Lecture 16: Scattering States and the Step Potential

B. Zwiebach
April 19, 2016

Contents

1 The Step Potential

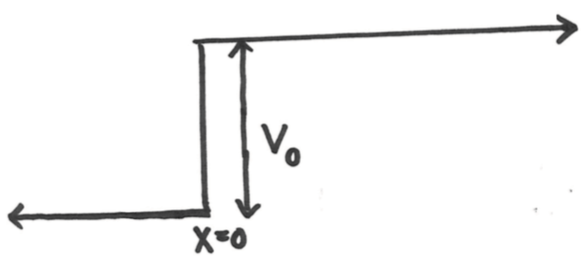

Figure 1: The step potential.

We now begin our detailed study of scattering states. These are un-normalizable energy eigenstates. They simply cannot be normalized, just like momentum eigenstates. These energy eigenstates are not states of particles, one must superpose scattering states to produce normalizable states that can represent a particle undergoing scattering in some potential. Here we examine the step potential (Figure 1), defined by

$$V(x) = \begin{cases} 0\,, & x < 0\,, \\ V_0\,, & x \geq 0\,. \end{cases} \tag{1.1}$$

Our solutions to the Schrödinger equation with this potential will be scattering states of definite energy E. We can consider two cases: $E > V_0$ and $E < V_0$. In both cases the wavefunction extends infinitely to the left and is non-normalizable. Let us begin with the case $E > V_0$.

2 Step Potential with $E > V_0$

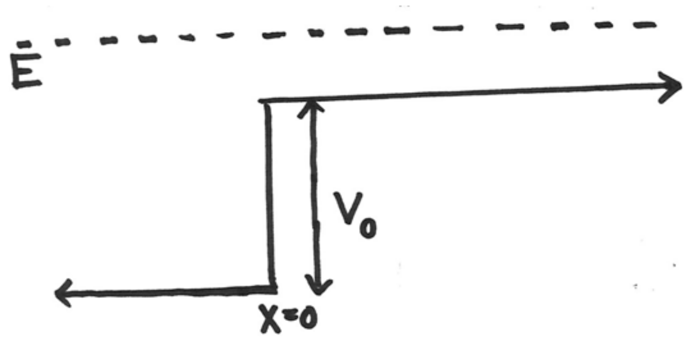

Figure 2: The energy E of the stationary state is greater than the step V_0. The full x axis is classically allowed.

The stationary state with energy E is of the form

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}, \tag{2.2}$$

and we will focus first on the unknown $\psi(x)$. In order to write a proper ansatz for $\psi(x)$ we visualize a physical process in which we have a wave incident on the step barrier from the left. Given such a wave traveling in the direction of increasing x, we would expect a reflected wave and a transmitted wave. The reflected wave, moving in the direction of decreasing x, would exist for $x < 0$. The transmitted wave, moving in the direction of increasing x, would exist for $x > 0$. The ansatz for the energy eigenstate must therefore contain all three pieces:

$$\psi(x) = \begin{array}{ll} Ae^{ikx} + Be^{-ikx} & x < 0\,, \\ Ce^{i\bar{k}x} & x > 0\,. \end{array} \tag{2.3}$$

Recall that e^{ikx}, with $k > 0$, represents a wave moving in the direction of increasing x, given the universal time dependence above. Therefore A is the coefficient of the incident wave, B is the coefficient of the reflected wave, and C is the coefficient of the transmitted wave. The waves for $x < 0$ have wavenumber k and the wave for $x > 0$ has wavenumber $\bar{k}$. These wavenumbers are fixed by the Schrödinger equation

$$k^2 = \frac{2mE}{\hbar^2}\,, \qquad \bar{k}^2 = \frac{2m(E-V_0)}{\hbar^2}\,. \tag{2.4}$$

There are two equations that constrain our coefficients A, B, and C: both the wavefunction and its derivative must be continuous at $x = 0$. With these two conditions we can solve for B and C in terms of A. This is all we could expect to do: because of linearity the overall scale of these three coefficients must remain undetermined. In fact, we can think of A as the input value and B and C as output values. Let us begin:

- $\psi(x)$ must be continuous at $x = 0$. Thus

$$A + B = C\,. \tag{2.5}$$

- $\psi'(x)$ must be continuous at $x = 0$. Thus

$$ikA - ikB = i\bar{k}C \quad \rightarrow \quad A - B = \frac{\bar{k}}{k}\,C\,. \tag{2.6}$$

Solving for B and C in terms of A, we get

$$\boxed{\frac{B}{A} = \frac{k-\bar{k}}{k+\bar{k}}, \qquad \frac{C}{A} = \frac{2k}{k+\bar{k}}.} \tag{2.7}$$

If A is real B and C are real. For $E = V_0$, we have $\bar{k} = 0$ and equations (2.7) give $B = A$ and $C = 2A$. Therefore, for $E = V_0$ the energy eigenstate is

$$E = V_0 : \qquad \psi(x) = \begin{cases} 2A\cos(kx) & x < 0\,, \\ 2A & x > 0\,, \end{cases} \tag{2.8}$$

and looks like this:

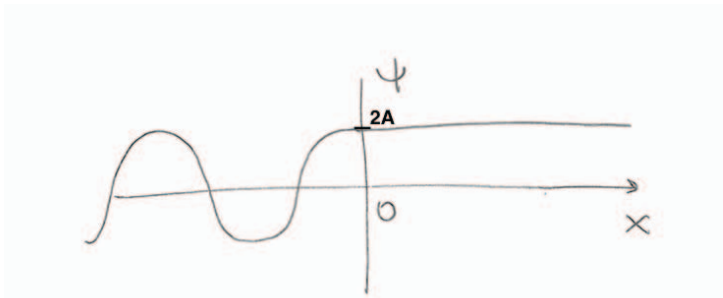

Figure 3: Energy eigenstate for $E = V_0$.

We get further insight into the solution by evaluating the probability current to the left and to the right of the $x = 0$ step. Recall the form of the probability current for a wavefunction ψ is

$$J = \frac{\hbar}{m}\text{Im}\left(\psi^* \frac{\partial \psi}{\partial x}\right) \tag{2.9}$$

A short calculation shows that the current J_L to the left of the step is

$$J_L = \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right) = J_A - J_B\,, \quad J_A = \frac{\hbar k}{m}|A|^2\,, \quad J_B = \frac{\hbar k}{m}|B|^2\,. \tag{2.10}$$

There is no interference arising from the incident and reflected waves. The total current to the left of the step is simply the current J_A associated with the incident wave minus the current J_B associated with the reflected wave. The current J_R to the right of the step is

$$j_R = \frac{\hbar\bar{k}}{m}\,|C|^2 \;=\; J_C\,. \tag{2.11}$$

In any stationary solution there cannot be accumulation of probability at any region of space because the probability density ρ is manifestly time-independent. While probability is continuously flowing in scattering solutions, it must be conserved. From the conservation equation $\frac{\partial J}{\partial x} + \frac{\partial \rho}{\partial t} = 0$, the time independence of ρ implies that the current J must be x-independent. In particular, our solution (2.7) must imply that $J_L = J_R$. Let us verify this:

$$\begin{aligned} J_L &= \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right) = \frac{\hbar k}{m}\left(1 - \left(\frac{k-\bar{k}}{k+\bar{k}}\right)^2\right)|A|^2 \\ &= \frac{\hbar k}{m}\left(\frac{4k\bar{k}}{(k+\bar{k})^2}\right)|A|^2 = \frac{\hbar\bar{k}}{m}\underbrace{\frac{4k^2}{(k+\bar{k})^2}|A|^2}_{|C|^2} \;=\; \hbar\bar{k}|C|^2 = J_R\,, \end{aligned} \tag{2.12}$$

as expected. The equality of J_L and J_R implies that

$$J_A - J_B = J_C \quad \rightarrow \quad J_A = J_B + J_C \quad \rightarrow \quad 1 = \frac{J_B}{J_A} + \frac{J_C}{J_A}\,. \tag{2.13}$$

We now define the *reflection coefficient* R to be the ratio of the probability flux in the reflected wave to the probability flux in the incoming wave:

$$\boxed{R \;\equiv\; \frac{J_B}{J_A} = \frac{|B|^2}{|A|^2} = \left(\frac{k-\bar{k}}{k+\bar{k}}\right)^2 \leq 1\,.} \tag{2.14}$$

This ratio happens to be the norm squared of the ratio B/A, and it is manifestly less than one, as it should be. We also define the *transmission coefficient* T to be the ratio of the probability flux in the transmitted wave to the probability flux in the incoming wave:

$$\boxed{T \;\equiv\; \frac{J_C}{J_A} = \frac{\bar{k}}{k}\frac{|C|^2}{|A|^2} = \frac{\bar{k}}{k}\frac{4k^2}{(k+\bar{k})^2} = \frac{4k\bar{k}}{(k+\bar{k})^2}\,.} \tag{2.15}$$

The above definitions are sensible because R and T, given in terms of current ratios, add up to one:

$$R + T \;=\; 1\,, \tag{2.16}$$

as follows by inspection of (2.13). Note that $T \neq \frac{|C|^2}{|A|^2}$ because of wavenumbers to the right and to the left of the step are not the same.

Recall that for $E = V_0$ we found $\bar{k} = 0$. In that case we have full reflection: $R = 1$ and $T = 0$. Indeed the probability current associated with the *constant* wavefunction that exists for $x > 0$ (see (2.8)) is zero. Additionally we can give an argument from continuity. The coefficients R and T must be continuous functions of the energy E. For $E < V_0$ we expect $T = 0$ since the forbidden region is all of $x > 0$ and an exponentially decaying wavefuntion cannot carry probability flux. If $T = 0$ for any $E < V_0$ it must still be zero for $E = V_0$, by continuity.

3 Step Potential with $E < V_0$

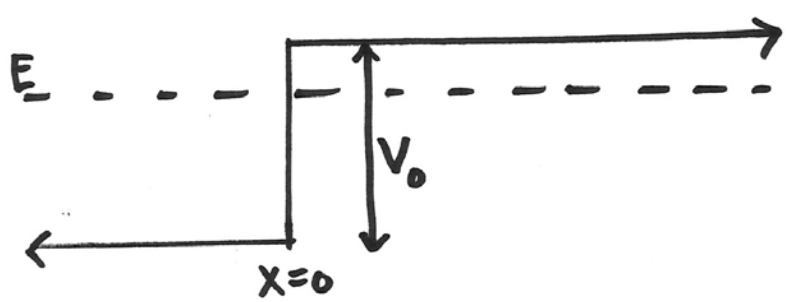

Figure 4: The step potential barrier.

When $E < V_0$ the region $x > 0$ is a classically forbidden region. Let us try to solve for the energy eigenstate without re-doing all the work involved in solving for B and C in terms of A. For this purpose we first note that the ansatz (2.3) for $x < 0$ can be left unchanged. On the other hand, for $x > 0$ the earlier solution

$$\psi(x) \;=\; Ce^{i\bar{k}x}\,, \qquad \bar{k}^2 \;=\; \frac{2m(E-V_0)}{\hbar^2}\,, \tag{3.17}$$

should become a decaying exponential

$$\psi(x) \; = \; Ce^{-\kappa x}\,, \qquad \kappa^2 \; = \; \frac{2m(V_0 - E)}{\hbar^2}\,. \tag{3.18}$$

We note that the former becomes the latter upon the replacement

$$\bar{k} \; \rightarrow \; i\,\kappa\,. \tag{3.19}$$

This means that we can simply perform this replacement in our earlier expressions for B/A and C/A and we obtain the new expressions. In particular from (2.7) we get

$$\frac{B}{A} = \frac{k - i\kappa}{k + i\kappa} \tag{3.20}$$

Therefore

$$\frac{B}{A} = \frac{i(k - i\kappa)}{i(k + i\kappa)} = -\frac{\kappa + ik}{\kappa - ik} \; = \; -\,e^{2i\delta(E)}\,, \tag{3.21}$$

with

$$\boxed{\delta(E) = \tan^{-1}\Big(\frac{k}{\kappa}\Big) = \tan^{-1}\Big(\sqrt{\frac{E}{V_0 - E}}\Big)\,.} \tag{3.22}$$

Since the magnitude of A is equal to the magnitude of B, we have $J_A = J_B$ and $J_C = 0$. Thus $T = 0$ and $R = 1$. As noted above, the ratio B/A is a pure phase. The phase of the numerator $\kappa + ik$ is $\delta(E)$ and the phase of the denominator $\kappa - ik$ is $-\delta(E)$, thus the total phase $2\delta(E)$ for the ratio. We did not absorb the minus sign into the phase; in this way $\delta(E) \to 0$ as $E \to 0$. Note that $\delta(E)$ is positive and does not exceed $\pi/2$. In fact a sketch of $\delta(E)$ is given in Figure 5.

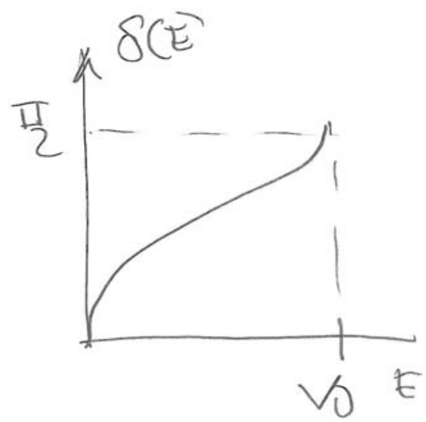

Figure 5: The phase $\delta(E)$ as a function of energy $E < V_0$.

The total wavefunction for $x < 0$ is interesting

$$\begin{aligned} \psi(x) \; &= \; Ae^{ikx} + (-Ae^{2i\delta(E)})e^{-ikx} \\ &= \; Ae^{i\delta(E)}\big(e^{-i\delta(E)}e^{ikx} - e^{i\delta(E)}e^{-ikx}\big) \\ &= \; 2iAe^{i\delta(E)}\sin(kx - \delta(E)) \end{aligned} \tag{3.23}$$

This means that the probability density is

$$|\psi|^2 \; = \; 4A^2\sin^2(kx - \delta(E))\,. \tag{3.24}$$

The point $x_0 > 0$ determined by the condition $kx_0 = \delta(E)$ is the point in the forbidden region where the extrapolation of the allowed-region solution would vanish. Of course in the forbidden region $x > 0$, the probability density $|\psi|^2$ is a decaying exponential.

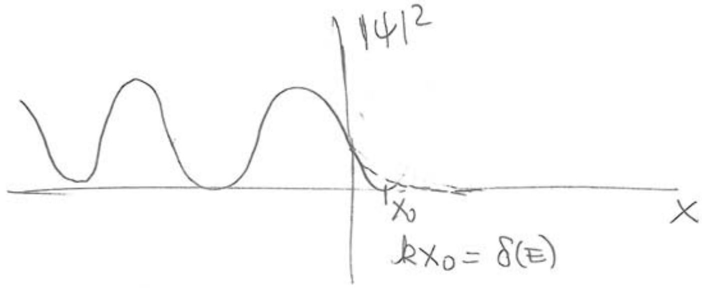

Figure 6: Norm squared for the energy eigenstate when $E < V_0$. For $x > 0$ the probability density decays exponentially with x. The point x_0 is the point where the extrapolation of the $x < 0$ probability density would have vanished.

For future use we record the derivative of the phase $\delta(E)$ with respect to the energy

$$\delta'(E) \equiv \frac{d\delta(E)}{dE} = \frac{1}{2}\sqrt{\frac{1}{E(V_0 - E)}}\,. \tag{3.25}$$

Note that this derivative becomes infinite both for $E \to 0$ and for $E \to V_0$.

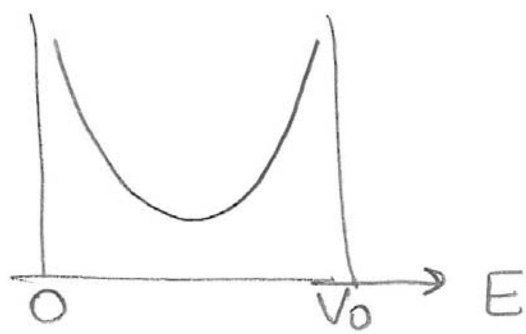

Figure 7: The derivative $\delta'(E)$ as a function of energy $E < V_0$.

4 Wavepackets in the step potential

Now we examine the more physical scenario. As we've seen with the free particle, the stationary states are not normalizable, and physical particles are actually represented by wavepackets built with an infinite superposition of momentum eigenstates. We can do similarly thing with our energy eigenstates. We will consider energy eigenstates with $E > V_0$ or equivalently with $k^2 > \hat{k}^2$, where

$$k^2 = \frac{2mE}{\hbar^2} > \frac{2mV_0}{\hbar^2} \equiv \hat{k}^2\,, \tag{4.26}$$

and we will superpose them. To begin we write the energy eigenstates in a slightly different form, including the time dependence. Setting $A = 1$ and using the values for the ratios B/A and C/A we find the solution

$$\Psi(x,t) = \begin{cases} \left(e^{ikx} + \frac{k-\bar{k}}{k+\bar{k}}\, e^{-ikx}\right) e^{-iE(k)t/\hbar}\,, & x < 0\,, \\ \frac{2k}{k+\bar{k}}\, e^{i\bar{k}x}\, e^{-iE(k)t/\hbar}\,, & x > 0\,. \end{cases} \tag{4.27}$$

We can form a superposition of these solutions by multiplying by a function $f(k)$ and integrating over k

$$\Psi(x,t) = \begin{cases} \int_{\hat{k}}^{\infty} dk\, f(k) \left(e^{ikx} + \frac{k-\bar{k}}{k+\bar{k}}\, e^{-ikx}\right) e^{-iE(k)t/\hbar}\,, & x < 0\,, \\ \int_{\hat{k}}^{\infty} dk\, f(k)\, \frac{2k}{k+\bar{k}}\, e^{i\bar{k}x}\, e^{-iE(k)t/\hbar}\,, & x > 0\,. \end{cases} \tag{4.28}$$

Here $f(k)$ is a real function of k that is essentially zero except for a narrow peak at $k = k_0$. Note that we have only included momentum components with energy greater than V_0 by having the integral's lower limit set equal to $\hat{k}$. The integral only runs over positive k because only in that case the e^{ikx} waves are moving towards positive x, and are therefore genuine incident waves. The above is guaranteed to be a solution of the Schrödinger equation.

We can split the solution into incident, reflected and transmitted waves, as follows.

$$\Psi(x,t) = \begin{cases} \Psi_{inc}(x,t) + \Psi_{ref}(x,t)\,, & x < 0\,, \\ \Psi_{trans}(x,t)\,, & x > 0\,. \end{cases} \tag{4.29}$$

Naturally both $\Psi_{inc}(x,t)$ and $\Psi_{ref}(x,t)$ exist for $x < 0$ and $\Psi_{trans}(x,t)$ exists for $x > 0$. We then have, explicitly

$$\begin{aligned} \Psi_{inc}(x<0,t) &= \int_{\hat{k}}^{\infty} dk\, f(k) e^{ikx} e^{-iE(k)t/\hbar}\,, \\ \Psi_{ref}(x<0,t) &= \int_{\hat{k}}^{\infty} dk\, f(k) \left(\frac{k-\bar{k}}{k+\bar{k}}\right) e^{-ikx} e^{-iE(k)t/\hbar}\,, \\ \Psi_{trans}(x>0,t) &= \int_{\hat{k}}^{\infty} d\bar{k}\, f(\bar{k}) \left(\frac{2k}{k+\bar{k}}\right) e^{i\bar{k}x} e^{-iE(k)t/\hbar}\,. \end{aligned} \tag{4.30}$$

How does the peak of $\Psi_{inc}(x,t)$ move? For this we look for the main contribution to the associated integral which occurs when the total phase in the integrand is stationary for $k \approx k_0$. We therefore require

$$\frac{d}{dk}\left(kx - \frac{\hbar^2 k^2}{2m}\frac{t}{\hbar}\right)\Big|_{k_0} = 0 \quad \rightarrow \quad x - \frac{\hbar k_0}{m} t = 0 \implies x = \frac{\hbar k_0}{m}\, t\,. \tag{4.31}$$

This is the relation between t and x satisfied by the peak of Ψ_{inc}. It describes a peak moving with constant velocity $\hbar k_0/m > 0$. Since $\Psi_{inc}(x,t)$ requires that $x < 0$, the above condition shows that we get the peak only for $t < 0$. The peak of the packet gets to $x = 0$ at $t = 0$. For $t > 0$, $\Psi_{inc}(x,t)$ is not zero, but it must be rather small, since the stationary phase condition cannot be satisfied for any x in the domain $x < 0$.

Consider now $\Psi_{ref}(x,t)$. This time the stationary phase condition is

$$\frac{d}{dk}\left(-kx - \frac{\hbar^2 k^2}{2m}\frac{t}{\hbar}\right)\Big|_{k_0} = 0 \quad \rightarrow \quad x + \frac{\hbar k_0}{m} t = 0 \implies x = -\frac{\hbar k_0}{m}\, t\,. \tag{4.32}$$

The relation represents a peak moving with constant negative velocity $-\hbar k_0/m$. Since $\Psi_{ref}(x,t)$ requires that $x < 0$, the above condition shows that we get the peak only for $t > 0$, as it befits a reflected wave. For $t > 0$, $\Psi_{ref}(x,t)$ is not zero, but it must be rather small, since the stationary phase condition cannot be satisfied for any x in the domain $x < 0$.

Finally, let us consider Ψ_{trans}. The stationary phase condition reads:

$$\frac{d}{dk}\left(\bar{k}x - \frac{\hbar^2 k^2}{2m}\frac{t}{\hbar}\right)\bigg|_{k_0} = 0 \quad \rightarrow \quad \frac{d\bar{k}}{dk}\bigg|_{k_0} x - \frac{\hbar k_0}{m} t = 0 \tag{4.33}$$

Using

$$\bar{k}^2 \;=\; k^2 - \frac{2mV_0}{\hbar^2} \quad \rightarrow \quad \frac{d\bar{k}}{dk} = \frac{k}{\bar{k}}\,, \tag{4.34}$$

back to the earlier equation we quickly find that

$$\text{Transmitted wave peak:} \quad x \;=\; \frac{\hbar\bar{k}}{m}\,t\,, \tag{4.35}$$

with $\bar{k}$ evaluated for $k = k_0$. Since $x > 0$ is the domain of Ψ_{trans} this describes a peak moving to the right with velocity $\hbar\bar{k}/m$ for $t > 0$. For $t < 0$, $\Psi_{trans}(x, t)$ is not zero, but it must be rather small, since the stationary phase condition cannot be satisfied for any x in the domain $x > 0$.

In summary, for large negative time Ψ_{inc} dominates and both Ψ_{ref} and Ψ_{trans} are very small. For large positive time, both Ψ_{ref} and Ψ_{trans} dominate and Ψ_{inc} becomes very small. These situations are sketched in figures 8 and 9. Of course for small times, positive or negative, all three waves exist and together they describe the complex process of collision with the step in which a reflected and a transmitted wave are generated.

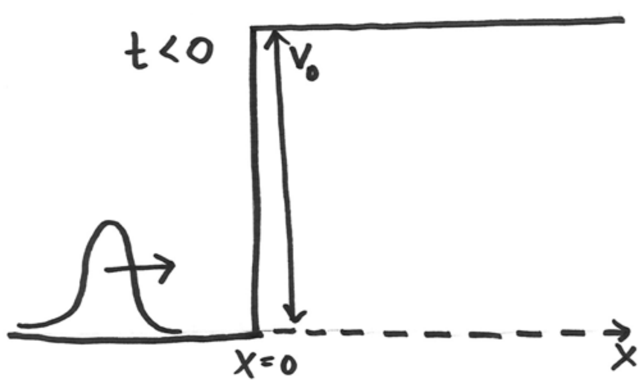

Figure 8: At large negative times an incoming wavepacket is traveling in the $+x$ direction.

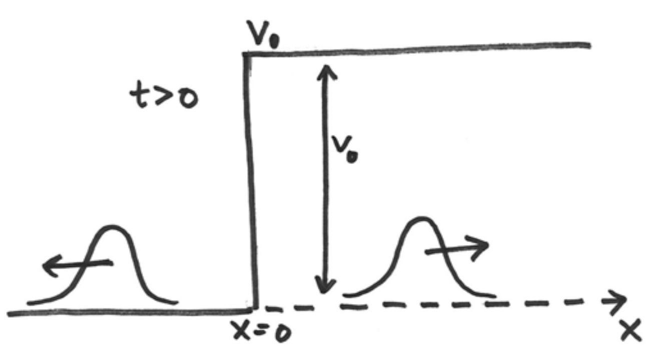

Figure 9: At large positive times we have a reflected wavepacket traveling in the $-\hat{x}$ direction and the transmitted wavepacket traveling in the $+\hat{x}$ direction.

Let us now examine a wavepacket built with energies $E < V_0$. Recall that in this situation $B/A = -e^{2i\delta(E)}$. Therefore for an incident wave, all of whose momentum components have energy less than V_0,

$$\Psi_{inc}(x<0,t) \;=\; \int_0^{\hat{k}} dk\, f(k)\, e^{ikx} e^{-iEt/\hbar}\,, \tag{4.36}$$

the associated reflected wavefunction is

$$\Psi_{ref}(x<0,t) \;=\; -\int_0^{\hat{k}} dk\, f(k)\, e^{2i\delta(E)} e^{-ikx} e^{-iEt/\hbar}\,. \tag{4.37}$$

Using the method of stationary phase again to find the evolution of the peak,

$$\frac{d}{dk}\Big(2\delta(E) - kx - \frac{Et}{\hbar}\Big)\Big|_{k_0} = 0 \quad\to\quad 2\delta'(E)\frac{\hbar^2 k_0}{m} - x - \frac{\hbar k_0 t}{m} \;=\; 0\,. \tag{4.38}$$

From this we quickly find

$$x \;=\; -\frac{\hbar k_0}{m}\big(t - 2\hbar\,\delta'(E)\big)\,, \tag{4.39}$$

where the derivative is evaluated at $E(k_0)$. The reflected wave packet is moving towards more negative x as time grows positive. This is as it should. But there is a time delay associated with the reflected packet, evident when we compare the above equation with $x = -\frac{\hbar k_0}{m}t$. The time delay is given by

$$\boxed{\text{time delay} \;=\; 2\hbar\,\delta'(E)\,.} \tag{4.40}$$

The derivative $\delta'(E)$ was evaluated in (3.25) and it is positive. We see that the delay is particularly large for wave packets of little energy or those with energies just below V_0.

We conclude the analysis of the step potential by discussing what it means to observe the particle in the forbidden region. It would be contradictory if the observer could make the following two statements:

1. The particle is located in the forbidden region.
2. The particle has energy less than V_0.

Both statements taken to hold simultaneously would imply that the particle has negative kinetic energy, something that is inconsistent. In particular with $E < V_0$ we would have a negative kinetic of magnitude $V_0 - E$.

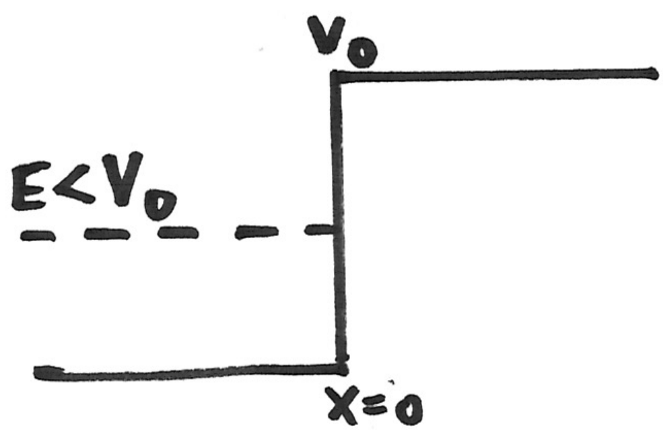

Figure 10: The step potential with potential energy V_0. If we could observe a particle in the forbidden region with energy E then the kinetic energy would be negative.

First note that in the solution the particle penetrates into the forbidden region a distance of about $1/\kappa$, where, you will recall that

$$\kappa^2 = \frac{2m(V_0 - E)}{\hbar^2}\,. \tag{4.41}$$

To be sure the particle is in the forbidden region its position uncertainty Δx must be smaller than the penetration depth:

$$\Delta x \leq \frac{1}{\kappa}\,. \tag{4.42}$$

The particle acquires some momentum p due to the position measurement:

$$p \geq \frac{\hbar}{\Delta x} \;\geq\; \hbar\kappa\,. \tag{4.43}$$

Due to this momentum induced by the position measurement there is some additional contribution E' to the kinetic energy

$$E' \;=\; \frac{p^2}{2m} \;\geq\; \frac{\hbar^2\kappa^2}{2m} = V_0 - E\,, \tag{4.44}$$

where we used (4.41). From this inequality we find that the total energy will exceed V_0

$$E_{tot} \;=\; E + E' \geq E + (V_0 - E) = V_0\,. \tag{4.45}$$

While the argument is heuristic, it gives some evidence that no negative kinetic energy will be detected for a particle that is found in the forbidden region.

Sarah Geller transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.