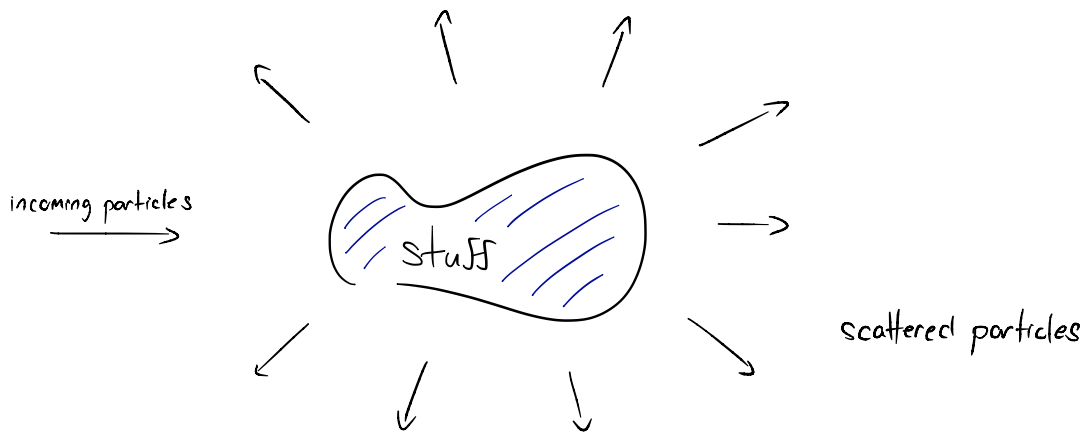
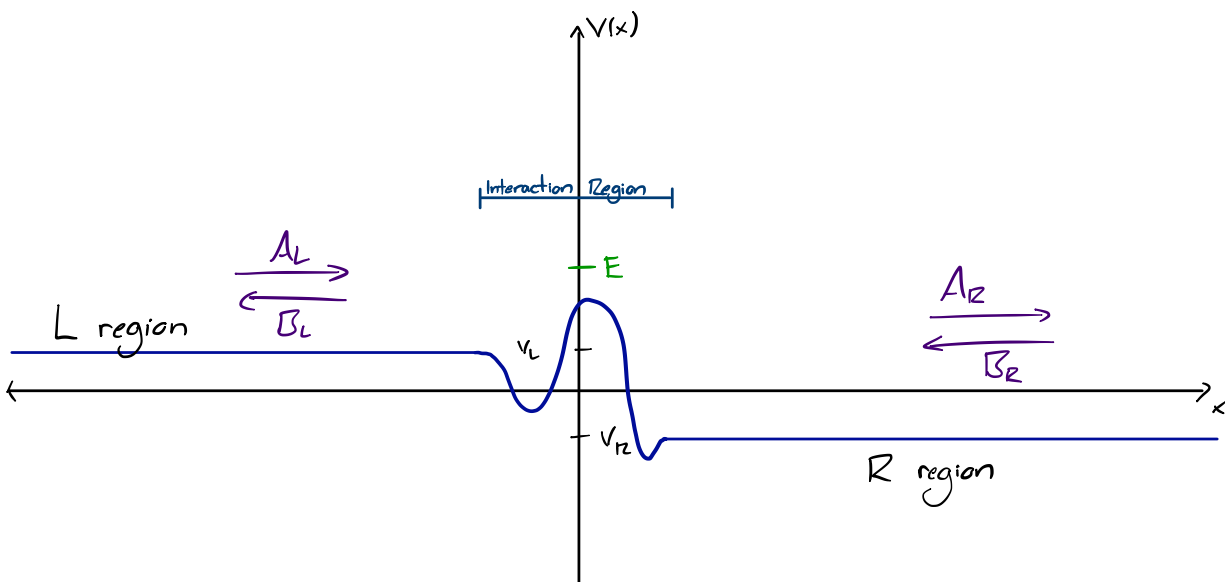


We mainly applied the WKB approximation to study stationary **bound states** of a particle subjected to some potential. There is another class of problems where some of our approximation methods can be brought to bear. These are "scattering" problems.



In general, want to fix momentum of incoming particles and predict probability to be scattered in some particular direction. When particle energy is conserved, this is **elastic scattering**.

We will consider the (somewhat artificial) 1-dimensional case. A more involved analysis is necessary in 2d or 3d, where angular dependence will be an important subject, adding a lot of complication.



We study this set-up using **non-normalizable, stationary states** (often called "scattering states"). There is a nice interpretation of this approach, but it's a little complicated to show that it is valid.

The time-independent Schrödinger equation has solutions in L & R regions given by plane waves:

$$\Psi_L(x) = A_L e^{\frac{i p_L x}{\hbar}} + B_L e^{-\frac{i p_L x}{\hbar}} \quad \text{with} \quad \frac{p_L^2}{2m} = E - V_L$$

$$\Psi_R(x) = A_R e^{\frac{i p_R x}{\hbar}} + B_R e^{-\frac{i p_R x}{\hbar}} \quad \text{with} \quad \frac{p_R^2}{2m} = E - V_R$$

Solving in the interaction region will give a relation b/w (A_L, A_R) and (B_L, B_R) . (Necessarily a linear relation that is a function of the energy, E .)

Our interpretation of this solution utilizes the probability current and density, and conservation equation

$$\left. \begin{aligned} \triangleright j &= \frac{\hbar}{2mi} (\bar{\Psi} \partial_x \Psi - \Psi \partial_x \bar{\Psi}) \\ \triangleright \rho &= |\Psi|^2 \end{aligned} \right\} \partial_x j + \partial_t \rho = 0 \Rightarrow \partial_x j = 0 \text{ in stationary states.}$$

In plane wave, $Ae^{\frac{i}{\hbar} p x} \rightarrow j = |A|^2 \cdot \frac{p}{m} = |A|^2 \cdot (\text{velocity})$. We interpret this as the flow rate of a beam of particles past a point x . Then the continuity equation says:

$$\frac{p_L}{m} (|A_L|^2 - |B_L|^2) = \frac{p_R}{m} (|A_R|^2 - |B_R|^2) \iff \underbrace{\frac{p_L}{m} |A_L|^2}_{\text{flow rate in}} + \underbrace{\frac{p_R}{m} |B_R|^2}_{\text{flow rate out}} = \frac{p_L}{m} |B_L|^2 + \frac{p_R}{m} |A_R|^2$$

If we specialize to a localized potential (so $V_L = V_R$) we have $p_L = p_R$, so the simpler relation

$$|A_L|^2 + |B_R|^2 = |A_R|^2 + |B_L|^2$$

Now we have a linear relation b/w (A_L, B_L) and (A_R, B_R) , and by continuity condition this can't be $A_R = B_L, A_L = B_R$. Consequently, there will be a linear relation b/w (A_L, B_R) and (A_R, B_L) :

$$\text{"out states"} \begin{pmatrix} A_R \\ B_L \end{pmatrix} = \underset{\substack{\uparrow \\ 2 \times 2 \text{ matrix}}}{S} \begin{pmatrix} A_L \\ B_R \end{pmatrix} \text{"in states"}$$

The conservation condition tells us that S is norm-preserving, so S is unitary. ($S^* = S^{-1}$). This is crucial for the interpretation as a kind of asymptotic time evolution (which is made more precise using the so-called "interaction picture").

A case of special interest is $B_R = 0$ (or $A_L = 0$), so particle(s) incident from one side. Say $B_R = 0$, then

$$A_L \rightarrow (B_L, A_R)$$

Def. The reflection and transmission coefficients are defined as (doesn't require $V_L = V_R$)

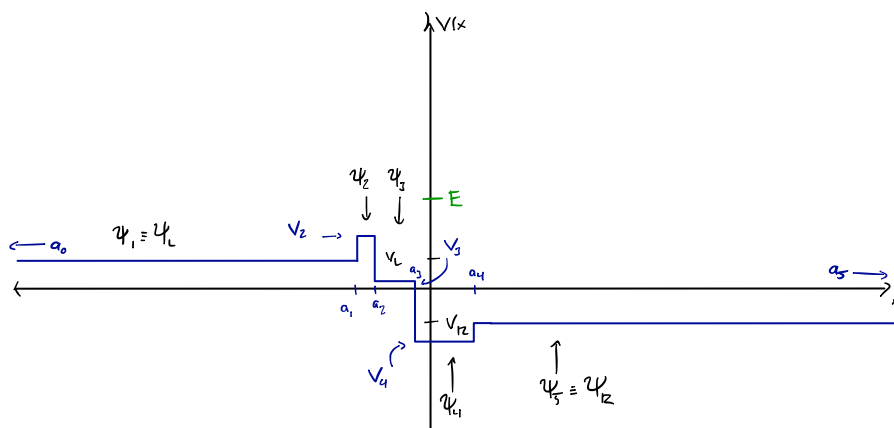
$$\triangleright R = \frac{|B_L|^2}{|A_L|^2} \quad \triangleright T = \frac{|A_R|^2}{|A_L|^2} \quad (\text{or } \frac{p_R |A_R|^2}{p_L |A_L|^2} \text{ if } V_L \neq V_R)$$

Conservation equation implies $R + T = 1$. (R is "percent particles reflected", T is "percent particles transmitted".) For potential scattering with an S -matrix

$$S = \begin{pmatrix} S_{++} & S_{-+} \\ S_{+-} & S_{--} \end{pmatrix} \rightarrow T = |S_{++}|^2 \quad R = |S_{-+}|^2$$

Similarly, $|S_{--}|^2$ and $|S_{+-}|^2$ are transmission and reflection coefficients for right-to-left scattering.

A completely solvable class of examples are step function potentials.



$V(x) = V_i \in \mathbb{R}$, $x \in (a_{i-1}, a_i)$ with $a_0 = -\infty$, $a_n = +\infty$; $V_1 = V_L$, $V_2 = V_R$. In each interval we have plane wave solutions:

$$\psi_j = A_j e^{ik_j x} + B_j e^{-ik_j x}, \quad \frac{\hbar^2 k_j^2}{2m} = E - V_j \quad \text{in } [a_{j-1}, a_j]$$

Then the coefficients are related by $\psi_j(a_j) = \psi_{j+1}(a_j)$, $\psi_j'(a_j) = \psi_{j+1}'(a_j)$. This is a linear relation for the (A_j, B_j) , so we will have

$$\begin{pmatrix} A_j \\ B_j \end{pmatrix} = M_j \begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix}$$

To relate $(A_L, B_L) = (A_1, B_1)$ to $(A_R, B_R) = (A_n, B_n)$ we just have to compose these matrices.

$$\begin{pmatrix} A_L \\ B_L \end{pmatrix} = M_1 M_2 \cdots M_{n-1} \begin{pmatrix} A_R \\ B_R \end{pmatrix}$$

We can then reconstruct the S -matrix if we so desire. Let $M = M_1 M_2 \cdots M_{n-1} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$. Then you can quickly check that we have:

$$S = \begin{pmatrix} \frac{1}{M_{11}} & -\frac{M_{12}}{M_{11}} \\ \frac{M_{21}}{M_{11}} & \frac{\det(M)}{M_{11}} \end{pmatrix}$$

So as a practical matter, to understand scattering from step-function potentials the necessary input is the matrix M_i . This can be recovered by direct calculation:

$$\psi_j(a) = \psi_{j+1}(a) \rightarrow A_j e^{ik_j a_j} + B_j e^{-ik_j a_j} = A_{j+1} e^{ik_{j+1} a_j} + B_{j+1} e^{-ik_{j+1} a_j}$$

$$\psi_j'(a) = \psi_{j+1}'(a) \rightarrow k_j (A_j e^{ik_j a_j} - B_j e^{-ik_j a_j}) = k_{j+1} (A_{j+1} e^{ik_{j+1} a_j} - B_{j+1} e^{-ik_{j+1} a_j})$$

Solving, we find:

$$M_j = \frac{1}{2k_j} \begin{pmatrix} s_j e^{-id_j a_j} & d_j e^{-is_j a_j} \\ d_j e^{is_j a_j} & s_j e^{id_j a_j} \end{pmatrix} \quad \text{with } s_j = k_j + k_{j+1}, \quad d_j = k_j - k_{j+1}$$

We've been assuming $E > V_j$ for each j , so in all intervals plane waves are the appropriate solutions. But we can accommodate classically forbidden intervals by a simple substitution:

▷ if $E < V_j$ for some j , define $\frac{\hbar^2 \ell_j^2}{2m} = (V_j - E)$ and let $K_j = -i\ell_j$.

We adopt a convention that $\ell_j \geq 0$, so:

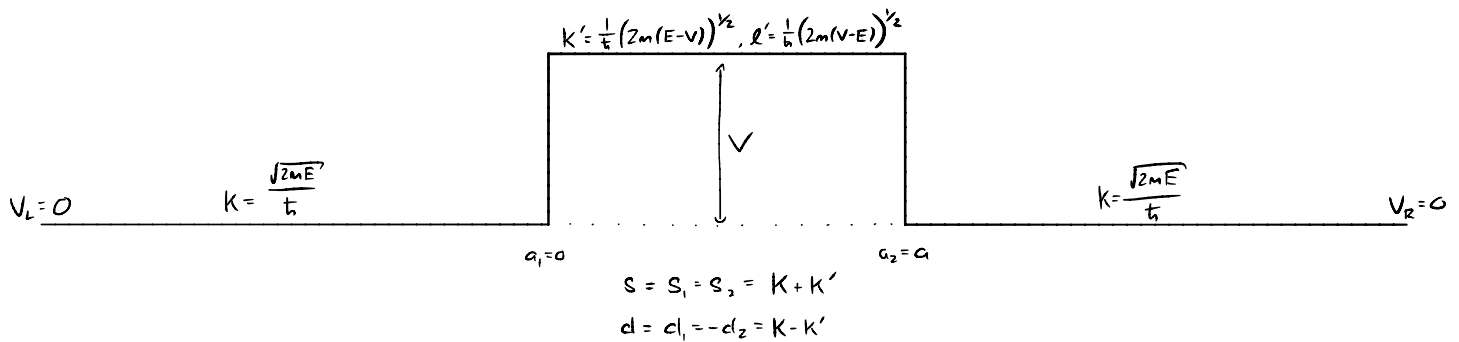
▷ $e^{iK_j x} = e^{\ell_j x}$: right-moving $\longleftrightarrow$ exponentially growing

▷ $e^{-iK_j x} = e^{-\ell_j x}$: left-moving $\longleftrightarrow$ exponentially falling

All manipulations hold identically, so M_j takes the same form with this replacement.

Let's see the "basic" examples:

I: single barrier, $V_L = V_R = 0$, $a_1 = 0$, $a_2 = a$ ($n=3$):



$$\left. \begin{aligned} M_1 &= \frac{1}{2K} \begin{pmatrix} s & d \\ d & s \end{pmatrix} \\ M_2 &= \frac{1}{2K'} \begin{pmatrix} s e^{i d a} & -d e^{-i s a} \\ -d e^{i s a} & s e^{-i d a} \end{pmatrix} \end{aligned} \right\} M = M_1 M_2 = \frac{1}{4KK'} \begin{pmatrix} s^2 e^{i d a} - d^2 e^{i s a} & s d (e^{-i d a} - e^{-i s a}) \\ s d (e^{i d a} - e^{i s a}) & s^2 e^{-i d a} - d^2 e^{-i s a} \end{pmatrix}$$

$$M_{11} = \frac{s^2 e^{i d a} - d^2 e^{i s a}}{(s^2 - d^2)} = e^{i K a} \left[\frac{-(K'^2 - K'^2)(2i \sin(K'a)) + 2KK'(\cos(K'a))}{4KK'} \right] \rightarrow |M_{11}|^2 = \frac{(K'^2 - K'^2)^2 \sin^2(K'a) + 4K'^2 \cos^2(K'a)}{4K'^2 K'^2}$$

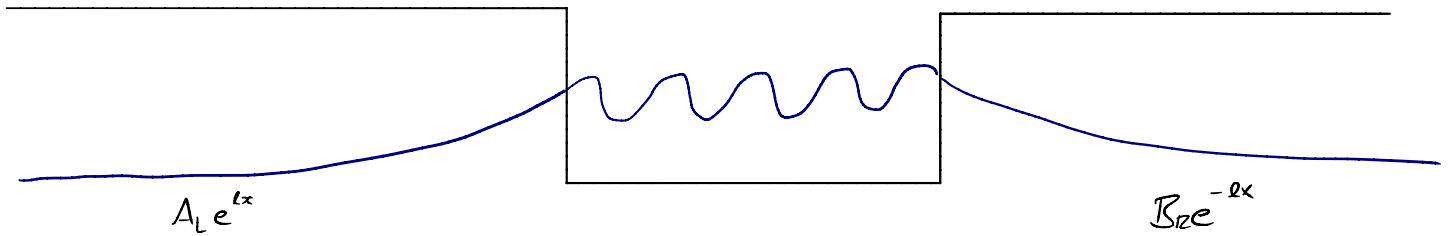
$$M_{21} = \frac{s d (e^{i d a} - e^{i s a})}{(s^2 - d^2)} = e^{i K a} \left[\frac{(K^2 - K'^2)(-2i \sin(K'a))}{4KK'} \right] \rightarrow |M_{21}|^2 = \frac{\sin^2(K'a) (K^2 - K'^2)^2}{4K^2 K'^2}$$

Combining: $T = \frac{1}{|M_{11}|^2} = \frac{4K^2 K'^2}{(K^2 - K'^2)^2 \sin^2(K'a) + 4K^2 K'^2 \cos^2(K'a)}$ & $R = \frac{|M_{21}|^2}{|M_{11}|^2} = \frac{(K^2 - K'^2)^2 \sin^2(K'a)}{(K^2 - K'^2)^2 \sin^2(K'a) + 4K^2 K'^2 \cos^2(K'a)}$, $T + R = 1$.

k and k' are implicitly functions of E , so this gives amplitudes for reflection and transmission as functions of E . When we take $E < V_0$, $k' \rightarrow i\ell'$ and we get the modification

$$T = \frac{1}{|M_{11}|^2} = \frac{4k^2\ell^2}{(k^2 - \ell^2)^2 \sinh^2(\ell a) + 4k^2\ell^2 \cosh^2(\ell a)} \quad \& \quad R = \frac{|M_{21}|^2}{|M_{11}|^2} = \frac{(k^2 - \ell^2)^2 \sinh^2(\ell a)}{(k^2 - \ell^2)^2 \sinh^2(\ell a) + 4k^2\ell^2 \cosh^2(\ell a)}, \quad T + R = 1.$$

Nonzero T in this range is "quantum tunnelling" through the barrier. Exponential suppression in T from the denominator. Further reducing $E < 0$, we can describe bound states for the case $V_0 < 0 < E$. Now we have $k \rightarrow -i\ell$ and $k' \in \mathbb{R}$.



Now if we look at the defining relation for the S -matrix, we see

$$S \begin{pmatrix} A_L \\ B_R \end{pmatrix} = \begin{pmatrix} A_R \\ B_L \end{pmatrix} \stackrel{!}{=} 0 \quad \text{for normalizable bound state.}$$

So zeroes of S -matrix at $k = -i\ell \in -i\mathbb{R}_{\geq 0}$ encode bound states of the potential! (In our case, this requires $\det(S) = 0$, which is $\frac{M_{22}}{M_{11}} = 0$.) Similarly, if we set $k = i\ell \in i\mathbb{R}_{\geq 0}$, we will see bound states as **poles**.

$$\frac{M_{22}}{M_{11}} = \frac{s^2 e^{-ida} - d^2 e^{-isa}}{s^2 e^{ida} - d^2 e^{isa}} \xrightarrow{k=-i\ell} -e^{-2a\ell} \left\{ \frac{(k^2 - \ell^2) \sin(k'a) - 2k'\ell \cos(k'a)}{(k^2 - \ell^2) \sin(k'a) + 2k'\ell \cos(k'a)} \right\} = 0$$

This is a shadow of a very general phenomenon in quantum mechanical scattering theory, where analytic properties of scattering amplitudes encode a wealth of physical information. This is even more the case in relativistic scattering theory/QFT.