1D Scattering

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We begin with an incoming wave (from the left) which is incident on a 1D "step" potential, V_0, at $x \geq 0$. As long as the width of the step is $\ll \lambda$, then this is a good approximation. The situation is similar to the classical problem of reflection and refraction, and we take the incoming wave to be a Gaussian

$$\Psi_I(x,0) = \frac{1}{(\pi\Delta^2)^{1/4}} e^{ik_0(x+a)} e^{-(x+a)^2/2\Delta^2}$$

here $\langle x \rangle = -a$, $\langle p \rangle = \hbar k_0$, with the widths $\Delta x = \frac{\Delta}{\sqrt{2}}$, $\Delta p = \frac{\hbar}{\sqrt{2}\Delta}$.
In the case for large Δ, p is well defined and $\frac{\Delta p}{p} \ll 1$. Then $p = \hbar k_0$ and $E = \frac{\hbar^2 k_0^2}{2m}$.
We will examine the case where $E > V_0$. The packet hits the barrier at time $t \approx a/v = am/p_0$. We will look for the reflected wave (Ψ_R), the transmitted wave (Ψ_T), the reflection coefficient (R), and the transmition coefficient (T). The coefficients are given by

$$R = \int |\Psi_R|^2 \, dx \;\; as \;\; t \to \infty; T = 1 - R$$

We solve the plane wave solution through the following steps:
1) Find the normalized eigenfunctions of **H**
2) Find the overlap $\langle \Psi_E | \, \Psi_I \rangle$
3) Time propagate it $|\psi(t)\rangle = \sum_E e^{-iHt/\hbar} |\Psi_E\rangle \langle \Psi_E | \, \Psi_I \rangle$
4) Identify Ψ_R, Ψ_T, and find R and T

Normalized Eigenfunctions
In the region to the left

$$\Psi_E(x) = Ae^{ik_1 x} + Be^{-ik_1 x} \quad k_1 = \frac{\sqrt{2mE}}{\hbar}$$

and in the region to the right

$$\Psi_E(x) = Ce^{ik_2 x} + De^{-ik_2 x} \quad k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

We can set $D = 0$ since there is no wave on the right side of the potential barrier traveling left. Next we look at the boundary conditions

$$A + B = C \;\; continuity \; of \; the \; wave$$

$$ik_1(A - B) = ik_2 C \;\; continuity \; of \; the \; derivative$$

$$\therefore B = \frac{k_1 - k_2}{k_1 + k_2} A \quad C = \frac{2k_1}{k_1 + k_2} A$$

Checking our limits
1) $V_0 \to 0 \Rightarrow k_2 = k_1$, $B = 0$, and $C = 1$
2) $V_0 \to E \Rightarrow k_2 = 0$, $B = 1$, and $C = 2$
then the normalized eigenfunction is

$$\Psi_E(x) = \frac{1}{\sqrt{2\pi}} \left[\left(e^{ik_1 x} + \frac{B}{A} e^{-ik_1 x} \right) \Theta(-x) + \frac{C}{A} e^{ik_2 x} \Theta(x) \right]$$

Overlap
We now look at the overlap of the eigenfunction with our incoming wave function

$$a(k_1) = \langle \Psi_{k_1} | \, \Psi_I \rangle = \frac{1}{\sqrt{2\pi}} \left[\int_{-\infty}^{\infty} \left(e^{-ik_1 x} + \left(\frac{B}{A}\right)^* e^{ik_1 x} \right) \Theta(-x) \Psi_I(x) dx + \int_{-\infty}^{\infty} \left(\frac{C}{A}\right)^* e^{-ik_2 x} \Theta(x) \Psi_I(x) \right]$$

Now the beauty of using a Gaussian for the incoming wave is that $\Psi(x) = 0 \;\forall\; x > 0$, so the second term goes away. Also there's no momentum overlap $\Rightarrow \left(\frac{B}{A}\right)^* e^{ik_1 x} = 0$. The first term and $\Psi_I(x)$ will overlap only when they are within the Gaussian width. With this our overlap function becomes

$$a(k_1) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik_1 x} \frac{1}{(\pi\Delta^2)^{1/4}} e^{ik_0(x+a)} e^{-(x+a)^2/2\Delta^2} dx$$

we can solve this with a couple substitutions, $u = x + a$ $\alpha = 1/2\Delta^2$ $\beta = ik_0 - ik_1$

$$a(k_1) = \frac{1}{\sqrt{2\pi}} \frac{1}{(\pi\Delta^2)^{1/4}} \int_{-\infty}^{\infty} e^{ik_1 a} e^{\beta u - \alpha u^2} du$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{(\pi\Delta^2)^{1/4}} e^{ik_1 a} e^{\beta^2/4\alpha} \int_{-\infty}^{\infty} e^{-\alpha(x-\beta/2\alpha)^2} dx$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{(\pi\Delta^2)^{1/4}} e^{ik_1 a} e^{\beta^2/4\alpha} \sqrt{\frac{\pi}{\alpha}}$$

so our overlap function is

$$a(k_1) = \left(\frac{\Delta^2}{\pi}\right)^{1/4} e^{ik_1 a} e^{-(k_1-k_0)^2\Delta^2/2}$$

Time Propagation

We now apply time propagation to our overlap function to get

$$\Psi(x,t) = \int |\Psi_{k_1}\rangle \langle\Psi_{k_1}| e^{-iE_{k_1}t/\hbar} |\Psi_I\rangle \, dk_1 = \int_{-\infty}^{\infty} \Psi_{k_1} e^{-iE_{k_1}t/\hbar} a(k_1) dk_1$$

doing the full expansion gives

$$\Psi(x,t) = \left(\frac{\Delta^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\hbar^2 k_1^2 t/2m\hbar} e^{-(k_1-k_0)^2\Delta^2/2} e^{ik_1 a} \left[e^{ik_1 x}\Theta(-x) + \frac{B}{A} e^{-ik_1 x}\Theta(-x) + \frac{C}{A} e^{ik_2 x}\Theta(x) \right] dk_1$$

Finding Ψ_R, Ψ_T, R, and T

Finding the integral for the first term in the brackets, we realize that this is the original Gaussian evolved in time, except for the step function $\Theta(-x)$. From the first semester (see also Shankar), we know that a Gaussian wave package evolves by moving to the right with velocity $\hbar k_0/(2m)$ while broadening due to its momentum width $\Delta p = \frac{\hbar}{\sqrt{2}\Delta}$. Since $\Delta p << p$, we can assume that after sufficiently long time ($t \to \infty$), the wave packet is completely located on the r.h.s., at $x > 0$. After applying the factor $\Theta(-x)$, this means that this part of the integral simply disappears as $t \to \infty$: The incoming wave is "swallowed up" and replaced by the reflected and the transmitted wave.

For the second term we use the fact that $e^{-(k_1-k_0)^2\Delta^2/2}$ is sharply peaked at k_0. Then

$$\frac{\Delta p}{p} \ll 1 \;\Rightarrow\; \frac{\Delta k_0}{k_0} \ll 1 \;\Rightarrow\; \frac{B}{A} \approx \left.\frac{B}{A}\right|_{k_1=k_0} \equiv const.$$

Apart from this factor, the second term then describes a Gaussian wave package that starts on the r.h.s. at $x = a$ and travels to the *left* with momentum $-k_0$. This can be seen directly by replacing the integration variable k_1 with $-k_1$ everywhere which of course doesn't change the integral, which then reads

$$\Psi_{II}(x,t) = \frac{B}{A}\Theta(-x)\left(\frac{\Delta^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\hbar^2 k_1^2 t/2m\hbar} e^{-(k_1+k_0)^2\Delta^2/2} e^{ik_1(x-a)} dk_1 =: \Psi_R(x,t).$$

Since this Gaussian packet will move to more and more negative x with time, the Theta-function will equal to 1 and we simply have a left-moving packet representing the reflected wave.

Finding R,

$$\lim_{t\to\infty} R = \int |\Psi_R|^2 \, dx = \left|\frac{B}{A}\right|^2_{k_0} = \left(\frac{\sqrt{E_0} - \sqrt{E_0 - V_0}}{\sqrt{E_0} + \sqrt{E_0 - V_0}}\right)^2 = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

Remember that this is only a good approximation for a plane wave
Now for T

$$T = 1 - R = \left(\frac{C}{A}\right)^2\bigg|_{k_0} \sqrt{\frac{E_0 - V_0}{E_0}} = \frac{4\sqrt{E_0}\sqrt{E_0 - V_0}}{(\sqrt{E_0} + \sqrt{E_0 - V_0})^2} = \frac{4k_1^2}{(k_1 + k_2)^2}$$

Looking at the probability currents

$$j_I = |A_0|^2 \frac{\hbar k_0}{m}$$

$$j_R = |B_0|^2 \frac{\hbar k_0}{m}$$

$$j_T = |C_0|^2 \frac{\hbar k_0}{m}$$

$$R = \frac{j_R}{j_I} = \frac{|B_0|^2}{|A_0|^2}$$

$$T = \frac{j_T}{j_I} = \frac{|C_0|^2}{|A_0|^2}\frac{k_2}{k_0} = \frac{|C_0|^2}{|A_0|^2}\frac{\sqrt{E_0 - V_0}}{\sqrt{E_0}}$$

Remember that this was all for $E > V_0$. If $V_0 > E$, then we have the decaying exponential, $Ce^{-\kappa x}\Theta(x)$, which was looked at last semester for 1D potentials.