Notes on Scattering Theory

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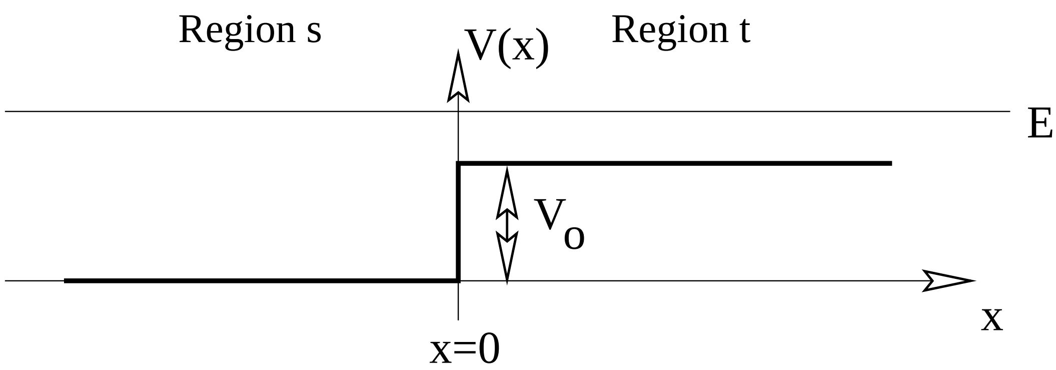

Figure 1: A potential with no bound states

1 Introduction

So far, we have dealt with bound states, those stationary states where a particle has vanishing probability of being found at infinite distance. As we noted in our analysis of the square well, not all stationary states in a potential are bound. The potential in Figure 1, for instance, has *no* bound states. For any $E > 0$, the particle has enough energy to exist classically at infinitely large distances to the left. The wave function in this region will be of the simple, non-decaying oscillatory form associated with classically allowed regions. The particle is not "bound" to any finite region about $x = 0$. A complete understanding of quantum mechanics must include dealing with such unbound states. Such states are referred to as *scattering states* and are the subject of this set of lecture notes.

The solutions of the TISE answer two very important questions about a system. First, they determine the values which will be found in measurements of the energy of a system. Second, the time evolution of the state of a system may be written as a superposition of solutions to the TISE with the appropriate time dependent phases attached. For scattering states, the question of the allowed energies has a simple answer. In Section 3.2, we discuss how *all* values of energy in the scattering range of the spectrum are allowed. We will then proceed to spend most of our effort addressing the issue of the time evolution of the scattering states of the system.

Because we are no longer dealing with bound states, the time evolution of a system is no longer restricted to a probability distribution which sloshes back and forth in a confined region of space. In Figure 2 we show an example of the typical time evolution of scattering states. The figure shows the time evolution of the spatial probability distribution of finding a particle subjected to the potential of Figure 1. These distributions were determined by numerical integration of the Time Dependent Schrödinger Equation.

The figure shows that repeated measurements of the position of the particle at time $t = 0$ yield a Gaussian distribution centered to the left of the origin $x = 0$. The initial state of the particle has a non-zero average velocity in the $+x$ direction. At time $t = 1$, the center of the distribution has shifted to the right. During the intervening interval the distribution has spread in accordance with the Heisenberg Uncertainty Principle.

As time progress to $t = 2$, the center of the packet has reached the step. This time we shall refer to as t_c, the time of the collision. At time $t = 3$, after the collision, the particle is no longer likely to be found at the step, and the probability distribution now takes on two peaks, one to the left and one to the right of the step. As time progresses from $t = 3$ to $t = 4$, the final behavior of the probability distribution is evident. The two peaks in the distribution now move away from the step, spreading in accordance with the HUP.

In interpreting these results, it is important to keep in mind that the *particle* has not split into two parts which then move either to the left or right, it is merely *the probability distribution* which has split. Repeated experiments will show that after the collision at $t = t_c$, the entire particle

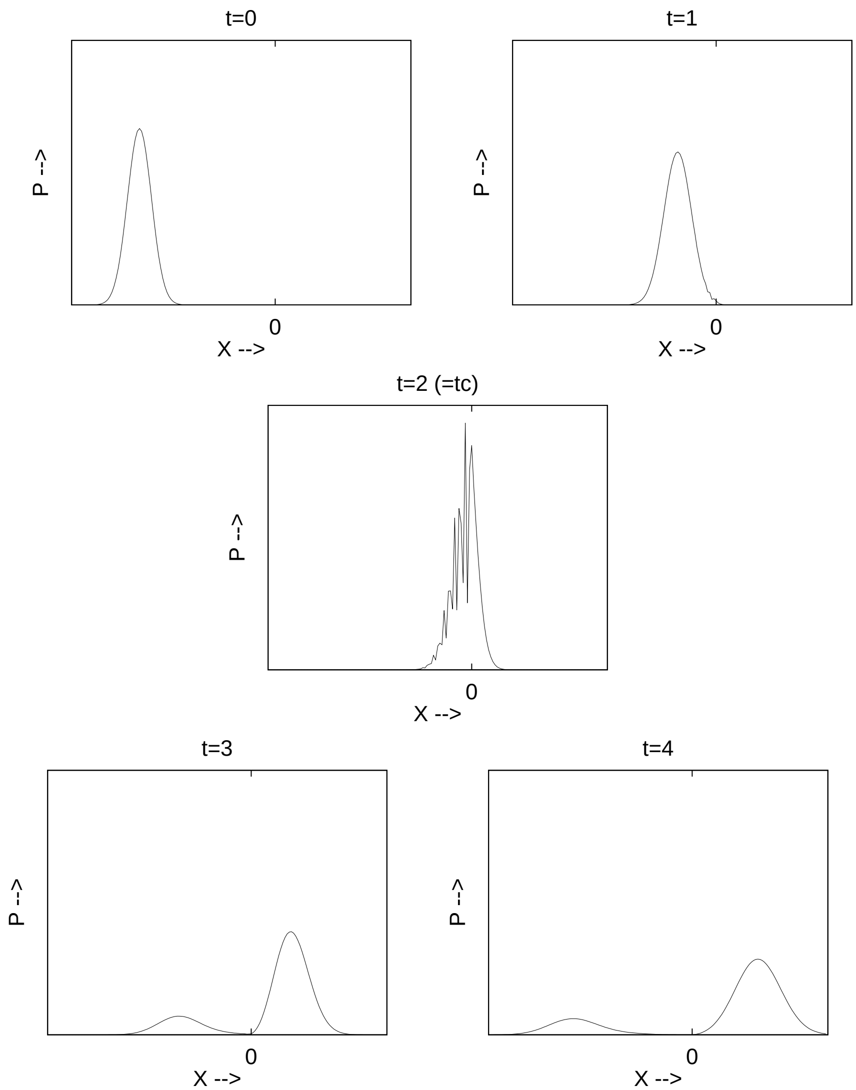

Figure 2: Example of time evolution of a particle approaching a potential step

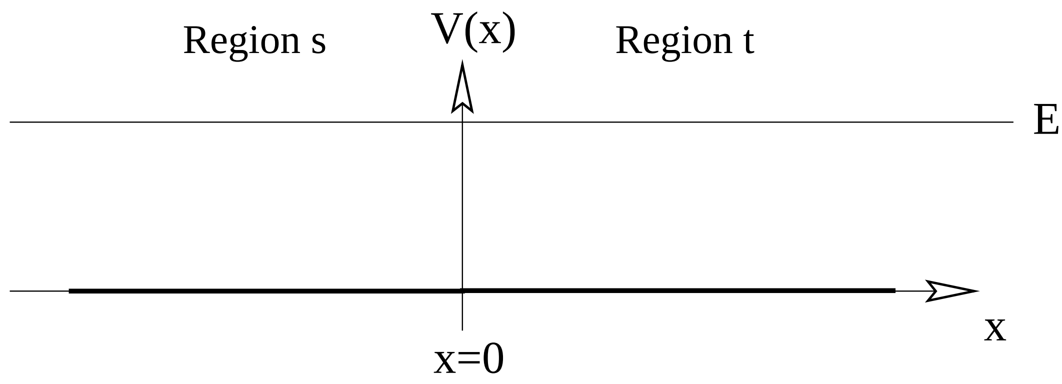

Figure 3: Potential and total energy for a free particle

randomly either continues forward (is *transmitted* by the step) or reverses course and returns along their original path (is "*reflected*" by the step). The probability of reflection or transmission is in direct proportion to the areas of the two peaks moving away from the step after the collision.

There are two more subtle effects of interest which we may study. There may be a delay of the scattered packets in the region of the step before they emerge. This delay if often supposed in science fiction stories to be zero during quantum tunneling events, thus allowing faster than light travel. It is also possible that the interaction with the step induces an additional spreading in the reflected and transmitted packets above and beyond what we normally expect for a packet propagating in free space. We will study this effect as well.

We will begin our discussion in in Section 2 with a full discussion of the simplest class of scattering states, particles propagating in free space ($V(x) = 0$). Although, the solution in this case is the familiar spreading wave packet, we will take a fresh look at the problem. In Section 3 we will develop the general theory of scattering, and finally, in Section 4 we will apply our general theory to the specific the problem of scattering from the potential step in Figure 1.

2 Propagation of a Wave Packet in Free Space

2.1 Solutions to the Time Independent Schrödinger Equation (TISE)

In the case of a free particle ($V(x) = 0$, Figure 3), energies $E < 0$ correspond to solutions everywhere classically forbidden. Such solutions will grow exponentially either as $x \to -\infty$ or $x \to \infty$ and place ever-growing probabilistic weight of finding the particle at infinite distances. Such wave functions do not correspond to probability distributions and thus do not describe physically allowed states. We reject them.

For $E > 0$, on the other hand, the entire space becomes classically allowed, and we find two linearly independent solutions of the form

$$\phi_k(x) \equiv A e^{ikx}, \tag{1}$$

where k may take either value $k = \pm\sqrt{2mE/\hbar^2}$, and A is a normalization constant. These states we recognize as physical; they are the pure states of momentum $p = \hbar k$.

2.2 Normalization of the solutions

Because the $\phi_k(x)$ are pure states with respect to momentum, we expect to find find complete uncertainty in position. Indeed, the probability distribution associated with these functions is constant in space,

$$\mathcal{P}(x) = |\phi_k(x)|^2 = |A|^2. \tag{2}$$

Strictly speaking, in an infinite space, these functions are not normalizable,

$$\int_{-\infty}^{\infty} \mathcal{P}(x)\, dx = |A|^2 \int_{-\infty}^{\infty} dx \to \infty.$$

However, this form of unnormalizability is much milder than that of the exponentially growing wave functions and is manageable. We may imagine placing our experiment in an extremely large box of size L. For sufficiently large L (several billion light years, for instance), we do not expect such a box to affect the small scale physics we study in quantum mechanics. And, as long as L is finite, the states $\phi_k(x)$ will be normalizable. We thus accept our plane wave solutions $\phi_k(x)$ as physical, realizing that they are an idealization in much the same way as is the idea of a an infinite straight line.

Although we cannot insist on the normalization condition $\int |\phi|^2\, dx = 1$, it is still useful at times to have a normalization convention for such states. We will discuss such a convention when we turn to our general discussion of scattering in 3.

2.3 Allowed energies

In contrast to the case of bound states, scattering states naturally remain finite at large distances without the imposition of boundary condition constraints. The TISE, being a second order differential equation then produces two physical solutions for each value of $E > 0$. This stands in stark contrast to the always *non*-degenerate solutions of bound states in one dimension.

2.4 Physical Interpretation of the Solutions to the TISE

The spatial probability distributions $\mathcal{P}(x)$ associated with the $\phi_k(x)$ are uniform and constant. Yet, we associate these states with particular values of momentum. It is the probability *current*,

$$j(x) = \frac{\hbar}{m} \Im \left\{ \psi^*(x) \partial_x \psi(x) \right\},$$

which shows the flow of particles associated with these states.

Evaluating the current for the $\phi_k(x)$ gives

$$\begin{aligned} j(x) &= \frac{\hbar}{m} \Im \left\{ \left(A^* e^{-ikx} \right) \left(Aike^{ikx} \right) \right\} \\ &= \frac{\hbar}{m} \Im \left\{ ik|A|^2 \right\} \\ &= |A|^2 \frac{\hbar k}{m} \\ j(x) &= \mathcal{P} v_{cl} \end{aligned} \tag{3}$$

In the last line, we have used the fact that the probability density of this state is $|A|^2$ and identified $v_{cl} = \hbar k/m = p/m$, the velocity which we would classically expect to be associated with a particle of mass m traveling with momentum $\hbar k$.

The form (3) for $j(x)$ gives a clear physical interpretation for the $\phi_k(x)$. The represent constant beams of particles of density $\mathcal{P}$ traveling at velocity v_{cl}. It is important to keep in mind that the simple result (3) does not hold in general except for wave functions of the simple plane wave form Ae^{ikx}. Nonetheless, (3) is a good mnemonic for remembering an expression which we will use time and time again in scattering theory.

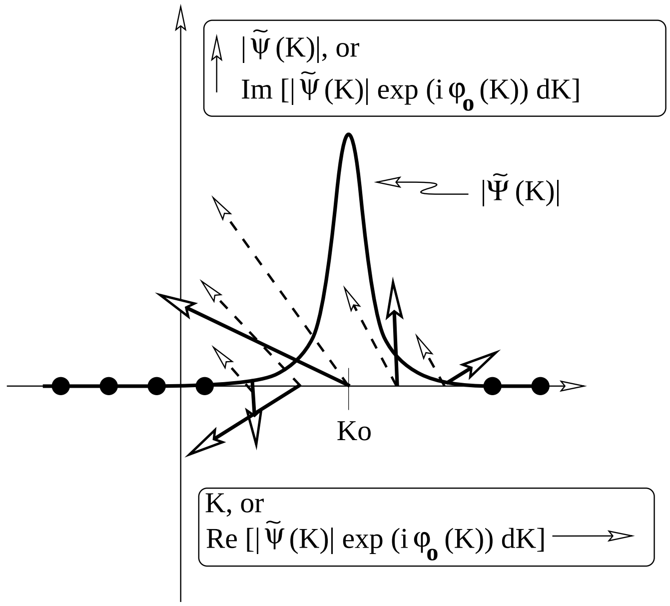

Figure 4: Integrand of an integral to be analyzed using the method of stationary phase

2.5 Wave packets

The direct connection between the physical interpretation of $\phi_k(x)$ as a beam of particles and our formal theory comes through the TDSE. The pure states $\phi_k(x)$ of energy are stationary, and the connection between them and the dynamical evolution pictured in Figure 2 is not direct. Producing a wave packet with an identifiable location in space requires taking superpositions of the states $\phi_k(x)$.

Mathematically, a wave packet evolving under the TDSE is such a superposition of pure energy states times multiplied with the appropriate time-dependent phase factors,

$$\Psi(x,t) = \int \frac{dk}{\sqrt{2\pi}} \tilde{\psi}(k) e^{ikx} e^{-i\frac{\hbar k^2}{2m}t}, \tag{4}$$

where $|\tilde{\psi}(k)|$ is sharply peaked near $k = k_o$. The mathematical form of the integral (4) naturally guarantees that the resulting wave packet $\Psi(x,t)$ will be confined to a particular region of space because the integral is essentially essentially a sum of complex numbers with varying phases. For most values of x, these phases vary rapidly, resulting in much cancellation and a small absolute value of the integral.

To sketch the behavior of the integral, we write $\tilde{\psi}(k)$ as the product of its amplitude and a complex phase

$$\tilde{\psi}(k) \equiv |\tilde{\psi}(k)| e^{i\phi_o(k)},$$

where $\phi_o(k)$ describes the phase of the packet. Note $|\tilde{\psi}(k)|$ is peaked about $k = k_o$ as in Figure 4.

With this separation we may rewrite (4) as the integral of the product of real amplitudes with complex phases,

$$\Psi(x,t) = \int dk \frac{|\tilde{\phi}(k)|}{\sqrt{2\pi}} e^{i\phi_o(k)} e^{ikx} e^{-i\frac{\hbar k^2}{2m}t}. \tag{5}$$

Such integrals are best analyzed using the method of stationary phase as described in the next section.

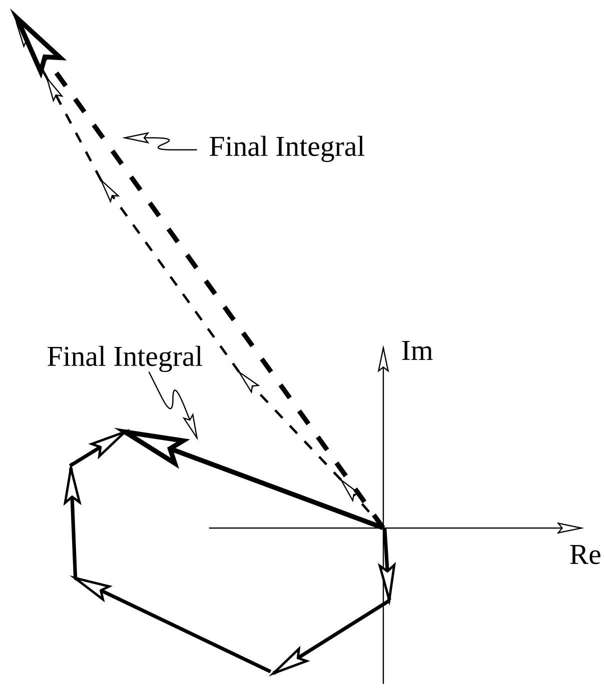

Figure 5: Total integral analyzed using stationary phase

2.6 The Method of Stationary Phase: Location of the packet

Figure 4 gives a representation of the integrand in (5). The integrand at each value of k, $|\tilde{\psi}(k)|\, e^{i\phi_o(k)} e^{ikx} e^{-i\frac{\hbar k^2}{2m}t}/\sqrt{2\pi}$, is sketched as a complex vector with its base placed at the corresponding point k along the real axis. The significant contributions to the integral all come from the points near k_o where the amplitude of the numbers is most significant. The figure shows two cases. In one case (the solid arrows), the phases vary rapidly across the region of significant contributions, whereas in the second case (the dashed arrows), the phases vary slowly in the region of significance.

The value of the integral is the sum of these vector obtained by adding them tail-to-head as in Figure 5. In the case where the phases vary rapidly near k_o, relatively little net progress is made away from the origin of the complex plane as the contributing vectors spin around. The result of this behavior is a small magnitude for the wave function, $|\Psi(x,t)|$. In the second case where the phases vary slowly, on the other hand, the vectors all line up to produce a large final magnitude for the wave function $|\Psi(x,t)|$.

We see, therefore, that the largest $|\Psi(x,t)$ come when the phase is as constant, as *stationary*, as possible in the region where $|\tilde{\psi}(k)|$ is most significant. Defining $\Phi(k)$ as the total phase of the integrand, this is the condition that

$$
\begin{aligned}
0 &= \partial_k \left(\Phi(k)\right|_{k_o} &(6)\\
&= \partial_k \left(\phi_o(k) + kx - \frac{\hbar k^2}{2m}t\right|_{k_o}\\
&= \phi_o'(k_o) + x - \frac{\hbar k_o}{m}t &(7)
\end{aligned}
$$

Applying the general condition (6) to locate the regions of greatest contribution from an integral is referred to as *The Method of Stationary Phase.*

In our specific case, the great magnitude of $|\Psi(x,t)|$ occurs when (7) is satisfied, when

$$x(t) = \frac{\hbar k_o}{m} t - \phi_o'(k_o).$$

The most probable location for the particle follows the same trajectory in time as does a classical particle traveling with the velocity $v_{cl} = \hbar k_o/m$. The physical interpretation of the states near $\phi_{k_o}(x)$ as beams of particles traveling with the classically expected velocity is indeed correct!

The analysis here further gives the location of the packet at time $t = 0$,

$$x_o = -\phi_o'(k_o),$$

and the time t_o when the center of the packet crosses the origin,

$$t_o = \frac{1}{v_{cl}} \phi_o'(k_o).$$

The three lessons of general applicability to be taken from this section are

1. Beams of particles $\phi_k(x)$ carry wave packets at the classically expected velocity.
2. *The Method of Stationary Phase* tells us that the most significant contributions from the integral of a complex integrand come when the phase of the integrand does not vary at the point of its maximum magnitude.
3. The initial location of a wave packet and the time when it crosses $x = 0$ are both determined by the derivative of the phase of the weights of superposition $\tilde{\psi}$ evaluated at the momentum where the packet is concentrated.

3 General Features of *Scattering* States

After having reviewed the propagation of packets in free space in detail and developed new general methods, we are in a position to discuss the general theory of scattering states. In the next section, we will apply these general principles to the case of scattering from a potential step.

3.1 Summary

Here we gather summarize the main results of what follows in this section.

To determine the scattering properties of a particular potential, one first divides space into three regions as in Figure 7. The potential is taken to be constant in the "source" region s, extending by convention from $x = -\infty$ to $x = 0$. This is the region from which particles from an external *source* come to interact with the potential. It is also this region into which particles reflect back. The potential is also be taken constant in the "transmitted" region t, extending by convention from $x = L$ to $x = \infty$. This is the region into which particles originating from the source in Region s may be *transmitted*. Finally, in Region c, where the *collisions* generating the scattering takes place, the wave functions may take on arbitrarily complicated forms. Note that one may generalize our results to situations where the particles are incident onto the potential from the right by changing the direction the x-axis.

Once the potential is determined, the first step in analyzing the problem is to solve the TISE with *left-incident* boundary conditions, which state that the form of the wave function in Region t is just some pure beam state $t(k)e^{ikx}$ of particles traveling to the right. This determines the entire solution to the TISE, which, by multiplying through by a normalization constant, may always be put into the following general form,

$$\phi_k(x) = \begin{cases} \frac{e^{ikx}}{\sqrt{\hbar k/m}} + r(k)\frac{e^{-ikx}}{\sqrt{\hbar k/m}} & \text{Region } s \\ \text{something complicated} & \text{Region } c \\ t(k)\frac{e^{ik_t(k)(x-L)}}{\sqrt{\hbar k_t(k)/m}} & \text{Region } t \end{cases}, \tag{8}$$

where $k_t(k)$ is the wave vector in Region t written as a function of the incoming wave vector in Region s. Once the quantum amplitudes $r(k)$ and $t(k)$ for the reflected and transmitted beams, respectively, are determined, all of the relevant issues in scattering may be studied.

Probability of Reflection and Transmission– The magnitudes of the scattering amplitudes give the probabilities of a particle reflecting or transmitting,

$$\begin{aligned} P_r &= |r(k_o)|^2 \\ P_t &= |t(k_o)|^2, \end{aligned}$$

respectively, where k_o is the wave vector about which the incoming wave packet is centered.

Time delays– The time delays for transmission and reflection after the source packet collides with Region c are determined by the phases of the quantum amplitudes, which are defined through

$$\begin{aligned} r(k) &= |r(k)|e^{i\phi_r(k)} \\ t(k) &= |t(k)|e^{i\phi_t(k)}. \end{aligned}$$

The reflected packet emerges into Region s a time Δt_r after the source packet collides with Region c, and the transmitted packet emerges into Region t a time Δt_t after the source packet collides with Region c,

$$\Delta t_r = (\phi_r'(k_o))/v_{cl}^{(s)} \tag{9}$$

$$\Delta t_t = (\phi_t'(k_o))/v_{cl}^{(s)}, \tag{10}$$

Here, k_o is the wave vector about which the incoming wave packet is centered and $v_{cl}^{(s)} = \hbar k_o/m$ is the classical velocity expected of a particle propagating in Region s.

3.2 Solutions of the TISE

In general, *scattering states* are pure states of energy (solutions to the TISE) where there is a classically allowed region at either $x \to -\infty$ or $x \to +\infty$, or both. States with energies E_3 or E_4 in the Asymmetric Finite Square Well in Figure 6, for instance, are scattering states. On the other hand, a state with energy E_2 would *not* be a scattering state but rather a bound state because both regions $x \to \pm\infty$ are forbidden. Finally, a state with energy E_1 is forbidden from *all* regions, must always curve away from the x-axis and thus grows exponentially in at least one of the limits $x \to \pm\infty$ and would never be acceptable physically.

The TISE is a second order equation, we thus expect its general solutions to involve two degrees of freedom, one of which corresponds to the normalization of the wave function, leaving only one remaining degree of freedom in the solution. For bound state energies such as E_2, we impose two boundary conditions, that the exponentially component of the wave function be zero in decay exponentially in both forbidden regions $x \to \pm\infty$. It is in general impossible to satisfy both of these conditions with the one degree of freedom remaining to our solutions. This is why we find solutions for bound states only under very special circumstances, only at the allowed energies.

For scattering states such as E_3 where exactly one region of the two regions at infinity is forbidden, we need to impose only one boundary condition, exponential decay in the forbidden region. (The oscillatory form of the solutions in the classically allowed region always results in physically acceptable behavior.) The one boundary condition which we now impose may always be satisfied with the one remaining degree of freedom in the normalized solution of the TISE. The solution is thus completely determined, and there is exactly one solution for each energy in this range.

Finally, when we move to energies in the range of E_4, the states naturally remain oscillatory in both allowed regions as $x \to \pm\infty$. The one remaining degree of freedom corresponds to the fact that there are two linearly independent physical solutions to the TISE for each energy in this range which we may then mix together arbitrarily. This is precisely what we found for particles propagating in free space in Section 2.3.

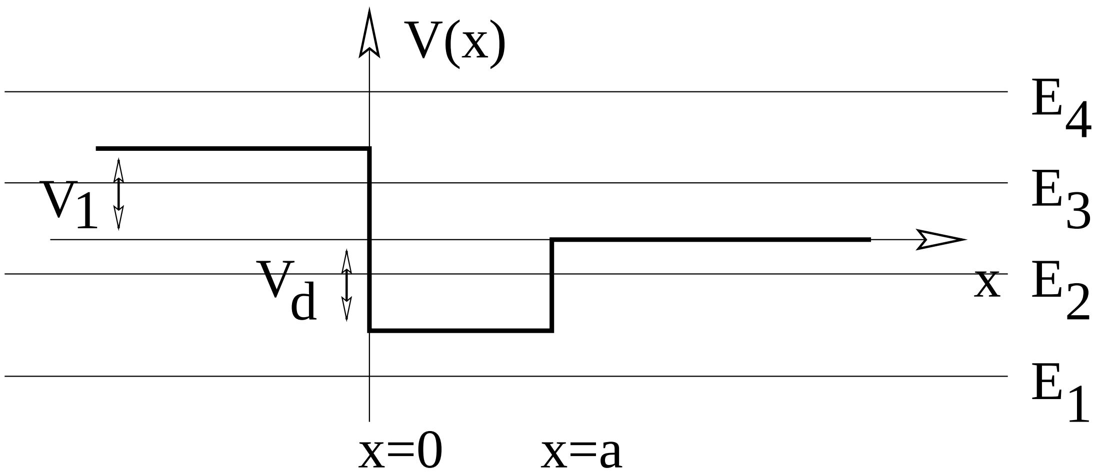

Figure 6: Ranges of disallowed, bound and scattering states in an Asymmetric Finite Square Well

3.3 Left- and right- incident boundary conditions

There is a standard choice for the two linearly independent solutions of the TISE in cases where the particle is classically allowed at infinite distances in both directions. Note that in the case of particles moving in free space, the solutions $\phi_k(x)$ for $k > 0$ contain only currents moving to the right as $x \to +\infty$. This is an appropriate state for when one imagines particles originating from a *source* on the far left of the system. The boundary condition that there be no left-moving currents for $x \to +\infty$ is termed the *left-incident boundary condition.* Setting this condition removes all freedom and specifies a unique solution to the TISE, once a convention for normalization have been specified. The *right-incident boundary condition*, that there be no right-moving currents as $x \to -\infty$, specifies another, linearly independent solution. These boundary conditions are sketched in Figure 7. As indicated in the figure, specifying either condition on one side of the system will in general generate solutions traveling in both directions on the other side.

As indicated in Figure 7, we may generally divide the problem into three regions. A scattering or *collision* region (Region c in the figure) where there is a disturbance in the potential, and two regions (Regions s and t), where particles propagate normally. Although the form of the wave function in Region c may be complicated, the solutions to the TISE in Regions s and t will be linear combinations of plane waves $\phi_k(x)$ with wave vectors given by $k_{s,t} \equiv \pm\sqrt{2m(E - V_{s,t})/\hbar^2}$, where $V_{s,t}$ is the value of the (constant) potential in the corresponding region. The precise form of the linear combination will be determined by the solution of the TISE in the scattering region.

For the left-incident case, which we will associate with values $k > 0$, in general we will find solutions to the TISE of the form,

$$\phi_k(x) = \begin{cases} Se^{ikx} + Re^{-ikx} & \text{Region } s \\ \text{something complicated} & \text{Region } c \\ Te^{ik_t(k)(x-L)} & \text{Region } t \end{cases}, \tag{11}$$

where we have taken care to follow our usual practice and centered our functions on the boundaries of the regions in which they are defined. In 11, k refers to the wave vector in region of the source,

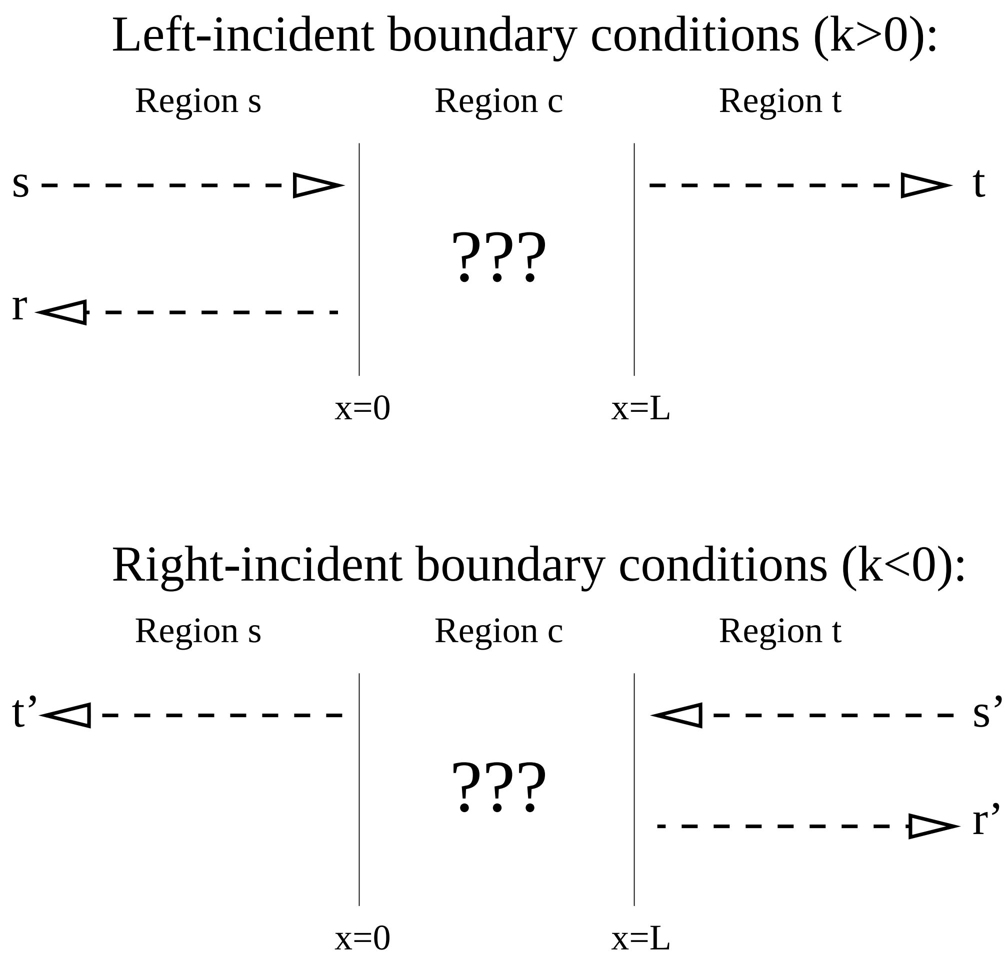

Figure 7: Left- (top) and Right- (bottom) Incident Boundary Conditions: The source, reflected and transmitted beams in either case are indicated by s, r and t, respectively. (We label the region $x < 0$ "Region s" because our convention is to work with left-incident boundary conditions.)

Region s. This wave vector determines the energy of the state and thus also the wave vector in Region t, which we have written as a function of the source wave vector, $k_t(k)$. The relation $E = \hbar^2 k^2/2m + V_s = \hbar^2 k_t^2/2m + V_t$ determines this function to be

$$k_t(k) = \sqrt{k^2 - \frac{2m}{\hbar^2}(V_t - V_s)} \equiv \sqrt{k^2 \mp Q_o^2}, \tag{12}$$

where $Q_o^2 \equiv \pm\frac{2m}{\hbar^2}(V_t - V_s)$ is a measure of the difference in potential going from Region s to Region t. This sign in the definition of Q_o is generally chosen so as to make Q_o a real number.

We have left the form of the solution in Region c unspecified because the form of the wave function in this region is not directly needed to determine the behavior of the wave packets entering and leaving the scattering region – only the final form of the solution to the TISE in the regions s and t. Currently, the factors S, R and T are undetermined because we have yet to choose a normalization convention for such states. Finally, we note that in the case where Region t classically forbidden, we insist upon exponentially decaying solutions, and only the factors S and R then play explicit roles in the scattering of particles.

3.4 Normalization Convention

In scattering theory the most natural choice of normalization is that the incoming "source" beam carry one particle per unit time. Note that according to 3, such a beam which carries a unit current, to the right or left respectively, always has the form $e^{+\pm ikx}/\sqrt{\hbar k/m}$. To produce a solution with this normalization of the incoming beam, we may simply multiplying any general solution of the form 11 through by the factor $1/(S\sqrt{\hbar k/m})$ to produce

$$\phi_k(x) = \begin{cases} \frac{e^{ikx}}{\sqrt{\hbar k/m}} + r(k)\frac{e^{-ikx}}{\sqrt{\hbar k/m}} & \text{Region } s \\ \text{something complicated} & \text{Region } c \\ t(k)\frac{e^{ik_t(k)(x-L)}}{\sqrt{\hbar k_t(k)/m}} & \text{Region } t \end{cases}, \tag{13}$$

where $r(k) \equiv (R/S)/sqrt\hbar k/m$ and $t(k) \equiv (T/S)\sqrt{k_t(k)/k}/\sqrt{\hbar k/m}$. Note that some extra care has been taken with the transmitted term to write it also in terms of a beam carrying unit current, so that all three beams of particles, source, reflected and transmitted are written a unit currents, with perhaps some prefactors attached. These prefactors have very simple physical interpretations and are thus given a special name. The factors $r(k)$ and $t(k)$ are called the *quantum amplitudes* for *reflection* and *transmission*, respectively.

Note that right-incident solutions, which we associate with values of $k < 0$, should also be written in this special normalized form,

$$\phi_k(x) = \begin{cases} t'(k)\frac{e^{-ikx}}{\sqrt{\hbar k/m}} & \text{Region } s \\ \text{something complicated} & \text{Region } c \\ \frac{e^{-ik_t(x-L)}}{\sqrt{\hbar k_t/m}} + r'(k)\frac{e^{ik_t(x-L)}}{\hbar k_t/m} & \text{Region } t \end{cases}.$$

Throughout the rest of these notes, we will consider problems with particles incident from the left and thus use *left-incident* boundary conditions. All results are easily generalized to the right-incident case by reflecting the problem about the point $x = L/2$.

3.5 Physical interpretation of the solutions of the TISE

The physical interpretation of the right-incident solutions (13), is that Region s contains two beams of particles, one, emanating from the source, carrying $j_s = 1$ particles per unit time toward the right, and the other, carrying $j_r = v_{cl}^{(s)}/(\sqrt{\hbar k/m})^2|r(k)|^2 = |r(k)|^2$ reflected particles per unit time toward the left. Region c is the scattering region about which we need say little. Finally, Region t contains a single beam of particles transmitted through the scattering region and carrying $j_t = v_{cl}^{(t)}/(\sqrt{\hbar k_t/m})^2 |t(k)|^2 = |t(k)|^2$ particles per unit time toward the right.

Knowing the magnitude of the currents gives the answer to the first question of scattering theory, the probability of a particle being scattered in either direction, to the left or to the right. The probability of reflection P_r is just the ratio of the number of particles reflected per unit time, j_r, to the total number of particles incident from the source per unit time, j_s. Similarly, the probability of transmission is the ratio of j_t to j_s. In either case $j_s = 1$ and thus we expect,

$$\begin{aligned} P_r &= |r(k)|^2 \\ P_t &= |t(k)|^2. \end{aligned} \tag{14}$$

Note that our original derivation of the form of the probability current $j(x,t) = (\hbar/m)\Im(\psi * \partial_x \psi)$ deals with the entire wave function $\psi(x,t)$ at point x and makes no distinction between different component parts of the wave function traveling in different directions whose currents may be evaluated separately. At present, the separation between the incoming and reflected currents is a new physical idea which we have brought into our formalism. We shall justify it fully in the next section where we show that in a solution to the TDSE made of an identifiable incoming wave packet one first finds a distinct wave packet traveling toward the collision region which is made up in such a way that the only significant contribution to the back in Region s comes from the incoming beam. Later, a partially reflected wave packet, to which only the reflected beam part of the solution to the TISE contributes, returns back toward the source. It is the fact that incoming and reflected beam parts are active at different times in the scattering of a wave packet which gives the ultimate justification for our physical separation of the two currents which occupy the same region of space. Below, we will see that (15) does not tell the whole story, but is really only valid in the approximation of an incoming wave packet which is nearly a pure state of momentum.

3.6 Wave packets

As in the free particle case, the time dependent wave packet solution to the TDSE is the general superposition of pure energy states with the appropriate time-dependent phase factors,

$$\Psi(x,t) = \int dk \, \frac{\sqrt{\hbar k/m}}{\sqrt{2\pi}} \, \tilde{\psi}(k) \phi_k(x) e^{-i\frac{\hbar k^2}{2m}t}, \tag{15}$$

$$= \int dk \, \frac{\sqrt{\hbar k/m}}{\sqrt{2\pi}} \, \tilde{\psi}(k) \left\{ \begin{array}{ll} \frac{e^{ikx}}{\sqrt{\hbar k/m}} + r(k)\frac{e^{-ikx}}{\sqrt{\hbar k/m}} & \text{Region } s \\ \text{something complicated} & \text{Region } c \\ t(k)\frac{e^{ik_t(k)(x-L)}}{\sqrt{\hbar k_t(k)/m}} & \text{Region } t \end{array} \right\} e^{-i\frac{\hbar k^2}{2m}t}, \tag{16}$$

where the factor $\sqrt{\hbar k/m}/\sqrt{2\pi}$ is just for normalization so that, as we show in the next paragraph, $\Psi(x,t)$ is normalized so long as is $\tilde{\psi}(k)$. Also, we again regard $|\tilde{\psi}(k)|$ as sharply peaked near some value of incoming momentum, $k = k_o$.

There are three terms in this expression, associated with either the source, the reflected or the transmitted packet. Each is an integral of the form we analyzed in free space in Section 2. Explicitly, the three terms are

$$\Psi_s(x,t) = \int \frac{dk}{\sqrt{2\pi}} \, \tilde{\psi}(k) e^{ikx} e^{-i\frac{\hbar k^2}{2m}t} \tag{17}$$

$$\Psi_r(x,t) = \int \frac{dk}{\sqrt{2\pi}} \, \tilde{\psi}(k) r(k) e^{-ikx} e^{-i\frac{\hbar k^2}{2m}t} \tag{18}$$

$$\Psi_t(x,t) = \int \frac{dk}{\sqrt{2\pi}} \, \tilde{\psi}(k) \sqrt{\frac{k}{k_t(k)}} t(k) e^{ik_t(k)(x-L)} e^{-i\frac{\hbar k^2}{2m}t}. \tag{19}$$

The complete scattering solution may be reassembled from these integrals,

$$\Psi(x,t) = \begin{cases} \Psi_s(x,t) + \Psi_r(x,t) & \text{Region } s \\ \text{something complicated} & \text{Region } c \\ \Psi_t(x,t) & \text{Region } t \end{cases} . \tag{20}$$

3.7 Location of the packets

The phases of the three packets 17-19 are

$$\Phi_s(k) = \phi_o(k) + kx - \frac{\hbar k^2}{2m}t \tag{21}$$

$$\Phi_r(k) = \phi_o(k) + \phi_r(k) - kx - \frac{\hbar k^2}{2m}t \tag{22}$$

$$\Phi_t(k) = \phi_o(k) + \phi_t(k) + k_t(k)(x-L) - \frac{\hbar k^2}{2m}t,$$

respectively. Evaluating the corresponding stationary phase conditions gives

$$\begin{aligned} 0 &= \Phi_s'(k_o) \\ &= \phi_o'(k_o) + x - \frac{\hbar k_o}{m}t \\ \Rightarrow & \\ x_s(t) &= -\phi_o'(k_o) + \frac{\hbar k_o}{m}t \end{aligned}$$

for the location of the source packet,

$$\begin{aligned} 0 &= \Phi_r'(k_o) \\ &= \phi_o'(k_o) + \phi_r'(k_o) - x - \frac{\hbar k_o}{m}t \\ \Rightarrow & \\ x_r(t) &= \phi_o'(k_o) + \phi_r'(k_o) - \frac{\hbar k_o}{m}t \end{aligned}$$

for the location of the reflected packet, and

$$\begin{aligned} 0 &= \Phi_t'(k_o) \\ &= \phi_o'(k_o) + \phi_t'(k_o) + k_t'(k_o)(x-L) - \frac{\hbar k_o}{m}t \\ &= \phi_o'(k_o) + \phi_t'(k_o) + \frac{k_o}{k_t(k_o)}(x-L) - \frac{\hbar k_o}{m}t \\ \Rightarrow & \\ x_t(t) &= L - \frac{k_t(k_o)}{k_o}\left(\phi_o'(k_o) + \phi_t'(k_o)\right) + \frac{\hbar k_t(k_o)}{m}t \end{aligned}$$

for the transmitted packet. For evaluation of the expression for the transmitted packet, we have used the identity,

$$\frac{dk_t(k)}{dk} = \frac{d}{dk}\sqrt{k^2 \mp Q_o^2\alpha} = \frac{k}{\sqrt{k^2 \mp Q_o^2}} = \frac{k}{k_t(k)}, \tag{23}$$

where as in Section 3.3, $Q_o^2 \equiv \pm\frac{2m}{\hbar^2}(V_t - V_s)$.

We first note that in all three cases, we find packets traveling with the expected classical velocities, $v_{cl}^{(s)} = \hbar k_o/m$, $-v_{cl}^{(s)} = -\hbar k_o/m$ and $v_{cl}^{(t)} = \hbar k_t(k_o)$, for the source, reflected and transmitted packets, respectively.

Let us call $t = 0$ a time when the source packet $\Psi_s(x,t)$ is entirely within Region s. The source packet then begins at $x_s(0) = -\phi_o'(k_o) < 0$ and then propagates to the right, until at time

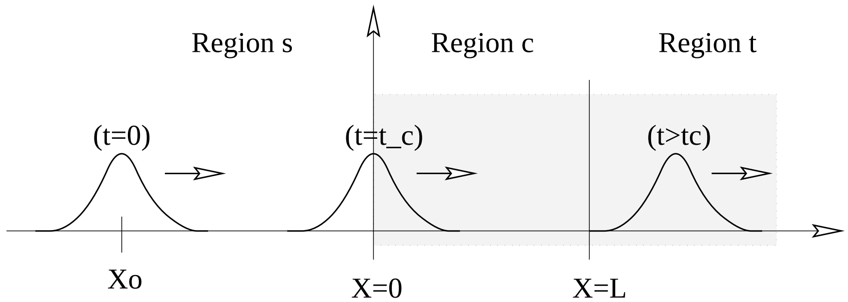

Figure 8: Evolution of the source packet in a general scattering problem

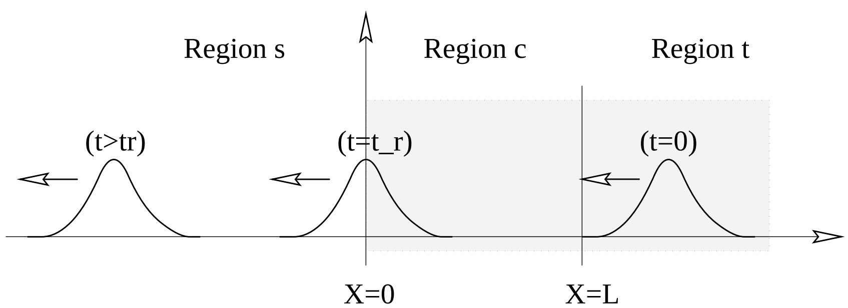

Figure 9: Evolution of the reflected packet in a general scattering problem

$t_c = \phi_o'(k_o)/v_{cl}^{(s)}$, its center reaches the point $x = 0$ where the particle first "collides" with the collision region. (See Figure 8.) At this moment, half of the packet extends into Region c. Note that because $\Psi_s(x,t)$ is only evaluated in Region s in (20), the part of the source packet extending into Region c makes no contribution to the final wave function $\Psi(x,t)$. As time goes on, $\Psi_s(x,t)$ eventually enters Regions c and t entirely, at which point the source packet entirely disappears from the problem.

The location of the reflected packet at time $t = 0$ is $x_r(0) = \phi_o'(k_o) + \phi_r'(k_o)$, which then must be entirely within Regions c and t. At this point in time, the reflected packet makes no contribution to the problem. ($\Psi_r(x,t)$ is only evaluated in Region s in (20).) As this packet then travels to the left, eventually, at time $t_r = (\phi_o'(k_o) + \phi_r'(k_o))/v_{cl}^{(s)} = t_c + \phi_r'(k_o)/v_{cl}^{(s)}$, it reaches the point $x = 0$ and emerges into Region s, from where it continues back toward the source. (See Figure 9.) Note that the time t_r at which the reflection emerges into the problem may is delayed by a period

$$\Delta t_r = \phi_r'(k_o)/v_{cl}^{(s)}$$

from the moment when the source packet first collides with the scattering region.

At $t = 0$, the transmitted packet $\Psi_t(x,t)$ is located at $x_t(0) = L - \frac{k_t(k_o)}{k_o}\left(\phi_o'(k_o) + \phi_t'(k_o)\right)$ and contained within within Regions s and c. This packet eventually emerges into the problem at the moment when $x_t(0) = L$, at time $t_t = \frac{k_t(k_o)}{k_o}\left(\phi_o'(k_o) + \phi_t'(k_o)\right)/v_{cl}^{(t)} = \left(\phi_o'(k_o) + \phi_t'(k_o)\right)/v_{cl}^{(s)} =$

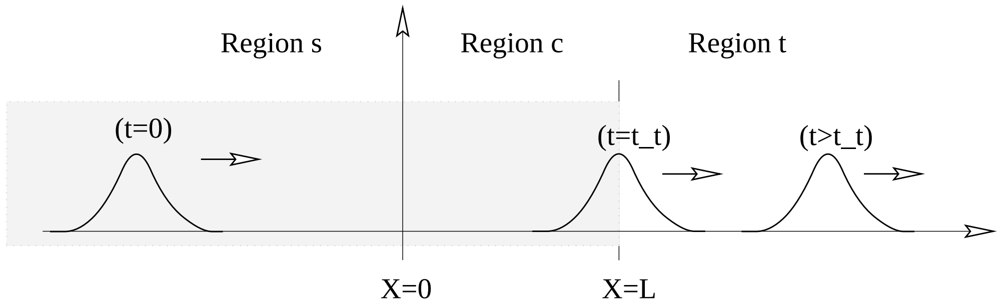

Figure 10: Evolution of the transmitted packet in a general scattering problem

$t_c + \phi_t'(k_o)/v_{cl}^{(s)}$, which is a period

$$\Delta t_t = \phi_t'(k_o)/v_{cl}^{(s)}$$

later than the moment t_c when the source packet collides with the scattering region. (See Figure 10.)

Taken all together, $\Psi(x,t)$ describes the following sequence of events. First, there is only a packet from the source traveling to the right in Region s at velocity $v_{cl}^{(s)}$. Then, at time $t_c = \phi_o'(k_o)/v_{cl}^{(s)}$ determined by the initial conditions, this packet collides with the scattering region, Region c. A period $\Delta t_r = \phi_r(k_o)/v_{cl}^{(s)}$ later, which is characteristic of the scattering potential only, a reflected packet emerges back from Region c into Region s and then continues to move to the left with velocity $-v_{cl}^{(s)}$. An additional transmitted packet emerges into Region t a period $\Delta t_t = (\phi_s'(k_o) - \phi_t'(k_o))/v_{cl}^{(s)}$, which again is a characteristic of the scattering potential only, after the collision at time $t = t_c$ and travels to the right with velocity $v_{cl}^{(t)}$. The order in which the reflected and transmitted packets emerge depends on the sizes of Δt_r and Δt_t.

3.8 Normalization of the Packets

We now complete our general discussion of scattering theory by verifying explicitly that the formulae (15), which were derived from different beam components of a single stationary solution to the TISE do indeed give the correct normalizations of the reflected and transmitted parts of an incoming wave packet.

The total probability associated with each of the packets is best determined in momentum space. From 17 is it clear that the momentum space wave function representation of the source packet at time t is

$$\tilde{\Psi}_s(k,t) = \tilde{\psi}(k) e^{-i\frac{\hbar k^2}{2m}t},$$

so that the total probability associated with the source packet is

$$P_s = \int dk\, |\tilde{\Psi}_s(x,t)|^2 = \int dk\, |\tilde{\psi}(k)|^2 = 1.$$

We know that the total probability associated with Ψ_s must be one because for $t << 0$, this is the only one of the packets which makes a contribution to the time dependent wave function, which always much be normalized.

To determine the momentum space representation of $\Psi_r(x,t)$, for the purpose of finding the probability of reflection P_r, we must manipulate (18) into the form of a standard Fourier transform. We may accomplish this by making the change of variables $k \to -k$. Under such a change of variables, $\int_{-\infty}^{\infty} dk\, I(k) \rightarrow \int_{\infty}^{-\infty} (-dk)\, I(-k) = \int_{-\infty}^{\infty} dk\, I(k)$, so that k is simply replaced by $-k$ in the integrand $I(k)$. Applying this to (18) then gives us

$$\begin{aligned}
\Psi_r(x,t) &= \int \frac{dk}{\sqrt{2\pi}}\, \tilde{\psi}(-k) r(-k) e^{ikx} e^{-i\frac{\hbar k^2}{2m}t} \\
&\Rightarrow \\
\tilde{\Psi}_r(k,t) &= \tilde{\psi}(-k) r(-k) e^{-i\frac{\hbar k^2}{2m}t} \\
&\Rightarrow \\
P_r &= \int dk\, |\tilde{\psi}(-k)|^2 |r(-k)|^2 \\
&= \int dk\, |\tilde{\psi}(k)|^2 |r(k)|^2,
\end{aligned} \tag{24}$$

where in the last step we have changed back to the original k variable by making the change $k \rightarrow -k$ once again. This is the complete, *exact* expression for the reflection probability. Generally, we deal in the *narrow packet approximation* under which $|\tilde{\psi}(k)|$, much like a Dirac $\delta-$function is so concentrated about $k = k_o$ that neither $r(k)$ nor $t(k)$ vary significantly over the range of k for which $|\tilde{\psi}(k)|$ is appreciable. Under these circumstances, $|r(k)|$ may be replaced to a good approximation by its value at $k = k_o$, so that

$$\begin{aligned}
P_r &\approx \int dk\, |\tilde{\psi}(k)|^2 |r(k_o)|^2 \\
&= |r(k_o)|^2 \int dk\, |\tilde{\psi}(k)|^2 \\
&= |r(k_o)|^2,
\end{aligned}$$

which is what we found in (15) based on the probability current.

To determine the full, *exact* form of the probability of transmission P_t, we require the momentum space representation of $\Psi_t(x,t)$. To do this we note that (19) does not appear in the standard momentum representation form because the variable of integration, k, is not the same wave vector which appears describing the pure momentum states, k_t. To produce the more familiar form, we should thus change the variable of integration to k_t. (12) gives the relationship between k and k_t so that we may perform the change of variables in (19).

$$\begin{aligned}
\Psi_t(x,t) &= \int \frac{dk}{\sqrt{2\pi}}\, \tilde{\psi}(k) \sqrt{\frac{k}{k_t(k)}} t(k) e^{ik_t(k)(x-L)} e^{-i\frac{\hbar k^2}{2m}t} \\
&= \int \frac{\frac{dk_t}{(dk_t/dk)}}{\sqrt{2\pi}}\, \tilde{\psi}(k(k_t)) \sqrt{\frac{k(k_t)}{k_t}} t(k(k_t)) e^{ik_t(x-L)} e^{-i\frac{\hbar k^2(k_t)}{2m}t} \\
&= \int \frac{\frac{dk_t}{(k/k_t)}}{\sqrt{2\pi}}\, \tilde{\psi}(k(k_t)) \sqrt{\frac{k(k_t)}{k_t}} t(k(k_t)) e^{ik_t(x-L)} e^{-i\frac{\hbar k^2(k_t)}{2m}t} \\
&= \int \frac{dk_t}{\sqrt{2\pi}}\, \tilde{\psi}(k(k_t)) \sqrt{\frac{k_t}{k(k_t)}} t(k(k_t)) e^{ik_t(x-L)} e^{-i\frac{\hbar k^2(k_t)}{2m}t},
\end{aligned}$$

where we have used $dk_t/dk = k/k_t$ from (23) and have taken care to write everything now as a function of k. If needed, the function $k(k_t)$ is easily determined by inverting (12). Now that we have the standard form of the momentum superposition, we may pick-off the momentum space wave function, now in terms of k_t instead of k, thereby using in effect Parseval's theorem to determine the normalization of transmitted packet,

$$\tilde{\Psi}(k_t,t) = \sqrt{\frac{k_t}{k(k_t)}} t(k(k_t)) \tilde{\psi}(k(k_t)) e^{-ik_tL} e^{-i\frac{\hbar k^2(k_t)}{2m}t}$$

$$\Rightarrow$$

$$\begin{aligned} P_t &= \int dk_t\, \frac{k_t}{k(k_t)} |t(k(k_t))|^2 |\tilde{\psi}(k(k_t))|^2 \qquad (25) \\ &= \int dk_t\, \frac{1}{\frac{dk_t}{dk}} |t(k(k_t))|^2 |\tilde{\psi}(k(k_t))|^2 \\ &= \int dk\, |t(k)|^2 |\tilde{\psi}(k)|^2. \end{aligned}$$

Here again, we have used the identity (23), and in our last step changed the integration variable back to k. This is the full, *exact* expression for P_t. As with the reflected packet, it is easy to determine the transmission probability when working in the *narrow packet limit*,

$$\begin{aligned} P_t &\approx \int dk\, |t(k_o)|^2 |\tilde{\psi}(k)|^2 \\ &= |t(k_o)|^2 \int dk\, |\tilde{\psi}(k)|^2 \\ &= |t(k_o)|^2, \end{aligned}$$

which is what we found in (15) based on the probability current.

There are two important lessons to be learned from this section. First, the results (15) determined using the simpler idea of monitoring the transmitted and reflected contributions to the current were indeed correct, but only when the packet is very narrowly distributed in momentum space. It is important to keep this caveat in mind. In some cases in scattering theory, particularly in the study of resonance, $r(k)$ and $t(k)$ become very sharply peaked, so that it becomes very demanding to produce incoming wave packets with $|\tilde{\psi}(k)|$ which is truly narrowly peaked in comparison. The second lesson is that there are more exact expressions available (24,25) for the reflection and transmission probabilities in cases where the packet is not so narrow.

4 Example: Scattering from a Potential Step

Let us now carry out the program outlined in Section 3.1 for the example of the potential step first introduced in Figure 1, thereby in effect producing the results in Figure 2 for which until now we had to rely on a computer generated solution.

4.1 Solutions to the TISE

In this case we only have two regions separated by a point discontinuity in the potential at $x = 0$. Region s ends at $x = 0$ and Region t begins at $x = 0$. Region c is just the point $x = 0$.

The *left-incident* boundary conditions at $\pm\infty$ set the form of the wave function in Region t to a wave of the form $te^{ik_t x}$, where $k_t^2 = 2m(E - V_o)/\hbar$.

The general form of the solutions in Region s are oscillatory with wave vector $k_s \equiv k = 2mE/\hbar^2$. The most convenient form of such solutions for matching the boundary conditions at $x = 0$ is a combination of sine and cosine centered at $x = 0$, giving

$$\psi(x) = \begin{cases} A\cos kx + B\sin kx & x < 0 \\ e^{ik_t x} & x > 0 \end{cases}.$$

Matching boundary conditions at $x = 0$ gives the solution,

$$\begin{aligned} \psi_s(0) = \psi_t(0): &\qquad A = 1. \\ \psi_s'(0) = \psi_t'(0): &\qquad kB = ik_t \Rightarrow B = i\frac{k_t}{k}. \end{aligned}$$

A and B determine our full solution. To determine s and r, we now expand the sines and cosines in complex exponentials,

$$\begin{aligned}\psi_s(x) &= A\cos kx + B\sin kx \\ &= \left(\frac{e^{ikx}+e^{-ikx}}{2}\right) + i\frac{k_t}{k}\left(\frac{e^{ikx}-e^{-ikx}}{2i}\right) \\ &= \frac{1}{2}\left(1+\frac{k_t}{k}\right)e^{ikx} + \frac{1}{2}\left(1-\frac{k_t}{k}\right)e^{-ikx} \\ \psi_t(x) &= e^{ik_t x},\end{aligned} \tag{26}$$

where for completeness, we have also included the present form of the transmitted solution.

Given the raw solution 26, the next step in the solution process is to set the overall normalization of the solution. To extract proper quantum amplitudes, we must have a unit incoming current. The we achieve by multiplying the *entire* raw solution through by $2/(1+k_t/t)/\sqrt{\hbar k/m}$ resulting in

$$\begin{aligned}\psi_s(x) &= \frac{e^{ikx}}{\sqrt{\hbar k/m}} + \frac{1-k_t/k}{1+k_t/k}\frac{e-ikx}{\sqrt{\hbar k/m}} \\ \psi_t(x) &= \frac{2}{1+k_t/k}\frac{e^{ik_t x}}{\sqrt{\hbar k/m}}.\end{aligned}$$

This form now has a unit incoming current. In addition, we have the reflected beam expressed as a simple factor times the *unit* reflected beam $e^{-ikx}/\sqrt{\hbar k/m}$. The one difficulty with this form is that the transmitted beam is not also written in terms of a unit current beam because the wave vector in the transmitted part $e^{ik_t x}$ does not match the wave vector appearing in the normalizing square-root $\sqrt{\hbar k/m}$. To rectify this situation, we rearrange the factors in ψ_t, taking care to do absolutely nothing to change the final value of this part of the wave function, which is set entirely by Schrödinger's equation, our boundary conditions and the normalization to unit incoming current,

$$\begin{aligned}\psi_s(x) &= \frac{e^{ikx}}{\sqrt{\hbar k/m}} + \frac{1-k_t/k}{1+k_t/k}\frac{e-ikx}{\sqrt{\hbar k/m}} \\ \psi_t(x) &= \frac{2}{1+k_t/k}\sqrt{\frac{k_t}{k}}\frac{e^{ik_t x}}{\sqrt{\hbar k_t/m}}.\end{aligned}$$

Our final wave function, after some minor algebra of gathering factors and clearing fractions, is

$$\psi(x) = \begin{cases} \frac{e^{ikx}}{\sqrt{\hbar k/m}} + \frac{k-k_t}{k+k_t}\frac{e-ikx}{\sqrt{\hbar k/m}} & x<0 \\ \frac{2\sqrt{kk_t}}{k+k_t}\frac{e^{ik_t x}}{\sqrt{\hbar k_t/m}} & x>0 \end{cases}. \tag{27}$$

The quantum amplitudes for reflection and transmission are thus

$$\begin{aligned}r(k) &= \frac{k-k_t}{k+k_t} \\ t(k) &= \frac{2\sqrt{kk_t}}{k+k_t}\end{aligned} \tag{28}$$

4.2 Physical interpretation of the solution: probabilities of reflection and transmission and discussion

Physically, (27) corresponds to a source current of one particle impinging on the step per unit time, which then results in a current of $j_r = |r(k)|^2$ particles reflected per unit time and $j_t = |t(k)|^2$ particles transmitted per unit time. The probabilities of reflection and transmission are thus respectively $P_r = |r(k)|^2$ and $P_t = |t(k)|^2$.

We now have two cases to consider. In the case where $E > V_o$, both k and k_t are real numbers. We then have,

$$\begin{aligned} P_r &= \frac{(k-k_t)^2}{(k+k_t)^2} \\ P_t &= \frac{4kk_t}{(k+k_t)^2}. \end{aligned}$$

It is always good practice to check that the transmission and reflection probabilities sum to unity. In this case, we have

$$P_r + P_t = \frac{(k-k_t)^2 + 4k^2k_t^2}{(k+k_t)^2} = \frac{(k+k_t)^2}{(k+k_t)^2} = 1.$$

In the case where $E < V_o$, the solution in Region t is a decaying exponential. Such a function is a real function and the expression for the current $j_t = (\hbar/m)\Im\{\psi^* \partial_x \psi\}$ gives zero when ψ is a real function. Thus $P_t = 0$. For P_r we must take care to note that the wave vector in Region t is now imaginary, $k_t \equiv +i\alpha_t$, where

$$\alpha_t \equiv \sqrt{Q_o^2 - k^2}. \tag{29}$$

We verify our choice of k_t by noting that with this choice, $e^{ik_tx} = e^{-\alpha x}$, a proper exponentially decaying solution. With k_t determined in this way, we then have

$$P_r = \frac{|k - i\alpha_t|^2}{|k + i\alpha_t|^2} = \frac{k^2 + \alpha_t^2}{k^2 + \alpha_t^2} = 1.$$

Thus, also when $E < V_o$, we find $P_t + P_r = 1$.

Our full formula for the reflection probability may be written out as

$$P_r = \left| \frac{k - \sqrt{k^2 - \frac{2m}{\hbar^2}V}}{k + \sqrt{k^2 - \frac{2m}{\hbar^2}V}} \right|^2 = \left| \frac{1 - \sqrt{1 - V/\frac{\hbar^2k^2}{2m}}}{1 - \sqrt{1 + V/\frac{\hbar^2k^2}{2m}}} \right|^2 = \left| \frac{1 - \sqrt{1 - V/T}}{1 + \sqrt{1 - V/T}} \right|^2,$$

where T is the kinetic energy of the incoming particle. This quantity sets the basic energy scale for the problem. Plotting the scattering probabilities in terms of V/T, which is the strength of the potential in terms of the kinetic energy of the incoming particles, gives the results in Figure 11.

First we notice, that as expected, when there is no step ($V_o = 0$), there is perfect transmission, $P_T = 1$ and $P_R = 0$. For negative values of V_o/T, we have a downward step, and surprisingly (in classical terms) there is a non-zero probability of reflection. In fact, as $V_0/T \to -\infty$, $P_R \to 1$, and nearly all particles are reflected. From the wave-propagation point of view, this is not surprising. The k's describe the nature of propagation of the wave in the different regions. A large step V_o results is a large difference in how the waves propagate in each region, which generates a large reflection.

For $V_o/T > 0$, we are studying reflections from an upward step in potential. As V_o increases P_R increases from zero until we reach the special point where $V_o = T$. After this point, the kinetic energy of the incoming particle is less than the height of the potential barrier, so that as we have seen, the reflection probability becomes $P_r = 1$.

4.3 Time delay

In the case $E > V_o$, (28) gives t and r as just real numbers because k and k_t are real. The phases on t and r are just $\phi_t = 0$ and $\phi_r = 0$ for $k > k_t$ (an upward step) or $\phi_r = \pi$ for $k < k_t$ (a downward step). For either an upward or downward step, so long as $E > V_o$, the phases ϕ_r and ϕ_t are independent of k and therefore, according to (10) there is no time lag in the generation of the transmitted or reflected packets.

The case $E < V_o$ is somewhat different. There is no transmitted packet propagating in the forbidden region. However, there is a reflected packet $\Psi_r(x,t)$ which we have already studied in

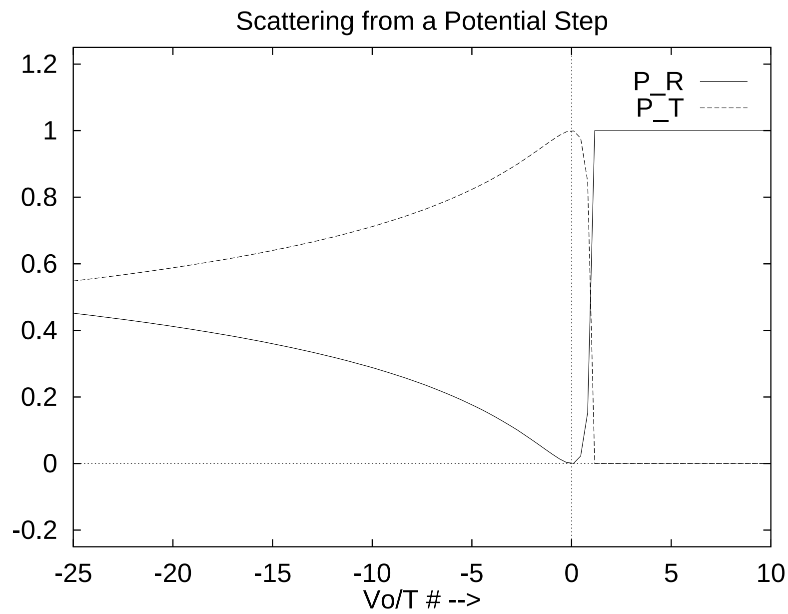

Figure 11: Scattering probabilities from a potential step of height Vo as a function of Vo/T, where T is the kinetic energy of the incoming particles.

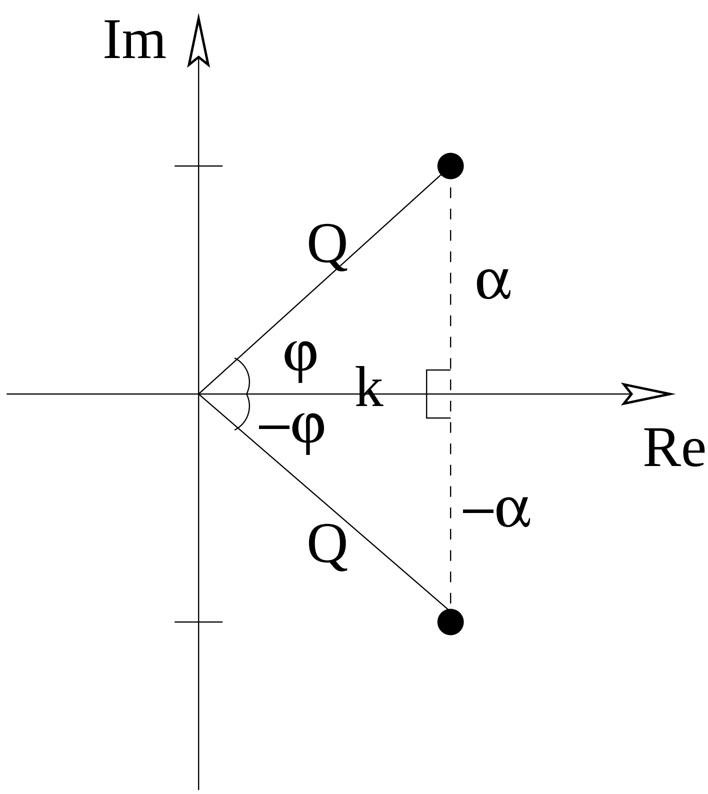

Figure 12: Components of ϕ_r in the complex plane

Section 3.7. There we showed that the time lag in the emergence of the reflected packet depends on the derivative of the phase of $r(k)$.

To help find this derivative we refer to Figure 12. As shown in the figure the complex numbers $k+i\alpha_t$ and $k-i\alpha_t$ appear opposite each other across the x-axis. Thus, if we denote the phase angle of $k+i\alpha_t$ by ϕ then then phase angle of $k-i\alpha_t$ will be $-\phi$. Now, because the phase angle of the ratio of two complex numbers is the difference between their phase angles and $r=(k-i\alpha_t)/(k+i\alpha_t)$, we have $\phi_r = -2\phi$. Next we note from (29) that $\alpha_t^2 + k^2 = Q_o^2$ which is also indicated in the figure as the length of the hypotenuse of each right triangle in the figure. From the figure we see that $\phi = \arccos(k/Q_o)$, and thus $\phi_r = -2\arccos(k/Q_o)$. Putting all of this together, we find

$$\begin{aligned}
\Delta t_r &= \frac{1}{v_{cl}^{(s)}}\partial_k \phi_r(k) \\
&= \frac{1}{v_{cl}^{(s)}}\partial_k \left(-2\arccos(k/Q_o)\right) \\
&= \frac{1}{v_{cl}^{(s)}} 2 \frac{\frac{1}{Q_o}}{\sqrt{1-(k/Q_o)^2}} \\
&= \frac{1}{v_{cl}^{(s)}} 2 \frac{1}{\sqrt{Q_o^2 - k^2}} \\
&= \frac{2/\alpha_t}{v_{cl}^{(s)}}.
\end{aligned}$$

For our labor we are rewarded with a simple result with a beautiful physical interpretation! The packet spends an extra time $(2/\alpha_t)/v_{cl}^{(s)}$ in the forbidden region. But, this is just the extra time the packet would take to penetrate a distance $1/\alpha_t$ into the forbidden region and then return. And, $1/\alpha_t$ is just the quantum penetration depth we expect into Region t!!!