-\varepsilon t}, & t \geq 0\\ 0, & t < 0,\end{cases} \tag{2.27}$$

where $\varepsilon \in \mathbb{R}^+$. For $t \geq 0$ and $\varepsilon \to 0^+$, we see that $|f(t)|^2 \to P(t)$. The reason we deal with $f(t)$ is that it is more well-behaved than the actual amplitude $\langle\varphi|\exp(-i\hat{H}t/\hbar)|\varphi\rangle$. The function is designed so that firstly, it vanishes at negative times prior to start of our thought experiment; and secondly, it vanishes as $t \to \infty$ due to the "regulator" ε. The latter enforces the idea that the bound state decays permanently into the continuum of free states, and is never repopulated by waves "bouncing back" from infinity.

We can determine $f(t)$ by first studying its Fourier transform,

$$F(\omega) \;=\; \int_{-\infty}^{\infty} dt\, e^{i\omega t}\, f(t) \;=\; \int_{0}^{\infty} dt\, e^{i(\omega+i\varepsilon)t}\, \langle\varphi|e^{-i\hat{H}t/\hbar}|\varphi\rangle. \tag{2.28}$$

Now insert a resolution of the identity, $\hat{I} = \sum_n |n\rangle\langle n|$, where $\{|n\rangle\}$ denotes the exact eigenstates of $\hat{H}$ (for free states, the sum goes to an integral in the usual way):

$$\begin{aligned}
F(\omega) &= \int_0^\infty dt\, e^{i(\omega+i\varepsilon)t}\, \sum_n \langle\varphi|e^{-i\hat{H}t/\hbar}|n\rangle\langle n|\varphi\rangle \\
&= \sum_n \langle\varphi|n\rangle \left(\int_0^\infty dt\, \exp\left[i\left(\omega - \frac{E_n}{\hbar} + i\varepsilon\right)t\right]\right)\langle n|\varphi\rangle \\
&= \sum_n \langle\varphi|n\rangle \frac{i}{\omega - \frac{E_n}{\hbar} + i\varepsilon}\langle n|\varphi\rangle \\
&= i\hbar\, \langle\varphi|\left(\hbar\omega - \hat{H} + i\hbar\varepsilon\right)^{-1}|\varphi\rangle.
\end{aligned} \tag{2.29}$$

In the third line, the regulator ε removes the contribution from the $t \to \infty$ limit, as desired. Hence, we obtain

$$\lim_{\varepsilon\to 0^+} F(\omega) = i\hbar\, \langle\varphi|\hat{G}(\hbar\omega)|\varphi\rangle, \tag{2.30}$$

where $\hat{G}$ is our old friend the causal Green's function. The fact that the *causal* Green's function shows up is due to our definition of $f(t)$, which is non-vanishing only for $t \geq 0$.

As discussed in the previous section, when the resonance condition is satisfied,

$$\langle\varphi|\,\hat{G}(E)\,|\varphi\rangle \approx \frac{1}{E - E_{\mathrm{res}} - i\mathrm{Im}[\Sigma]}, \tag{2.31}$$

where E_{res} is the resonance energy and Σ is the self-energy of the quasi-bound state. We can now perform the inverse Fourier transform

$$\begin{aligned}\lim_{\varepsilon\rightarrow 0^+} f(t) &= \lim_{\varepsilon\rightarrow 0^+} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, F(\omega) \\ &= \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\, \frac{e^{-i\omega t}}{\omega - (E_{\mathrm{res}} + i\mathrm{Im}[\Sigma])/\hbar} \\ &= \exp\left(-\frac{iE_{\mathrm{res}}t}{\hbar}\right)\, \exp\left(-\frac{|\mathrm{Im}[\Sigma]|}{\hbar}\, t\right).\end{aligned} \tag{2.32}$$

In deriving the last line, we performed a contour integration assuming that $\mathrm{Im}[\Sigma] < 0$; this assumption will be proven shortly. The final result is

$$P(t) = e^{-\kappa t}, \quad \text{where } \kappa = \frac{2|\mathrm{Im}[\Sigma]|}{\hbar}. \tag{2.33}$$

Let us now take a closer look at the self-energy Σ, which was defined in Eq. (2.21):

$$\Sigma(E) \equiv \lim_{\varepsilon\rightarrow 0^+} \sum_k \frac{|\langle\psi_k|\hat{V}_1|\varphi\rangle|^2}{E - E_k + i\varepsilon}, \tag{2.34}$$

where $|\varphi\rangle$ and $\{|\psi_k\rangle\}$ are the bound and free states of the model in the absence of $\hat{V}_1$, and E_k is the energy of the k-th free state. We can calculate the imaginary part as follows:

$$\begin{aligned}\mathrm{Im}\big[\Sigma(E)\big] &= \lim_{\varepsilon\rightarrow 0^+} \sum_k \left|\langle\psi_k|\hat{V}_1|\varphi\rangle\right|^2 \mathrm{Im}\left(\frac{1}{E - E_k + i\varepsilon}\right) \\ &= -\sum_k \left|\langle\psi_k|\hat{V}_1|\varphi\rangle\right|^2 \left[\lim_{\varepsilon\rightarrow 0^+} \frac{\varepsilon}{(E - E_k)^2 + \varepsilon^2}\right].\end{aligned} \tag{2.35}$$

The quantity in the square brackets is a Lorentzian function, which is always positive. Hence, $\mathrm{Im}(\Sigma) < 0$, as previously asserted. The Lorentzian function has the limiting form

$$\lim_{\varepsilon\rightarrow 0^+} \frac{\varepsilon}{x^2 + \varepsilon^2} = \pi\delta(x). \tag{2.36}$$

This is because the Lorentzian gets sharper as $\varepsilon \rightarrow 0^+$, but the area under it is π. Hence,

$$\mathrm{Im}\big[\Sigma(E)\big] = -\pi \sum_k \left|\langle\psi_k|\hat{V}_1|\varphi\rangle\right|^2 \delta(E - E_k). \tag{2.37}$$

Due to the delta function, non-vanishing contributions come only from values of k such that $E = E_k$. We can use this fact to further simplify the result. Consider the first term in the sum in Eq. (2.37), $\big|\langle\psi_k|\hat{V}_1|\varphi\rangle\big|^2$. It is k-dependent, but we can let

$$\overline{\big|\langle\psi_{k(E)}|\hat{V}_1|\varphi\rangle\big|^2}$$

denote its average value over the values of k for which $E = E_k$. Then we can approximate Eq. (2.37) by pulling that term out of the sum:

$$\mathrm{Im}\big[\Sigma(E)\big] \approx -\pi\, \overline{\big|\langle\psi_{k(E)}|\hat{V}_1|\varphi\rangle\big|^2} \left(\sum_k \delta(E - E_k)\right). \tag{2.38}$$

Hence, the quasi-bound state's decay rate is

$$\kappa \approx \frac{2\pi}{\hbar} \big|W(E_{\mathrm{res}})\big|^2 \rho(E_{\mathrm{res}}), \quad \text{where} \quad \left\{\begin{aligned} \big|W(E)\big|^2 &= \overline{\big|\langle\psi_{k(E)}|\hat{V}_1|\varphi\rangle\big|^2} \\ \rho(E) &= \sum_k \delta(E - E_k). \end{aligned}\right. \tag{2.39}$$

This result is called **Fermi's golden rule**. It states that the decay rate of a quasi-bound state is directly proportional to two factors. The first factor, $|W(E_{\mathrm{res}})|^2$, describes the strength of the coupling between the quasi-bound state and the free states. It is computed from $\langle\psi_k|\hat{V}_1|\varphi\rangle$, which called the **transition amplitude**, using free states meeting the resonance condition $E_k = E_{\mathrm{res}}$; the stronger the coupling, the faster the decay. The second factor, $\rho(E_{\mathrm{res}})$, is the number of free states per unit energy at energy E_{res}; the more free states available, the faster the decay.

Often, these two factors are estimated using further approximations. One common trick is to treat the free states as plane waves (we will see an example in the next section).

When using plane waves to approximate $\{|\psi_k\rangle\}$, the k labels are d-dimensional wave-vectors. In this case, it is convenient to amend Eq. (2.39) to treat k-space as a continuum, following the procedure discussed in Section II of the previous chapter: we introduce a k-space discretization $dk = 2\pi/L$, where L is the system size in each direction; then, as $L \to \infty$, the discrete sum $\sum_k$ appearing in the definition $\rho(E)$ in Eq. (2.39) can be turned into an integral. In place of $\rho(E)$, we can define the **density of states**

$$\mathcal{D}(E) = \int \frac{d^dk}{(2\pi)^d}\, \delta(E - E_k), \tag{2.40}$$

which counts the number of free states with energy E per unit energy and per unit volume.

After converting the sum to an integral, there is an inverse factor $\big[d^dk/(2\pi)^d\big]^{-1} = L^d$ left over, which has to be grouped with the $|W|^2$ term in Eq. (2.39). At the same time, we have to re-normalize the free states in the definition of $|W|^2$. If we follow the delta normalization convention discussed in Section II of the previous chapter,

$$|\psi_k\rangle^{(\mathrm{new})} = \left(\frac{L}{2\pi}\right)^{d/2} |\psi_k\rangle^{(\mathrm{old})}, \tag{2.41}$$

then Fermi's golden rule is re-expressed as

$$\kappa \approx \frac{2\pi}{\hbar}\,\big|\mathcal{W}(E_{\text{res}})\big|^2\,\mathcal{D}(E_{\text{res}}), \quad \text{where} \quad \begin{cases} \big|\mathcal{W}(E)\big|^2 = (2\pi)^d\,\overline{\big|\langle\psi_{k(E)}|\hat{V}_1|\varphi\rangle\big|^2} \\ \mathcal{D}(E) = \displaystyle\int \frac{d^dk}{(2\pi)^d}\,\delta(E-E_k). \end{cases} \tag{2.42}$$

V. FERMI'S GOLDEN RULE IN A 1D MODEL

Let us apply Fermi's golden rule to the simple 1D model of Section II. The potential is

$$V(x) = V_0(x) + V_1(x), \quad \text{where} \quad \begin{cases} V_0(x) = -U\,\Theta(a-|x|) \\ V_1(x) = \quad V_b\,\Theta(b-|x|) \\ \qquad 0 < U < V_b. \end{cases} \tag{2.43}$$

The finite square well $V_0(x)$ supports one or more bound states; for simplicity, we focus on the ground state, whose energy is denoted by E_0 (where $-U < E_0 < 0$). Its wavefunction is

$$\varphi(x) = \begin{cases} \mathcal{A}\,\cos(qx), & |x| < a \\ \mathcal{B}\,\exp\left(-\eta|x|\right), & |x| \geq a, \end{cases} \tag{2.44}$$

where $\mathcal{A}$ and $\mathcal{B}$ are constants to be determined, and

$$q = \sqrt{\frac{2m}{\hbar^2}(E_0+U)}, \quad \eta = \sqrt{\frac{2m}{\hbar^2}|E_0|}. \tag{2.45}$$

By matching $\varphi(x)$ and $d\varphi/dx$ across the $x = a$ interface, we can derive E_0, $\mathcal{A}$, and $\mathcal{B}$. The details are left as an exercise.

Once we have obtained $\varphi(x)$, we want to use it to find the transition amplitude $\langle\psi_k|\hat{V}_1|\varphi\rangle$, where $\psi_k(x)$ is a "representative" free eigenstate of $V_0(x)$ that the quasi-bound state decays to. We can estimate this with a series of tricks. First,

$$\langle\psi_k|\hat{V}_1|\varphi\rangle \;=\; \int_{-\infty}^{\infty} dx\,\psi_k^*(x)\,V_1(x)\,\varphi(x) \;=\; V_b\int_{-b}^{b} dx\;\psi_k^*(x)\,\varphi(x). \tag{2.46}$$

Next, because $\psi_k(x)$ and $\varphi(x)$ are orthogonal,

$$\int_{-\infty}^{\infty} dx\;\psi_k^*(x)\,\varphi(x) = 0 \quad \Rightarrow \quad \int_{-b}^{b} dx\;\psi_k^*(x)\,\varphi(x) = -\int_{|x|>b} dx\;\psi_k^*(x)\,\varphi(x). \tag{2.47}$$

The integral breaks into two pieces, which can be interpreted as the contribution from the quasi-bound state escaping to the left or to the right. We assume these contribute equally to the escape probability, so that

$$\big|\langle\psi_k|\hat{V}_1|\varphi\rangle\big|^2 \;\approx\; 2V_b^2\,\left|\int_b^{\infty} dx\;\psi_k^*(x)\,\varphi(x)\right|^2. \tag{2.48}$$

Outside the scatterer ($x > b$), the escaping free state can be approximated as an outgoing plane wave, with the delta-normalized form

$$\psi_k(x) \approx \frac{e^{ikx}}{\sqrt{2\pi}}, \tag{2.49}$$

where k is chosen such that

$$E_k = E_{\text{res}} \approx E_0 + V_b \quad \Rightarrow \quad k \approx \sqrt{\frac{2m}{\hbar^2}(E_0 + V_b)}. \tag{2.50}$$

Plugging Eqs. (2.44) and (2.49) into Eq. (2.48), and solving the integral, gives

$$\left|\langle\psi_k|\hat{V}_1|\varphi\rangle\right|^2 \approx \frac{1}{\pi} V_b^2 \mathcal{B}^2 \frac{e^{-2\eta b}}{k^2 + \eta^2}. \tag{2.51}$$

The other quantity we need for Fermi's golden rule is the density of free states. This can be found by taking $E_k \approx \hbar^2 k^2/2m$, and performing a change of variables:

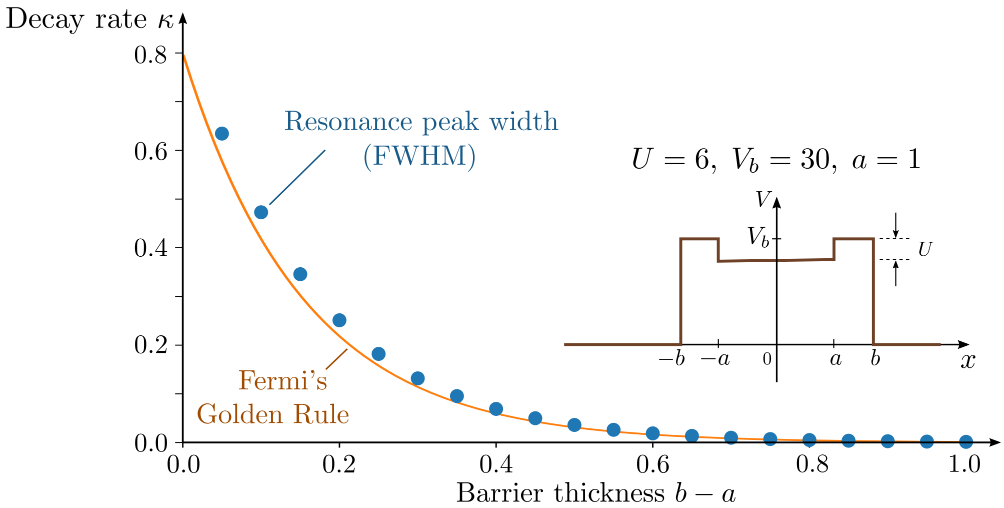
$$\mathcal{D}(E) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, \delta\left(E - \frac{\hbar^2 k^2}{2m}\right) \tag{2.52}$$

$$= 2 \cdot \frac{1}{2\pi} \int_0^{\infty} dE' \,\frac{dk}{dE'}\, \delta(E - E') \tag{2.53}$$

$$= \sqrt{\frac{m}{2\pi^2\hbar^2 E}}. \tag{2.54}$$

In Eq. (2.53), the factor of 2 accounts for the fact that for each E, both positive and negative k contribute to the density of states.

We can now plug Eqs. (2.51) and (2.54) into Fermi's golden rule, Eq. (2.42). In the figure below, the orange curve shows how the resulting decay rate, κ, varies with the barrier thickness $b - a$, with the other model parameters fixed at $U = 6$, $V_b = 30$, and $a = 1$:



For comparison, the blue dots show the values of κ taken from the width of the resonant scattering peak (see Section III). For this calculation, we use the transfer matrix method to compute the E-dependent transmittance for particles incident on one side of the scatterer (see Appendix B), and numerically extract the full-width at half-maximum (FWHM) for the peak near E_{res}.

Evidently, Fermi's golden rule (the orange curve) gives a very good estimate for the true decay rate based on the scattering peak width (the blue dots). The agreement is not exact, but after all the Fermi's golden rule result is based on a series of approximations, including the various assumptions in the derivation of Fermi's golden rule (discussed in Sections III and IV), as well as the approximations used in applying Fermi's golden rule (e.g., using plane waves to calculate the transition amplitude and density of states).

In this simple 1D example, it takes more or less the same amount of effort to estimate the decay rate from Fermi's golden rule or calculate it exactly. However, in other situations, such as higher-dimensional systems, the true decay rate may be very hard to compute, and Fermi's golden rule becomes valuable since it is both accurate and easy to calculate.

Exercises

1. Use the variational theorem to prove that a 1D potential well has at least one bound state. Assume that the potential $V(x)$ satisfies (i) $V(x) < 0$ for all x, and (ii) $V(x) \to 0$ for $x \to \pm\infty$. The Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x). \tag{2.55}$$

Consider a (real) trial wavefunction

$$\psi(x;\gamma) = \left(\frac{2\gamma}{\pi}\right)^{1/4} e^{-\gamma x^2}. \tag{2.56}$$

Note that this can be shown to be normalized to unity, using Gauss' integral

$$\int_{-\infty}^{\infty} dx\; e^{-2\gamma x^2} = \sqrt{\frac{\pi}{2\gamma}}. \tag{2.57}$$

Now prove that

$$\begin{aligned}\langle E\rangle &= \int_{-\infty}^{\infty} dx\; \psi(x)\,\hat{H}\,\psi(x) \\ &= \frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx\,\left(\frac{d\psi}{dx}\right)^2 + \int_{-\infty}^{\infty} dx\; V(x)\,\psi^2(x) \\ &= A\sqrt{\gamma}\left[\sqrt{\gamma} + B\int_{-\infty}^{\infty} dx\; V(x)\, e^{-\gamma x^2}\right],\end{aligned} \tag{2.58}$$

where A and B are positive real constants to be determined. By looking at the quantity in square brackets in the limit $\gamma \to 0$, argue that $\langle E\rangle < 0$ in this limit. Hence, explain why this implies the existence of a bound state.

Finally, try generalizing this approach to the case of a 2D radially-symmetric potential well $V(x, y) = V(r)$, where $r = \sqrt{x^2 + y^2}$. Identify which part of the argument fails in 2D. [For a discussion of certain 2D potential wells that *do* always support bounds states, similar to 1D potential wells, see Ref. [4].]

2. In this problem, you will investigate the existence of bound states in a 3D potential well that is finite, uniform, and spherically-symmetric. The potential function is

$$V(r,\theta,\phi) = -U\Theta(a-r), \tag{2.59}$$

where a is the radius of the spherical well, U is the depth, and (r,θ,ϕ) are spherical coordinates defined in the usual way.

The solution involves a variant of the partial wave analysis discussed in Appendix A. For $E < 0$, the Schrödinger equation reduces to

$$\begin{cases} \Big(\nabla^2 + q^2\Big)\psi(r,\theta,\phi) = 0 \;\; \text{where} \;\; q = \sqrt{2m(E+U)/\hbar^2}, & \text{for } r \le a \\ \Big(\nabla^2 - \gamma^2\Big)\psi(r,\theta,\phi) = 0 \;\; \text{where} \;\; \gamma = \sqrt{-2mE/\hbar^2}, & \text{for } r \ge a. \end{cases} \tag{2.60}$$

For the first equation (called the Helmholtz equation), we seek solutions of the form

$$\psi(r,\theta,\phi) = f(r)\, Y_{\ell m}(\theta,\phi), \tag{2.61}$$

where $Y_{\ell m}(\theta,\phi)$ are spherical harmonics, and the integers l and m are angular momentum quantum numbers satisfying $l \ge 0$ and $-l \le m \le l$. Substituting into the Helmholtz equation yields

$$r^2 \frac{d^2 f}{dr^2} + 2r\frac{df}{dr} + \big[q^2 r^2 - l(l+1)\big]\, f(r) = 0, \tag{2.62}$$

which is the **spherical Bessel equation**. The solutions to this equation that are non-divergent at $r = 0$ are $f(r) = j_\ell(qr)$, where j_ℓ is called a **spherical Bessel function of the first kind**. Most numerical packages provide functions to calculate these (e.g., `scipy.special.spherical_jn` in Scientific Python).

Similarly, solutions for the second equation can be written as $\psi(r,\theta,\phi) = g(r)\, Y_{\ell m}(\theta,\phi)$, yielding an equation for $g(r)$ called the **modified spherical Bessel equation**. The solutions which do not diverge as $r \to \infty$ are $g(r) = k_\ell(\gamma r)$, where k_ℓ is called a **modified spherical Bessel function of the second kind**. Again, this can be computed numerically (e.g., using `scipy.special.spherical_kn` in Scientific Python).

Using the above facts, show that the condition for a bound state to exist is

$$\frac{q j_\ell'(qa)}{j_\ell(qa)} = \frac{\gamma k_\ell'(\gamma a)}{k_\ell(\gamma a)}, \tag{2.63}$$

where j_ℓ' and k_ℓ' denote the derivatives of the relevant special functions, and q and γ depend on E and U as described above. Write a program to search for the bound state energies at any given a and U, and hence determine the conditions under which the potential does not support bound states.

3. In this problem, we will find the quasi-bound and free states for the model discussed in Section V, and use it to calculate the decay rate according to Fermi's golden rule.

Let $\varphi(x)$ be the bound state of a square well of width $2a$ and depth U, and let E_0 be the energy. This state satisfies the 1D time-independent Schrödinger wave equation,

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\varphi(x) = E_0\,\varphi(x), \tag{2.64}$$

where

$$V(x) = V_0(x) + V_1(x), \quad \text{where} \quad \begin{cases} V_0(x) = -U\,\Theta(a - |x|) \\ V_1(x) = \;\; V_b\,\Theta(b - |x|) \\ \quad 0 < U < V_b. \end{cases} \tag{2.65}$$

Take the ansatz

$$\varphi(x) = \begin{cases} \mathcal{A}\,\cos(qx), & |x| < a \\ \mathcal{B}\,\exp\left(-\eta|x|\right), & |x| \geq a. \end{cases} \tag{2.66}$$

(a) Using Eqs. (2.64)–(2.66), and the fact that both $\varphi(x)$ and $d\varphi/dx$ are continuous at $x = \pm a$, prove that E_0 can be obtained by solving the transcendental equation

$$q\tan(qa) = \eta, \quad \text{where} \quad \begin{cases} q = \sqrt{\dfrac{2m}{\hbar^2}(E_0 + U)} \\ \eta = \sqrt{\dfrac{2m}{\hbar^2}|E_0|}. \end{cases} \tag{2.67}$$

(b) By using the fact that $\varphi(x)$ is normalized to unity, prove that

$$\mathcal{B}^2 = \frac{\exp\left(2\eta a\right)}{a}\left[\frac{1 + \sin(2qa)/2qa}{\cos^2(qa)} + \frac{1}{\eta a}\right]^{-1}. \tag{2.68}$$

(c) Write a program to compute the decay rate based on Fermi's golden rule, by combining Eqs. (2.42), (2.51), (2.54), (2.67), and (2.68). Hence, reproduce the plot shown in Section V.

(d) Write a program to extract the decay rate from the width of the transmission peak, using the transfer matrix method (see Appendix B). Hence, investigate the accuracy of the Fermi's golden rule result for different values of U, V_b, and the other model parameters.

Further Reading

[1] Bransden & Joachain, §4.4, 9.2–9.3, 13.4

[2] Sakurai, §5.6, 7.7–7.8

[3] R. Courant and D. Hilbert, *Methods of Mathematical Physics* vol. 1, Interscience (1953). [link]

[4] B. Simon, *The bound state of weakly coupled Schrödinger operators in one and two dimensions*, Annals of Physics **97**, 279 (1976). [link]