

Notes on Feynman Diagrams for Scattering Problems in One Dimension

Tomás A. Arias

May 29, 1997

Massachusetts Institute of Technology

Department of Physics

Physics 8.04

May 29, 1997

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1 Introduction

At this point in our course we have developed our formal formulation of quantum mechanics directly from the de Broglie Hypothesis, verified that our formulation is consistent with all previously known experimental information, such as $F = ma$ from classical mechanics, and even gone on to make predictions of new phenomena using our formulation. It is important for the student to understand that our formulation of quantum mechanics is not unique, that there is more than one valid formulation of quantum mechanics. In fact there are three distinct formulations of quantum mechanics in common use today.

Each of these formulations is quite different in terms of the physics which it emphasizes. Given problems are usually most directly attacked within one of the formulations. Although these three formulations are quite different, they are all known to be equivalent. All three formulations include the following features a) events are viewed as probabilistic, b) the probability for the occurrence of an event is given by the complex magnitude squared of the corresponding *quantum amplitude*, and c) a prescription is given for computing the quantum amplitude associated with a given event. It is only in how the amplitudes are computed that the formulations differ. We know that all three formulations are equivalent because we can show that they all give the same quantum amplitudes.

The formulation which we have built up in this course is known as Wave Mechanics. This formulation, where amplitudes are computed by solving differential equations is due to Schrödinger. This formulation is most convenient when working with potentials of arbitrary form in one dimension. The second formulation is Matrix Mechanics, and is due to Heisenberg. We have had some exposure to this formulation in our treatment of the simple harmonic oscillator (SHO) where we used operator algebra rather than differential equations to determine the allowed states. In practice research physicists do not use matrix mechanics as originally formulated by Heisenberg. Rather, we usually work with operator algebra using a special notation developed by Dirac, known as “bra-ket” notation. This operator/bra-ket formulation of quantum mechanics is most convenient when working with problems with special symmetries such as the Simple Harmonic Oscillator, problems involving angular momentum and problems involving the spin of particles, and when dealing with multiple particle systems. In 8.05 and 8.059, you will be exposed heavily to this formulation. The third and final of the three equivalent formulations is due to Feynman. In this formulation, one computes amplitudes for events by summing over all ways in which the event may happen. In practice, this is done using Feynman diagrams. This formulation is extremely powerful and is mostly used in quantum field theory and in the study of many-particle systems such as those found in condensed matter physics. You will use this formulation in 8.323, 8.512 and 8.334. Table 1 summarizes the basic features of the three formulations.

2 The Sum Over Histories

The Feynman formulation of Quantum Mechanics builds three central ideas from the de Broglie hypothesis into the computation of quantum amplitudes: the probabilistic aspect of nature, superposition, and the classical limit. This is done by making the following three postulates:

1. *Events in nature are probabilistic with predictable probabilities P .*
2. *The probability P for an event to occur is given by the square of the complex magnitude of a quantum amplitude for the event, Q . The quantum amplitude Q associated with an event is the sum of the amplitudes q_h associated with every history leading to the event.*
3. *The quantum amplitude associated with a given history q_h is the product of the amplitudes f_i associated with each fundamental process in the history.*

Postulate (1) states the fundamental probabilistic nature of our world, and opens the way for computing these probabilities.

Postulate (2) specifies how probabilities are to be computed. This item builds the concept of superposition, and thus the possibility of quantum interference, directly into the formulation.

Formulation	Developer	Computation of Amplitudes	Best suited for	Course
Wave Mechanics	Schrödinger	Solve Diff Eq's	Arbitrary Potentials in One Dimension	8.04
Matrix Mechanics	Heisenberg/Dirac	Operator/Bra-ket Algebra	SHO, Angular Momentum, Spin	8.05, 8.059
Sum over Histories	Feynman	Feynman Diagrams	Field Theory, Many-body Physics	8.323, 8.512, 8.334

Table 1: Independent, equivalent Formulations of Quantum Mechanics

Specifying that the probability for an event is given as the magnitude-squared of a sum made from complex numbers, allows for negative, positive and intermediate interference effects. This part of the formulation thus builds the description of experiments such as the two-slit experiment directly into the formulation. A *history* is a *sequence* of fundamental processes leading to the the event in question. We now have an explicit formulation for calculating the probabilities for events in terms of the q_h , quantum amplitudes for individual histories, which the third postulate will now specify.

Postulate (3) specifies the quantum amplitude associated with individual histories in terms of *fundamental processes*. A *fundamental process* is any process which cannot be interrupted by another fundamental process. The *fundamental processes* are thus indivisible “atomic units” of history. With this constraint of the choice of *fundamental processes*, individual histories may always be divided unambiguously into ordered sequences of fundamental events, which is key to making a consistent prescription for computing the amplitudes of individual histories from *fundamental processes*. The fact that the definition of fundamental processes is not very specific is actually one of the strongest aspects of the Feynman approach. As we will see, we may sometimes discover that we may lump fundamental processes together into larger units which make up new fundamental processes. This procedure is know as renormalization and is one the the great central ideas in managing the infinities in quantum field theory.

The third postulate builds in the classical limit by allowing recovery of the classical physics notion that the probability of an *independent* sequence of events is the product of the probabilities for each event in the sequence. If we know the sequence of fundamental processes leading to an event, the only contributing history is that sequence of processes. In such a case, we have $Q = q_h = \prod f_i$ so that then $P = \prod |f_i|^2 = \prod p_i$, where the $p_i \equiv |f_i|^2$ are just the probabilities for the individual processes in the sequence, and we recover the usual classical probabilistic result.

What remains unspecified by these postulates is the specification of a valid set of fundamental processes and corresponding quantum amplitudes f_i for the phenomena we wish to describe. For this information, we must rely upon experimental observations. It is at this point that experimental information is input into the Feynman formulation much like how we inputted experimental information into our formulation when we produced the forms for our operators and the Schrödinger Equations.

A great appeal to the Feynman sum over histories approach is that often we are able to intuit the nature and amplitudes of the fundamental events. A natural way to build the de Broglie hypothesis $\lambda = h/p$ from the Davisson-Germer and G.P. Thomson experiments into the formulation, for instance, would be to ascribe a quantum amplitude of $p = \exp(ika)$ for the propagation of a particle with momentum $\hbar k$ across a distance a .

Another common way to infer the fundamental events and associated amplitudes is to determine the amplitudes for fundamental processes from the requirement that the Feynman formulation always give the same results as an already established approach, such as Schrödinger formulation. This latter procedure is referred as *construction of Feynman rules*, and is also how we determine that the Feynman approach is indeed equivalent to the other formulations of quantum mechanics. We shall follow this procedure in the next section.

3 Construction of Feynman Rules for One-Dimensional Scattering

In practice, the rules for formulating the Feynman approach within a given context are often derived from another established formulation. The overall procedure we shall follow here for scattering problems in one dimension is the same as employed in far more complicated contexts. The procedure for constructing Feynman rules is very intuitive and usually precedes by generalizing from specific examples. The example with which we shall work is scattering from a potential barrier as pictured in Figure 1.

The first stage in the process is agreeing on a pictorial notation for the relevant mathematical functions. This we do in Section . We then immediately, in Section 3.2, make use of our new diagrams to prove some very interesting theorems about how the transmission and reflection probabilities and delays compare when we approach a potential from both the left and the right.

Once we are familiar with the diagrams, we then use the diagrams to compute in a new way, but still within the Schrödinger formulation, the scattering amplitudes for a specific problem. This new approach (Section 3.3) to computing the scattering amplitudes is sufficiently close to the postulates of the Feynman formulation that in Section 3.4 we are able to prove that the Feynman formulation is indeed equivalent to the Schrödinger approach, for the specific problem which we have taken up. Section 3.5 then generalizes our results from the specific problem to arbitrary problems in one dimensional scattering theory. As the last topic in this section we then complete our discussion by specifying specific Feynman rules for scattering problems involving forbidden regions.

After developing the Feynman rules for one dimensional scattering, we then take up in Section 4 the mathematics of performing the resulting Feynman sums.

3.1 Construction of Feynman Diagrams

3.

From our Schrödinger formulation, we know that the allowed solutions to the TISE in the three regions (s), (c) and (t) of Figure 1 are forward and backward traveling plane waves with wave vectors k , k_c and k , where $k \equiv \sqrt{2mE/\hbar^2}$ and $k_c \equiv \sqrt{2m(E - V_o)/\hbar^2}$, respectively. We may generally choose to represent these components of the final wave function as

$$a(x) \equiv e^{ikx}/\sqrt{\hbar k/m} \quad \text{for } x < 0 \quad (1)$$

$$b(x) \equiv e^{-ikx}/\sqrt{\hbar k/m} \quad \text{for } x < 0 \quad (2)$$

$$c(x) \equiv e^{ik_c x}/\sqrt{\hbar k_c/m} \quad \text{for } 0 < x < a \quad (3)$$

$$d(x) \equiv e^{-ik_c x}/\sqrt{\hbar k_c/m} \quad \text{for } 0 < x < a \quad (4)$$

$$e(x) \equiv e^{ik_c(x-a)}/\sqrt{\hbar k_c/m} \quad \text{for } 0 < x < a \quad (5)$$

$$f(x) \equiv e^{-ik_c(x-a)}/\sqrt{\hbar k_c/m} \quad \text{for } 0 < x < a \quad (6)$$

$$g(x) \equiv e^{ik(x-a)}/\sqrt{\hbar k/m} \quad \text{for } x > a \quad (7)$$

$$h(x) \equiv e^{-ik(x-a)}/\sqrt{\hbar k/m} \quad \text{for } x > a. \quad (8)$$

We have taken care to make each of our eight component solutions $a(x) \dots h(x)$ to carry unit current and to center each at an appropriate point. We list two sets of solutions $c(x), d(x)$ and $e(x), f(x)$ for

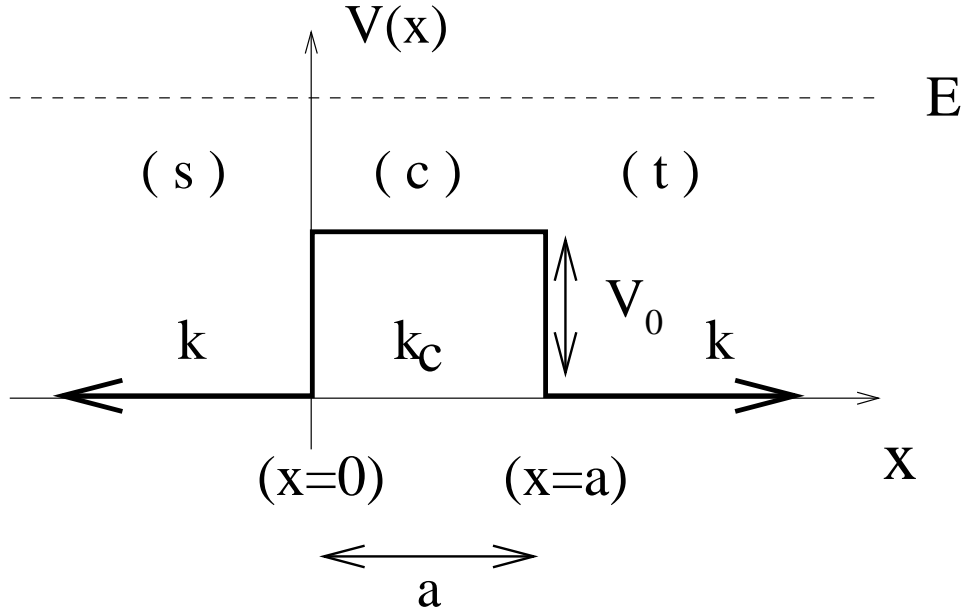


Figure 1: A potential barrier

region (c), as the solutions in the corresponding region generally must satisfy boundary conditions at the two end points, $x = 0$ and $x = a$.

The first step in developing the Feynman rules is to agree upon a short-hand diagrammatic representation for all of these functions. Figure 2 shows these eight *Feynman diagrams*. Each time we draw one of these diagrams, it is meant to represent one of the eight functions (1-8). We may then use these diagrams rather than algebraic functions to write down equations.

Two important equations relate $c(x)$ to $e(x)$ and $d(x)$ to $f(x)$. These pairs of functions represent the same physical state, a current flowing in Region (c) either to the right or left, respectively, and thus are related by a constant factors,

$$c(x) = e^{ik_c a} e(x) \tag{9}$$

$$f(x) = e^{ik_c x} d(x). \tag{10}$$

The complex exponential factor connecting these will appear so often in our analysis of scattering from this potential barrier that we give it a special name. As it represents the effect on the wave function of “propagating” across Region (c), we call the factor p for “propagation,”

$$p \equiv e^{ik_c a}. \tag{11}$$

We now make our first diagrammatic equations. To represent (9) and (10) *diagrammatically*, we use the definitions from Figure 2 to produce the two diagrammatic equalities in Figure 3.

3.2 Use of Feynman Diagrams to Prove General Theorems in Scattering Theory: Time Reversal and Parity

By giving us a short-hand notation, Feynman diagrams are very convenient for proving identities in quantum mechanics. In this section we apply the diagrams to investigate how the transmission and reflection probabilities and time delays compare when particles approach a collision potential from all possible directions. This will not only give us interesting insights into the physics of the scattering process but will also provide us with important identities for our later general discussion.

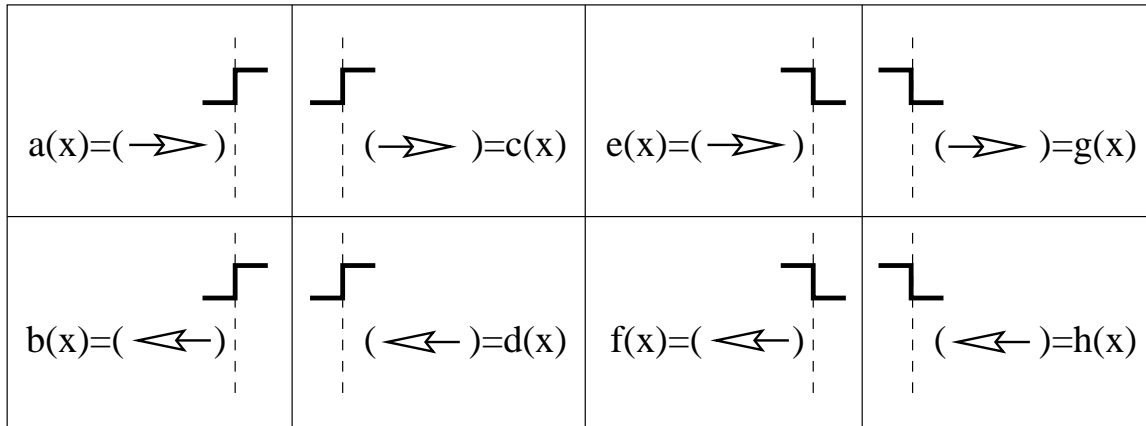


Figure 2: Eight *Feynman Diagrams* corresponding to the eight solutions to the TISE $a(x), b(x), \dots, h(x)$

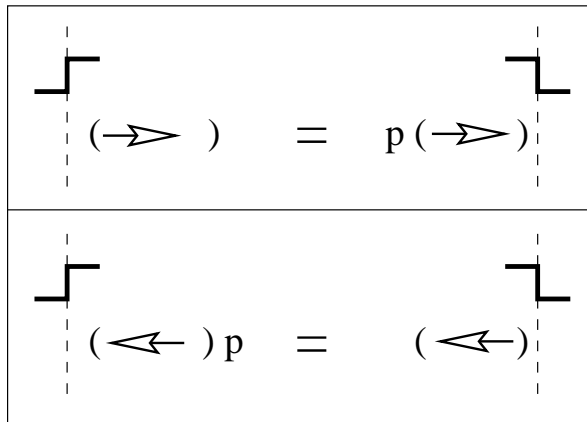


Figure 3: Diagrammatic Expression of Two Scattering Identities 9 and 10 (top and bottom panels, respectively)

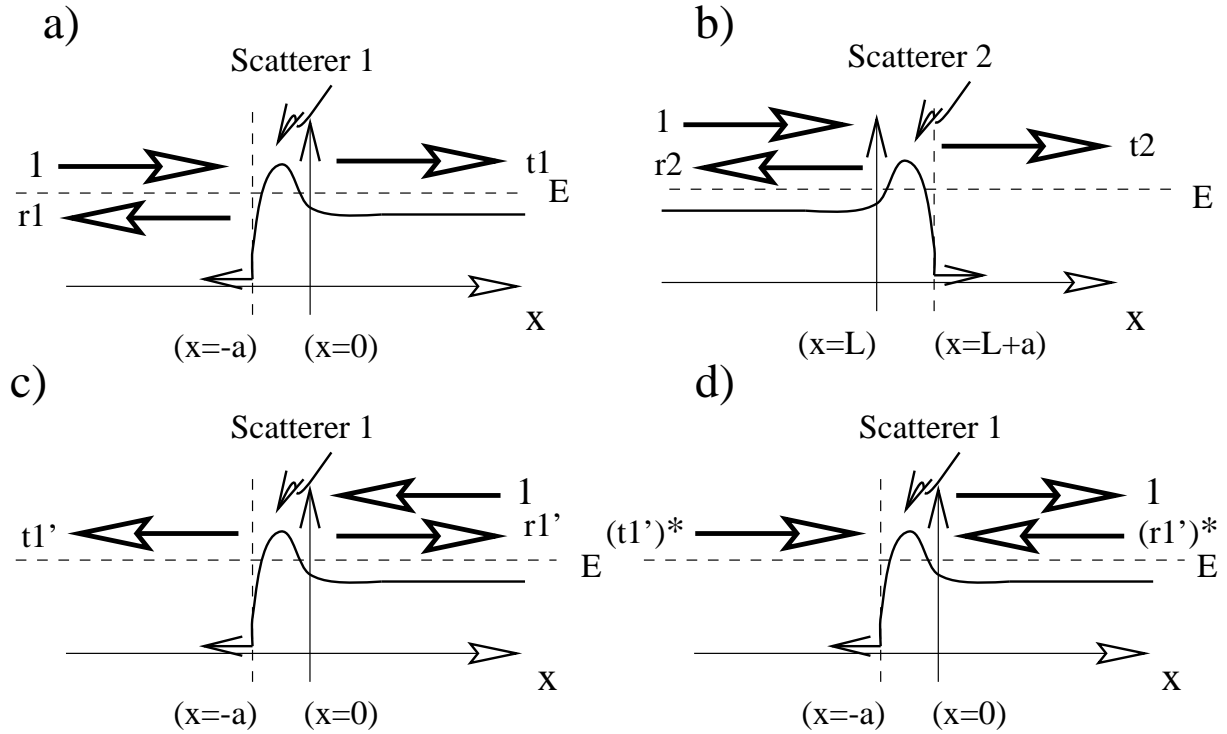


Figure 4: Scattering from a general potential from various directions: a) Initial approach to the first scatterer from the left (t_1, r_1), b) left-approach to the second, reflected scatterer (t_2, r_2), c) approach to the first scatterer from the right, d) time-reversal of c). The two scatterers have width a .

The results we find here are not necessary in our construction of the Feynman formulation, but appear here to help familiarize the student with representing wave functions as diagrams.

We first compare what happens when we approach an arbitrary collision potential from the left to what happens when we approach the mirror-image of that potential from the right, as in Figures 4b and 4c. By symmetry and physical reasoning, the transmission and reflection amplitudes and delays must be the same in both cases. As these two physical quantities determine both the magnitude and phase derivatives of the quantum amplitudes, the quantum amplitudes for reflection and transmission in these two situations may differ by at most a constant phase factor. Below in Section 3.2.1 we give a formal proof for the interested student using Feynman diagrams that the quantum amplitudes are precisely equal for both cases.

We then turn to what happens when we approach the same potential but from two different directions, as in Figures 4a and 4c. Now, when the overall potential is not symmetric, the situation is not so clear, and the results somewhat surprising. It turns out the the probabilities for transmission and reflection are in fact always identical, regardless of the direction from which we approach the potential! Although the time delays for reflection need not be identical, the time delays for transmission are always equal. Finally, the sum of the transmission delays for both directions must equal the sum of the two transmission delays. For the interested student, we use Feynman diagrams to prove these intriguing properties in Section 3.2.2 below.

Note on notation: Because the reflection amplitudes across a barrier are different in the two directions, we shall denote them by r and r' , where a “'” denotes right-incidence and the lack of one denotes left-incidence. Because a theorem shows that the transmission amplitudes must always be identical in both directions, it is not necessary is to make a distinction between t and t' . Nonetheless,

we will at times use both t and t' to remind us of the physical origin of the different factors.

3.2.1 (*) Scattering amplitudes from mirror-image potentials

Let us denote the potentials for Scatters 1 and 2 by $V_1(x)$ and $V_2(x)$, respectively. These two potentials are related to each other by reflection about the point $L/2$ so that $V_1(x) = V_2(L - x)$. This linear mapping may be verified by noting that under this transform the point $-a$ maps to $-a \rightarrow L + a$ and the point 0 maps to $0 \rightarrow L$, and from Figure 4, which are indeed the corresponding points in the two potentials.

If $\psi_1(x)$ is the scattering solution for $V_1(x)$, by symmetry we expect that $\phi(x) \equiv \psi_1(L - x)$ will be a solution for the scattering problem associated with the potential $V_2(x)$. This is verified by inserting $\phi(x)$ directly into the TISE for the potential $V_2(x)$,

$$\begin{aligned}
-\frac{\hbar^2}{2m}\partial_x^2\phi(x) + V_2(x)\phi(x) &= \\
&= -\frac{\hbar^2}{2m}\partial_x(\partial_x\psi_1(L-x)) + V_1(L-x)\phi_1(L-x) \\
&= -\frac{\hbar^2}{2m}\partial_x(-\psi_1'(L-x)) + V_1(L-x)\psi_1(L-x) \\
&= -\frac{\hbar^2}{2m}\psi_1''(L-x) + V_1(L-x)\psi_1(L-x) \\
&= E\psi_1(L-x) \quad ; \text{ from the TISE for state } \psi_1 \\
&= E\phi(x) \quad (!)
\end{aligned}$$

Algebraically, this means that if we start with the $\psi_1(x)$ pictured in 4c,

$$\psi_1(x) = \begin{cases} t'_1 \frac{e^{-ik(x+a)}}{\sqrt{\hbar k/m}} & x < -a \\ ?(x) & -a < x < 0 \\ \frac{e^{-ik_c x}}{\sqrt{\hbar k_c/m}} + r'_1 \frac{e^{ik_c x}}{\sqrt{\hbar k_c/m}} & 0 < x \end{cases}, \quad (12)$$

where $?(x)$ indicates the unspecified form for the solution within the scattering region, and then form $\phi(x) \equiv \psi(L - x)$, we find a solution to the TISE for Scatterer 2 of the form

$$\phi(x) = \begin{cases} t'_1 \frac{e^{-ik(L-x+a)}}{\sqrt{\hbar k/m}} & L-x < -a \\ ?(L-x) & -a < L-x < 0 \\ \frac{e^{-ik_c(L-x)}}{\sqrt{\hbar k_c/m}} + r'_1 \frac{e^{ik_c(L-x)}}{\sqrt{\hbar k_c/m}} & 0 < L-x \end{cases} = \begin{cases} t'_1 \frac{e^{ik(x-(L+a))}}{\sqrt{\hbar k/m}} & L+a < x \\ ??(x) & L < x < L+a \\ \frac{e^{ik_c(x-L)}}{\sqrt{\hbar k_c/m}} + r'_1 \frac{e^{-ik_c(x-L)}}{\sqrt{\hbar k_c/m}} & x < L \end{cases}$$

This algebraic relationship may be summarized in a very intuitive way by stating that we may flip around any Feynman diagram, as indicated in Figure 5, and produce a valid solution to the TISE.

The connection between the quantum amplitudes comes about when we inspect the result of the flipping process. The result in Figure 5 shows a perfect, properly normalized scattering wave function, with a unit wave approaching Scatterer 2 from the left and no returning current from the side opposite the source. We may therefore read the quantum amplitudes for left-incident reflection and transmission from Scatter 2 from the new diagram as r'_1 and t'_1 , respectively. However, from Figure 4c we see that these quantities were originally defined as r_2 and t_2 . Therefore we conclude

$$\begin{aligned}
r_2 &= r'_1 \\
t_2 &= t'_1,
\end{aligned}$$

that the quantum amplitudes for reflection and transmission when approaching mirror image potentials from opposite directions are exactly equal, which is consistent with what we expected on physical grounds.

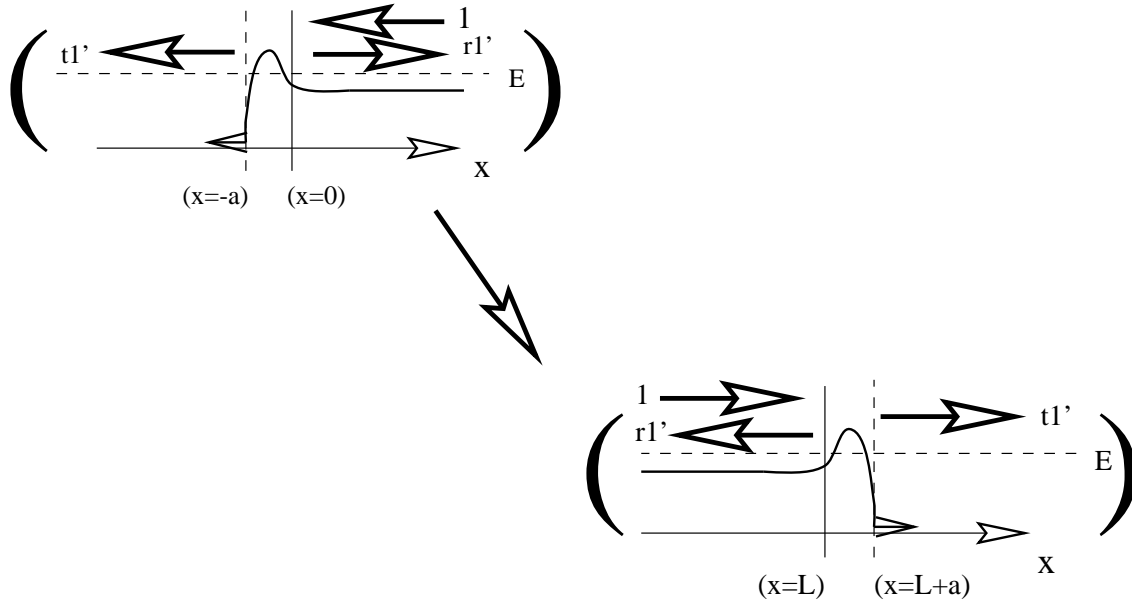


Figure 5: Reflection symmetry expressed in Feynman Diagrams

3.2.2 (*) Scattering of the same potential from two different directions: Time reversal symmetry

Approaching a potential from the left looks very much like what we expect to see when playing backwards a movie of what happens when we approach the potential from the right. We now use the idea of reversing time to study these two distinct processes. The only place where i appears in the TDSE is next to the time derivative operator,

$$i\hbar\partial_t\Psi = \left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x)\right)\Psi.$$

Reversing time (letting $t \rightarrow -t$) would simply change the sign on the first term in this equation. We could achieve the same effect more simply by just letting $i \rightarrow -i$. Inverting the sign on i like this is the process of complex conjugation. Thus, to study what happens when we reverse time, we consider what happens when we take the complex conjugate of the wave function. As we will see, this has precisely the intended effect: doing this to a solution to the TISE produces another valid solution, but one in which the direction of all currents is reversed.

The reason why complex conjugated wave functions also satisfy the TISE is that the TISE is a real differential equation,

$$-\frac{\hbar^2}{2m}\partial_x^2\psi(x) + V(x)\psi(x) = E\psi(x).$$

Because no factors of i appear explicitly in this equation, taking the complex conjugate of both sides gives,

$$-\frac{\hbar^2}{2m}\partial_x^2\psi^*(x) + V(x)\psi^*(x) = E\psi^*(x).$$

We thus see that if $\psi(x)$ is a solution to the TISE, then so is the function $\phi(x) \equiv \psi^*(x)$.

Algebraically, the result of doing this to the wave function (12) is

$$\phi(x) = \begin{cases} (t_1^*)^* \frac{e^{ik(x+a)}}{\sqrt{\hbar k/m}} & x < -a \\ ?^*(x) & -a < x < 0 \\ \frac{e^{ik_c x}}{\sqrt{\hbar k_c/m}} + (r_1^*)^* \frac{e^{-ik_c x}}{\sqrt{\hbar k_c/m}} & 0 < x \end{cases} \quad (13)$$

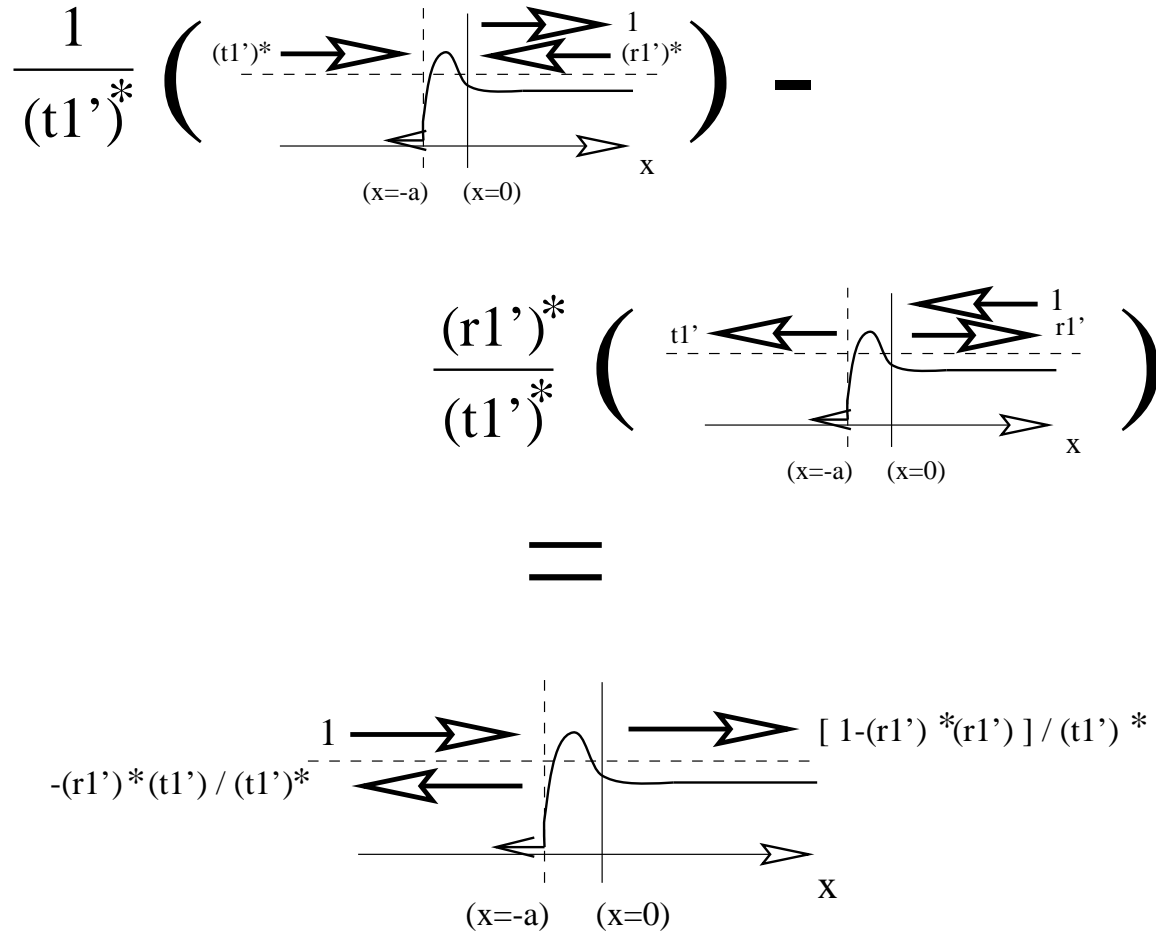


Figure 6: Use of time reversal symmetry to compute left- from right-scattering amplitudes

Figure 4d shows the corresponding Feynman diagram.

Our new solution to the TISE differs from the original in two ways. First, we have had the intended effect of reversing the direction of all currents in the wave function. A subsidiary effect is that the associated quantum amplitudes are all complex conjugated as well. Although we began with the wave function for scattering from Scatterer 1 from the right, inspection of the new solution which we have generated to the TISE shows that we cannot use it directly to determine the scattering amplitude for Scatterer 1 from the left. The new wave function describes an odd, but completely time reversed scenario, where particles now first approach the potential from both directions and then are transmitted out in a single beam moving to the right.

Although the new wave function which we have produced does not correspond to a familiar scenario, because the TISE is a linear equation, we may make a linear combination of the wave function (d) with the original wave function (c) and produce another solution to the TISE. By the proper choice of linear combination, we may arrange to reproduce an appropriate wave function for left-incident scattering. The appropriate combination is carried out diagrammatically in Figure 6, from which we may extract the reflection and transmission amplitudes for approaching Scatterer 1 from the left.

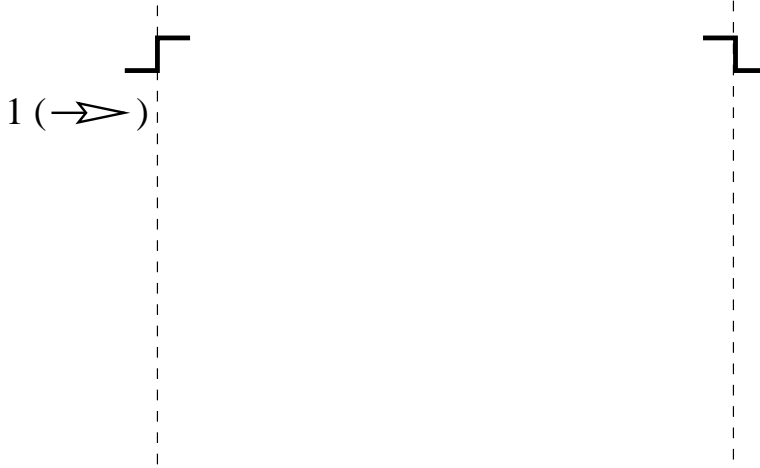


Figure 7: A unit left-incident current

Identifying terms from Figure 4a, we first conclude that

$$(t_1) = \frac{1 - (r_1')^*(r_1')}{(t_1')^*} = \frac{(t_1')^*(t_1')}{(t_1')^*} = (t_1'),$$

where we have used conservation of probability, $|r_1'|^2 + |t_1'|^2 = 1$. This result is somewhat surprising. Physically, the equality of left- and right-incident transmission amplitudes means that the *transmission* probabilities and time delays for a barrier are *independent of the direction* of approach. The barrier need not be symmetric!

Of course, if the transmission probabilities are the same for both directions, then the probabilities for reflection must be the same. The situation for the reflection time delays a little more subtle. Comparing Figures 4a and 6 shows that $(r_1) = -(r_1')^*(t_1')/(t_1')^*$. Rearranging and using the fact that $t_1 = t_1'$ leads to $(r_1)/(r_1')^* = -(t_1)/(t_1')^*$. Analyzing the phases in this relationship we see that $\phi_{r_1} + \phi_{r_1'} = \pi + \phi_{t_1} + \phi_{t_1'}$. Because the derivatives of these phases determine the time delays, *the sum of the time delays for reflection in both direction is exactly the same as the sum of the two time delays.*

An interesting special case is that of a symmetric scatterer. In this case, the reflection delays in both directions must be equal by symmetry, but then because they give the same sum as the two equal transmission delays, *the time delay for reflection and the time delay for transmission are identical for a symmetric scattering potential.*

3.3 Application of Diagrams to Compute Scattering Amplitudes

Let us now use our diagrams to compute the scattering amplitudes for the potential of Figure 1. We begin with an incoming wave from the source carrying a unit current, as expressed in Figure 7. This diagram represents the wave function $a(x)$, which is zero in Regions (c) and (t), and, as such, violates the boundary conditions at $x = 0$.

As we have learned, to satisfy the boundary conditions at $x = 0$, we must include both a transmitted and reflected current, with factors arranged to satisfy the boundary conditions in the presence of a unit incoming current. These are precisely the same conditions we impose when computing scattering from an upward step as in the “Notes on Scattering Theory.” Including reflected and transmitted waves, $r_1 \cdot b(x)$ and $t_1 \cdot c(x)$, with the same prefactors $r_1(k)$ and $t_1(k)$ as we found for scattering from a single upward step,

$$r_1(k) = \frac{k - k_c}{k + k_c} \tag{14}$$

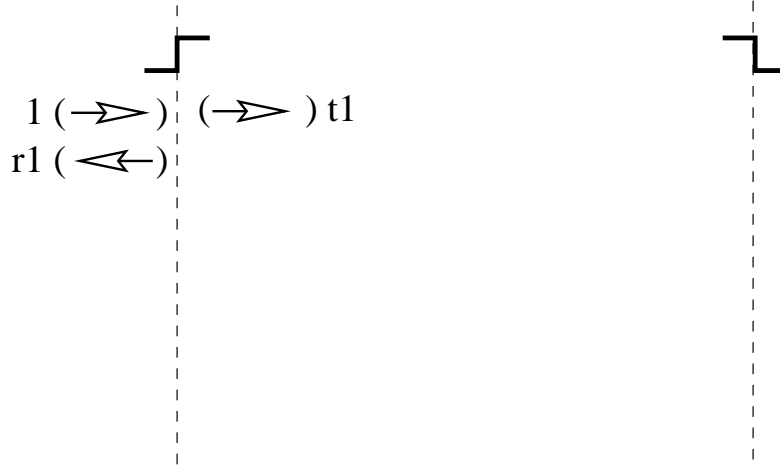


Figure 8: Satisfying the boundary conditions at $x = 0$

$$t_1(k) = \frac{2\sqrt{k k_c}}{k + k_c},$$

will therefore satisfy the boundary conditions at $x = 0$. The diagrammatic representation of the present stage in our solution to the TISE appears in Figure 8. Here, the factors r_1 and t_1 appearing next to the reflected and transmitted beams are multiplicative factors. As we will see in Section 3.4, this determines the appropriate quantum amplitudes for the fundamental events of reflecting and transmitting across the first step.

The wave function diagrammed in Figure 8 has been designed to satisfy the boundary condition at $x = 0$ but still represents a zero wave function in Region (t). The present solution now violates the boundary condition at $x = a$. To match this boundary condition, we follow a procedure similar to that in the previous paragraph. However, as our standardized form for scattering amplitudes is based upon current carrying functions centered at the point of matching boundary conditions, $x = a$ in this case, it is best to first use (9) to express our solution in Region (c) in a form centered at $x = a$. This results in the function $t_1 p \cdot e(x)$ as indicated in Figure 9. As we will see in Section 3.4, this determines the appropriate quantum amplitude for the fundamental event of propagating across the barrier.

Now we face the standard scattering boundary condition problem for a downward step in potential, except that rather than a unit incoming current, the incoming current carries a factor $t_1 p$. We know that the solution

$$\begin{aligned} \phi_c(x) &= e(x) + r_2(k)f(x) \\ \phi_t(x) &= t_2(k), \end{aligned}$$

satisfies these boundary conditions when $r_2(k)$ and $t_2(k)$ are the usual scattering amplitudes from a downward step,

$$\begin{aligned} r_2(k) &= \frac{k_c - k}{k + k_c} \\ t_2(k) &= \frac{2\sqrt{k k_c}}{k + k_c}. \end{aligned} \tag{15}$$

Because the TISE is linear, we may multiply this solution to the TISE by any constant factor and still satisfy the boundary conditions at $x = a$. To match our incoming wave $t_1 p e(x)$, the factor which we should use is clearly $t_1 p$. Doing this then generates the waves $t_1 p r_2 \cdot f(x)$ and $t_1 p t_2 \cdot g(x)$

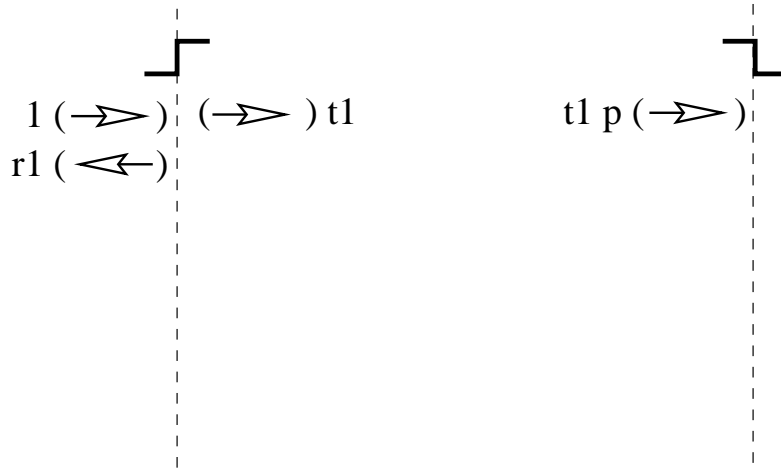


Figure 9: Propagating the solution to test boundary conditions at $x = a$

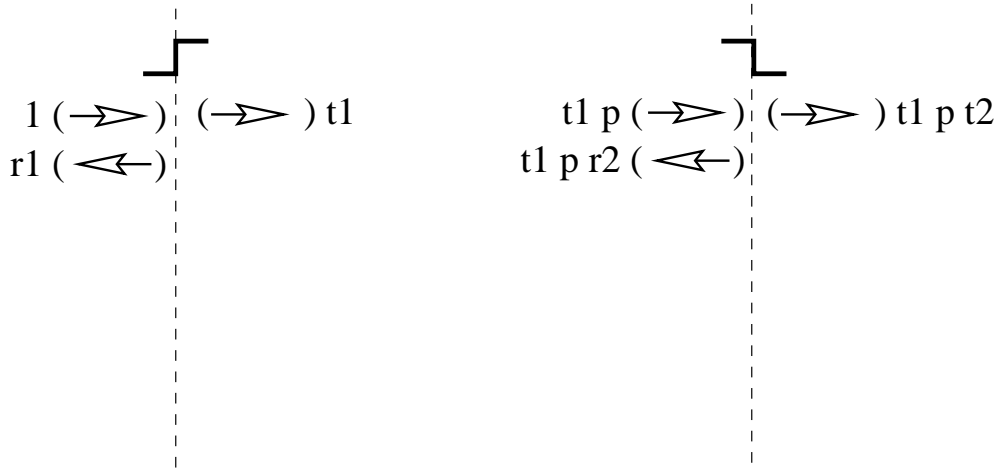


Figure 10: Satisfying the boundary conditions at $x = a$

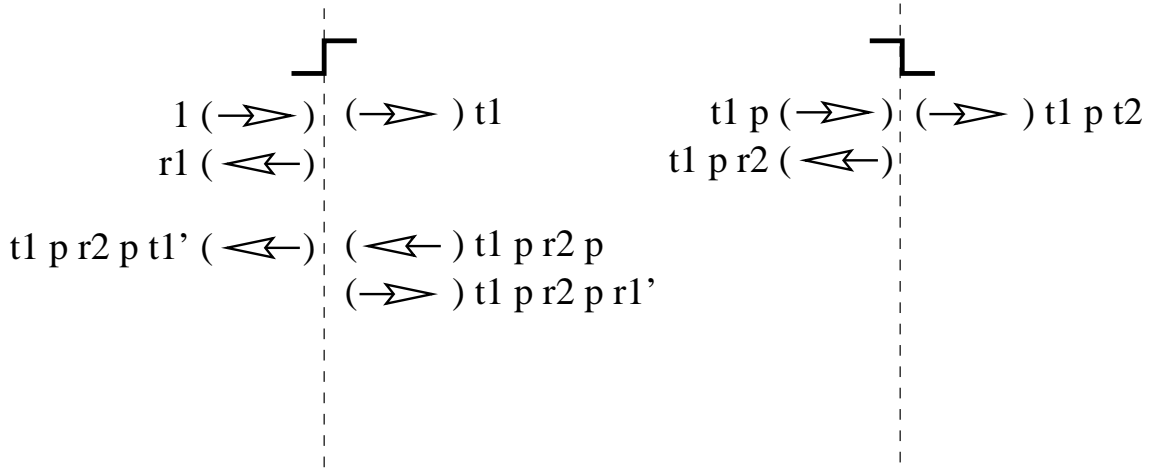


Figure 11: Propagating back to $x = 0$ and re-satisfying the boundary conditions

as diagrammed in Figure 10. As we will see in Section 3.4, this determines the appropriate quantum amplitudes for the fundamental events of reflecting and transmitting from the second step.

The wave function diagrammed in Figure 10 satisfies the boundary conditions at $x = a$; however, the new reflected current in Region (c) designed to satisfy the boundary condition at $x = a$ now violates the boundary condition at $x = 0$. To match this boundary condition, it is most convenient to use the identity (10) to re-express this solution in terms of a wave centered at $x = 0$, resulting in $t_1 p r_2 p \cdot d(x)$, as indicated in Figure 11. This now brings a new uncompensated current to the boundary conditions which previously had been in perfect balance at $x = 0$. Because the TISE is linear, to satisfy the boundary condition at $x = 0$ we need only add the reflected and transmitted waves corresponding to the *new* current $t_1 p r_2 p \cdot d(x)$. This new current now approaches a *downward* step from the *right*. As shown in Section 3.2.1, the quantum amplitudes r'_1, t'_1 for this are the same as those for approaching the mirror image from the right,

$$\begin{aligned}
 r'_1(k) &= \frac{k_c - k}{k + k_c} \\
 t'_1(k) &= \frac{2\sqrt{k k_c}}{k + k_c}.
 \end{aligned}
 \tag{16}$$

Making the appropriate adjustment for the fact that the incoming wave carried the factor $t_1 p r_2 p$ instead of 1, the reflected and transmitted parts needed to balance the boundary conditions at $x = 0$ are $t_1 p r_2 p r'_1 \cdot c(x)$ and $t_1 p r_2 p t'_1 \cdot b(x)$, respectively. This ultimately determines the quantum amplitudes for reflection and transmission when approaching the first step from inside the barrier.

These contributions are included in Figure 11. We now have two contributions to the final reflected current. Note that the presence of two forward arrows in Region (c) and two backward arrows in Region (s) (representing the functions $c(x)$ and $b(x)$ respectively) means that these terms should be added in producing the total wave represented by the diagram.

Having adjusted the boundary condition at $x = 0$, we have once again disturbed the boundary condition at $x = a$. Figure 12 shows the result of propagating this disturbance to the other side of the barrier and adjusting the boundary condition at $x = a$. The result is a second contribution to the final transmitted current and another term which will then require adjustment of the boundary condition at $x = 0$.

We may continue this process, alternately satisfying the boundary conditions at $x = 0$ and at $x = a$. At each stage in the process, some current leaks out of Region (c) so that the violation of the boundary condition at $x = 0$ or $x = a$ gets smaller and smaller. Continuing the processes *ad*

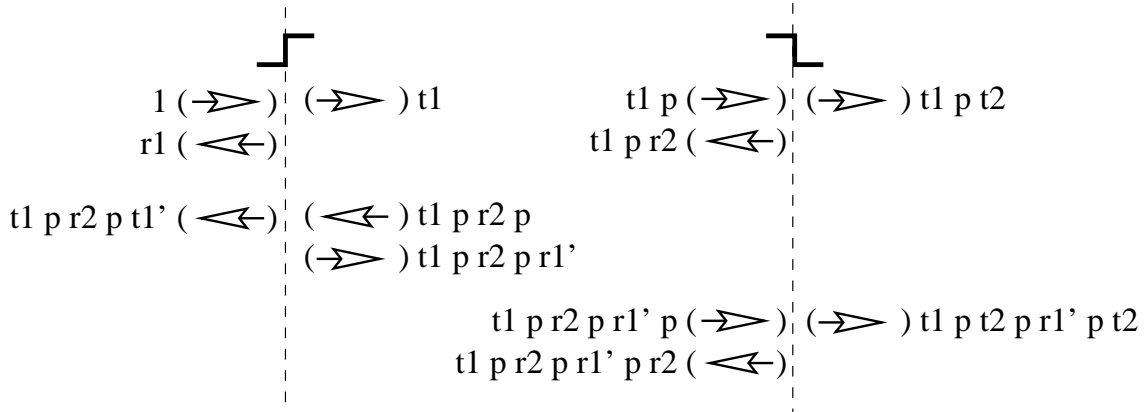


Figure 12: Propagating back to $x = a$ and re-satisfying the boundary conditions

infinitum eventually leads to a solution which satisfies all boundary conditions, and we will have built up a solution to the TISE with a proper unit left-incident current and no returning current from the far side of the source. The total of the factors multiplying the reflected current $b(x)$ and the final transmitted current $g(x)$ will then be quantum amplitudes for reflection $R(k)$ and transmission $T(k)$ from the *entire* barrier. As we see from Figure 12, these amplitudes are therefore

$$\begin{aligned} R(k) &= r_1 + t_1 p r_2 p t_1' + \dots \\ T(k) &= t_1 p t_2 + t_1 (p r_2 p r_1') p t_2 + \dots \end{aligned} \quad (17)$$

As we shall see in the next section, the Feynman formulation gives us an organized, extremely efficient short-hand for generating these factors.

3.4 Extracting the rules

Let us now see how the expressions (17) which we determined for the transmission and reflection amplitudes fit within the Feynman formulation. We first focus on the amplitude for transmission $T(k)$. Figure 12 shows the generation of two of the terms which contribute to the sum which gives the final transmission amplitude. According to Postulate (2) of the Feynman formulation, each of these terms corresponds to an individual history leading to transmission across the barrier.

From the form of the amplitude associated with the first term, $t_1 p t_2$, we know from Postulate (3) that three fundamental processes make up the first history. These processes (and associated quantum amplitudes) are 1) transmission across the first step (t_1), propagation across the barrier (p), 3) transmission across the second step (t_2). This sequence of fundamental processes is clearly one possible history which we associate with the final transmission of a particle across the barrier. Figure 13.1 shows a short-hand for representing this sequence of fundamental events. We now connect the arrows from Figure 13 and place the factor associated with each fundamental process on the diagram near where the corresponding process occurs. The amplitude associated with the Feynman diagram for this first history is simply the product of all factors written near it, where the values of these and the factors used below are given by (11,14,15,16).

The next term contributing to the transmission amplitude from Figure 12 is $t_1 p r_2 p r_1' p t_2$. This term was generated as we satisfied boundary conditions in the sequence of events which Figure 13.2 illustrates: transmission through the first step (t_1), propagation across the barrier (p), reflection from the second step (r_1), propagation back across the barrier (p), reflection from the first step as approached from the right (r_1'), propagation across the barrier (p) and transmission across the

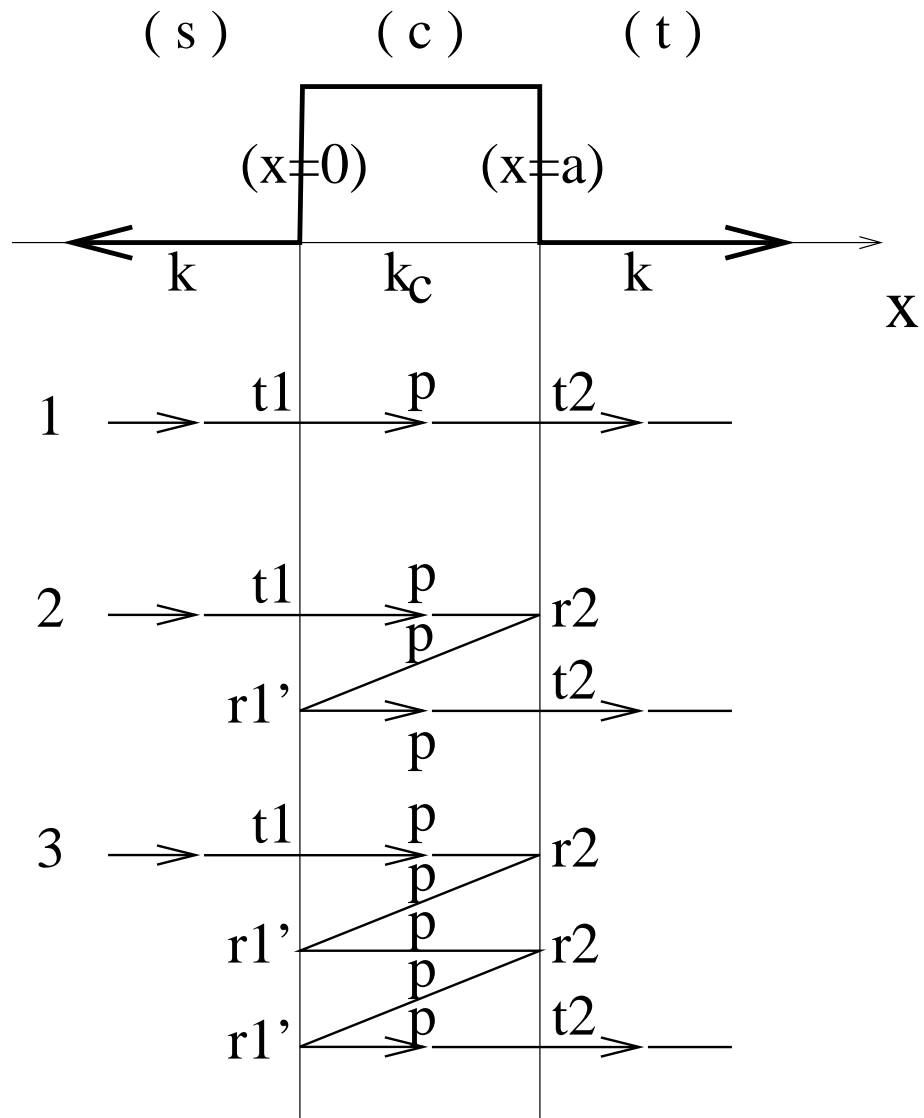


Figure 13: List of Histories Leading to a Transmission Event

second step t_2 . This again is another history which we associate with transmission across the barrier as we generate reflections and transmissions at all points for which there is a change in the potential and therefore the possibilities of a reflection. We also include factors for the processes of crossing the regions in between these scattering points. Clearly, as we continue to patch up unbalanced boundary conditions we may generate an arbitrary number of reflections back and forth within the barrier before the final transmission process occurs. The third order term in the sequence is also indicated in Figure 13.

The same logic applies for the terms leading to reflection. The *Feynman diagrams* for reflection from the barrier are shown in Figure 14. The first history, Figure 14.1, is just reflection from the first step (r_1) and corresponds to the first term contributing to the $b(x)$ wave function in Figure 12. The next history involves transmission through the first step (t_1), propagation across the barrier (p), reflection from the second step (r_2), propagation back across the barrier (p), and transmission through the first step approaching now from the right (t'_1). Successively higher terms then involve more ricochets within the barrier before the final transmission back into Region (s). Figure 14 also gives the digram for the third term.

3.5 General rules for all scattering problems in one dimension

To implement the Feynman Formulation as described in Section 2, we need rules for deciding what are the valid histories which we must consider in our sum for Postulate (2) and determining the fundamental events and their quantum amplitudes for Postulate (3). This section extracts general lessons from the specific rules which we determined in the discussion of the previous section of scattering from the barrier of Figure 1.

In Section 3.4 the histories which we considered for transmission or reflection from a collision potential arose from all ways in which a final transmission or reflection is eventually generated after all sequences of transmissions or reflections from the points in space for which we must generate reflections to match the proper boundary conditions. As we know, such reflections are generated wherever there is a disturbance in the potential. This then completes the specification of the histories which must be considered for Postulate (2) for any one-dimensional scattering problem:

The histories leading to the eventual reflection or transmission of interest for a scattering event in one dimension consist of all sequences of transmissions or reflections at points of disturbance in the potential.

The most common such disturbances include sudden steps (discontinuities) in the potential as in Figure 1 and also often consider reflection generating terms in our potential such Dirac δ -functions. In Section 6 we consider problems involving smoothly varying potentials.

With the allowed histories specified, we must then complete Postulate (3) by specifying the fundamental events which make up the histories and the associated quantum amplitudes. As we saw in Section 3.4, the final quantum amplitude for a given history consists of the product of the reflection and transmission amplitudes associated with each boundary condition and propagation factors between matching boundary conditions. The fundamental events are thus scattering from points of disturbance in potential and propagation across regions of constant potential.

The quantum amplitude for propagation is simple in form, we have seen that it is simply $p = \exp(ika)$, where a is the length of the region and k is the constant wave vector across the region. The quantum amplitudes for scattering from steps and δ -functions are simple to describe but must be solved for on an individual basis. As we saw in Section 3.4 the quantum amplitude for each fundamental reflection and transmission process is just what is required to satisfy the boundary conditions in the Schrödinger approach, and are therefore the same quantities which we originally defined as the quantum amplitudes for scattering from that disturbance in isolation.

Apart from the discussion of Feynman diagrams for classically forbidden regions in Section 3.6 (which is optional material provided for the interested student), this, completes the specification of Feynman rules for scattering in one dimension. We here state the final set of rules for Postulate (3) in their full general form including the treatment of classically forbidden regions.

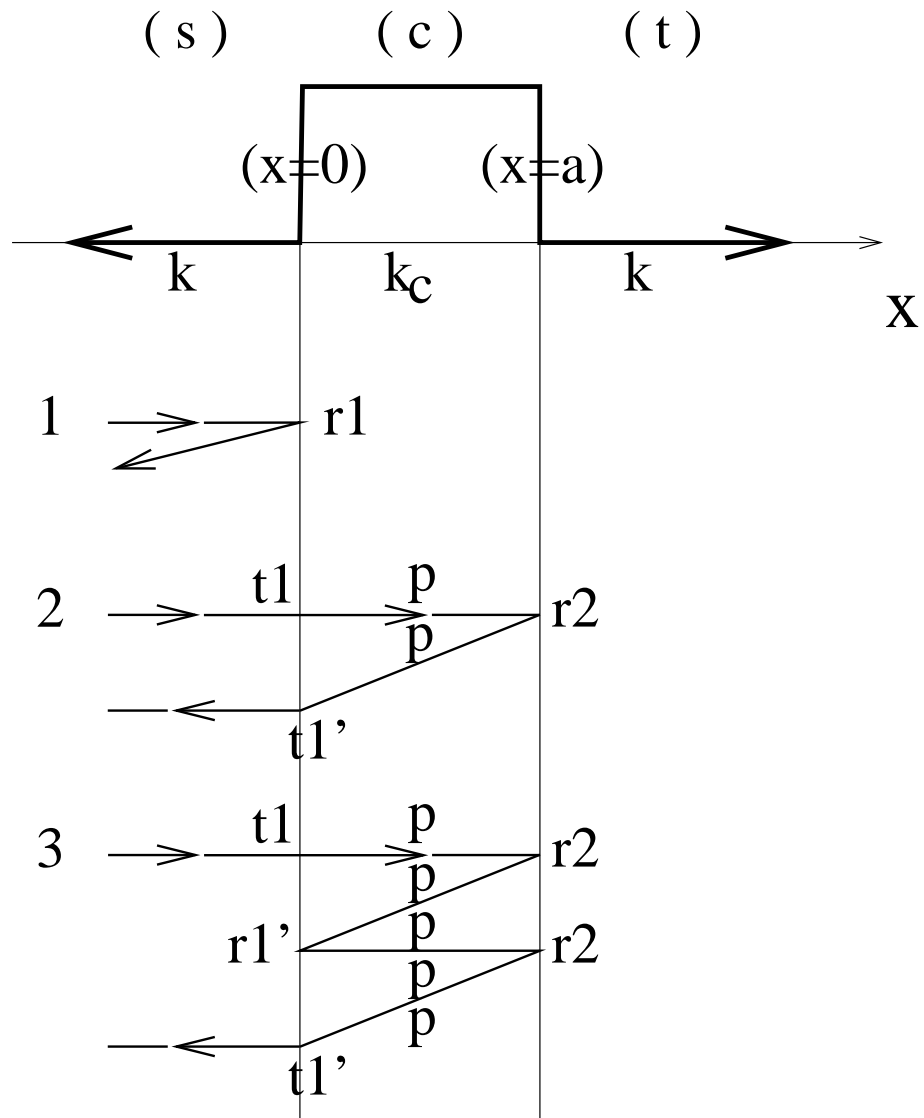


Figure 14: List of Histories Leading to a Reflection Event

The fundamental processes for Feynman histories in one dimensional scattering are the transmission and reflection at each disturbance in the potential and propagation (or penetration) events between the disturbances. The quantum amplitude for propagation (penetration) is $p = \exp(ikx)$ ($p = \exp(-\alpha x)$) where k (α) is the constant wave vector (decay constant) characteristic of the region crosses. The quantum amplitudes for the transmission and reflection at each disturbance are the usual scattering amplitudes for each disturbance in isolation.

3.6 (*) General Rules for Classically Forbidden Regions: Analytic Continuation

We have so far treated with the propagation factor across a classically allowed region, finding that whether the particle is moving to the left or the right, this factor is given by $p = \exp(ika)$ where a is the length of the region and k is the constant wave vector across the region. In general, we will also need a propagation factors for forbidden regions. The zero-centered form for an acceptable wave function for a forbidden region extending in the region $x > 0$ is $c(x) = \exp(-\alpha x)$ where $\alpha \equiv \sqrt{2m(V - E)}/\hbar$. A corresponding wave function centered at the point $x = a$ will be $e(x) = \exp(-\alpha(x - a))$. In the same way as we generated the propagation factor for a classically allowed (9) region, these two wave functions are related by the propagation factor for a classically forbidden region, $c(x) = pe(x)$ where $p = \exp(-\alpha a)$.

For classically forbidden regions the exponential solutions carry no current and we must decide which of the two exponential solutions $\exp(\pm \alpha x)$ we regard as traveling to the right and which as traveling left. We must also decide how to normalize the standard unit solution. Any choice of normalization is valid so long as we are consistent in our assignment of quantum amplitudes. However, we seek to make a choice in normalization which leads to the most natural assignment of quantum amplitudes.

As we observed in the previous paragraph, when a left incident particle collides with a forbidden region extending across the entire region $x > 0$, the only acceptable form for the solution for $x > 0$ is $\exp(-\alpha x)$, which therefore must play the role which the transmitted wave $\exp(ikx)$ plays in the classically allowed case. We thus identify $\exp(-\alpha x)$ as a solution “penetrating to the right” and $\exp(\alpha x)$ as a solution “penetrating to the left.” We then use these forms as the sole component of the solution in the transmitted region when scattering into a forbidden region from the left or right.

The mathematical way of expressing this identification is to use the concept of *analytic continuation*, which, in loose terms, simply means allowing a variable which we normally regard as real to take on complex values. Consider for example the wave vector $k \equiv \sqrt{2m(E - V_o)}/\hbar$ which insures that the functions $\exp(\pm ikx)$ satisfy the TISE for a potential V_o . In classically forbidden regions ($E < V_o$) we generally do not work with k because it becomes imaginary. However, there is no mathematical reason preventing us from working with imaginary k . The mathematics used in deriving our solutions to the TISE works just as well for complex numbers as it does for real numbers.

An imaginary k simply means that the solutions $\exp(\pm ikx)$ are actually the exponentially growing and shrinking solutions which we expect. In fact,

$$\begin{aligned} k &\equiv \sqrt{2m(E - V_o)}/\hbar \\ &= \sqrt{(-1)2m(V_o - E)}/\hbar \\ &= \pm i\sqrt{2m(V_o - E)}/\hbar \\ &\equiv \pm i\alpha, \end{aligned}$$

so that $\exp(\pm ikx) = \exp(\pm \alpha x)$, which is precisely correct. Similarly, we may take any wave function, which had been computed under the assumption that a given region is classically allowed, and by substituting $k = \pm i\alpha$ find a valid solution for the classically forbidden case. The only ambiguity which we must resolve is the choice of sign for k . To resolve this, note that if we take a classically allowed scattering solution, the wave function in the transmitted region appears as $\exp(ikx)$. If the transmitted region were actually forbidden, then the solution there must behave like $\exp(-\alpha x)$.

The only way for this to happen is if we make the choice in sign,

$$k = i\alpha. \tag{18}$$

This simple observation determines all of the rules for fundamental scattering processes involving forbidden regions. To determine the quantum amplitudes for a forbidden region, simply use the corresponding amplitudes for the classically allowed case and make the substitution (18). For instance, the quantum amplitude for *penetration* through a region a (as opposed to propagation) is then obtained as $p = \exp(ika) = \exp(i(i\alpha)x) = \exp(-\alpha x)$, consistent with our previous result. Similarly, the reflection and transmission amplitudes for crossing from an allowed region with wave vector k to a forbidden region with decay constant α , crossing from a forbidden region with decay constant α to an allowed region with wave vector k , and crossing from a forbidden region with decay constant α_1 to an other forbidden region with decay constant α_2 , are

$$\begin{aligned} r &= \frac{k - i\alpha}{k + i\alpha} & t &= \frac{2\sqrt{ik\alpha}}{k + i\alpha} \\ r &= \frac{i\alpha - k}{k + i\alpha} & t &= \frac{2\sqrt{ik\alpha}}{k + i\alpha} \\ r &= \frac{\alpha_1 - \alpha_2}{\alpha_1 + \alpha_2} & t &= \frac{2\sqrt{\alpha_1\alpha_2}}{\alpha_1 + \alpha_2}, \end{aligned}$$

respectively.

The alternate way of determining the quantum amplitudes is to follow the procedure given in Section 3.5, solve the TISE explicitly for the case of interest and then to pick off the prefactors multiplying the unit wave functions when there is a unit incident beam. This procedure depends on the choice of unit wave functions. The choice which is consistent with the amplitudes of the previous paragraph is obtained by analytic continuation of the unit current classically allowed functions,

$$\begin{aligned} \psi_l^{(f)}(x) &= \frac{e^{\alpha x}}{\sqrt{i\hbar\alpha/m}} \\ \psi_r^{(f)}(x) &= \frac{e^{-\alpha x}}{\sqrt{i\hbar\alpha/m}}, \end{aligned} \tag{19}$$

where $\psi_l^{(f)}$ and $\psi_r^{(f)}$ are the unit left- and right- penetrating wave functions, respectively.

4 Feynman Sums: two scattering centers

The Feynman rules at which we arrived in Section 3.5 are quite intuitive and we most likely could have guessed at them from the beginning based upon our physical intuition. The bulk of the discussion in Section 3 has been to demonstrate the equivalence of the Feynman and Schrödinger approaches for scattering in one dimension and to establish the Feynman rules. Once this is accomplished, it is a simple matter to draw out and label the diagrams in Figures 13 and 14. The final transmission and reflection amplitudes are then the sums over all the corresponding diagrams of the product of all of the labels. The result is precisely what we found in the Schrödinger formulation but now obtained in an extremely elegant and simple manner.

The raw power of the Feynman approach is illustrated by the fact that the sums (17) which we have derived are completely general. They are valid for any scattering potential made from two scattering centers, not merely the two equal but opposite steps which we originally had in mind. Figure 15 shows another example of a scattering potential involving two scattering centers made from the general barriers we studied in Section 3.2. As the figure shows, the quantum amplitudes for this far more complicated potential are described by precisely the same Feynman sum. The Feynman approach brings out the essential physics which this potential and the simple barrier share.

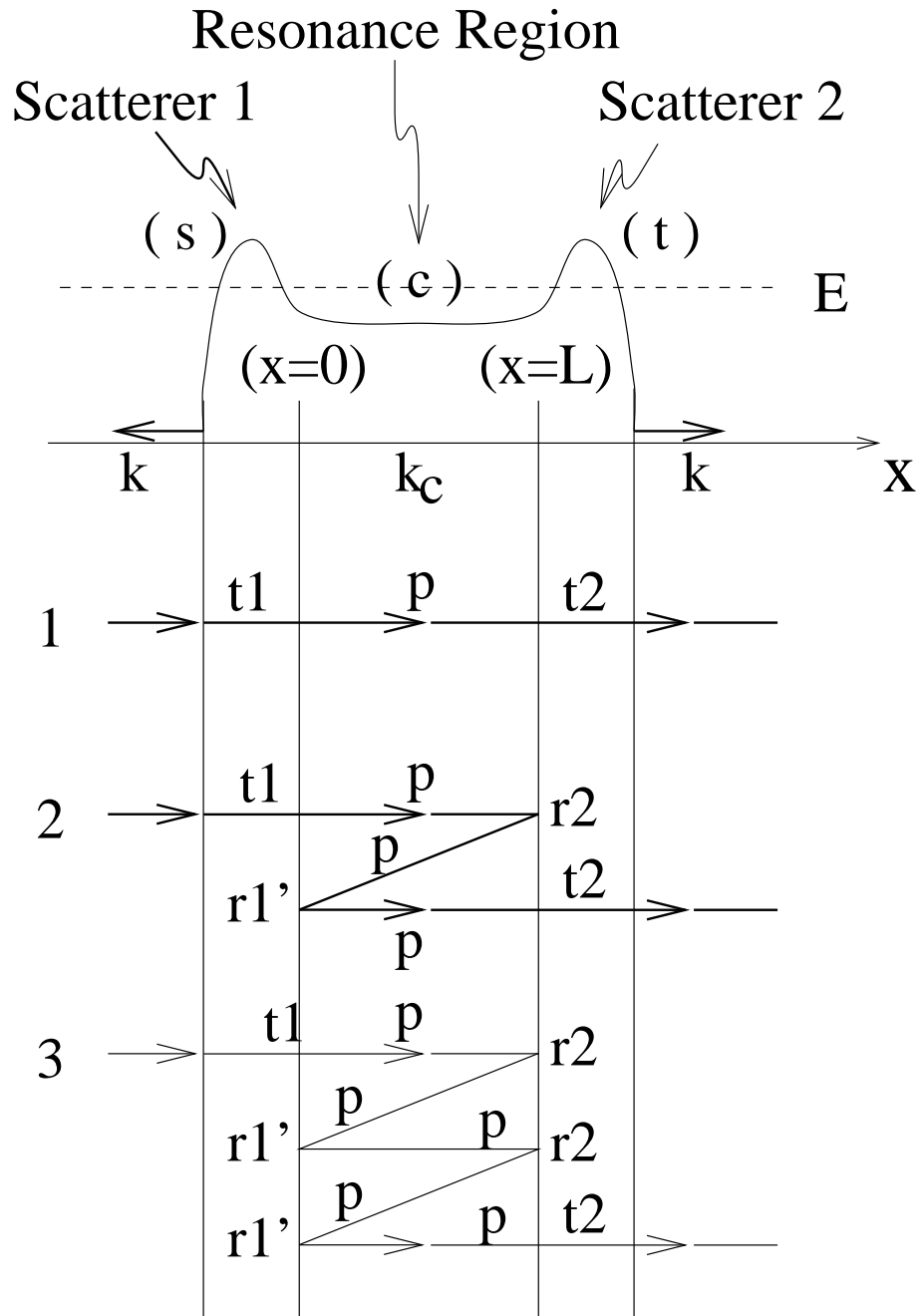


Figure 15: General Resonant Scatterer: two symmetric scatterers of width a separated by a propagating region of width L . Outside of the two scatterers, the potential is constant.

The sums (17) themselves are also rich in physical structure which we may exploit in determining their values. Each term in the transmission sum, for instance, involves transmission into the barrier region t_1 , some number (possibly zero) of repetitions of the basic ricochet sequence $pr_2pr'_1$, and then a final propagation across the scattering region and transmission out of the second scatterer pt' . Organizing the sum according to this physical principle, we find

$$T = t_1 \cdot pt_2 + t_1 \cdot (pr_2pr'_1) \cdot pt_2 + t_1 \cdot (pr_2pr'_1)(pr_2pr'_1) \cdot pt_2 + \dots \quad (20)$$

After factoring the common parts from the histories, we are left with an easily summed standard geometric series,

$$\begin{aligned} T &= t_1(1 + (pr_2pr'_1) + (pr_2pr'_1)^2 + (pr_2pr'_1)^3 + \dots)pt_2 \\ &= t_1 \cdot \frac{1}{1 - (pr_2pr'_1)} \cdot pt_2 \\ &= \frac{t_1pt_2}{1 - (pr_2pr'_1)}. \end{aligned} \quad (21)$$

This factoring into common end-point events and a basic repeating sequence is a common feature of most Feynman sums, even in far more complicated contexts. A basic repeating unit similar to the ricochet factor, for instance, appears in field theory to represent the self-energy of the electron and eventually leads to the theory of renormalization of the electron mass. Note that there is no mathematical need to write the ricochet factor as $pr_2pr'_1$. We could just as well write $r'_1r_2p^2$. The former form, however, helps us to keep in mind the physical origin of the term.

The sum for reflection is only slightly more complex. The first term is a different from the others because it is the only term which involves reflection when approaching the first barrier from the left (r_1). All of the other terms involve the processes needed to reach the second barrier and reflect back from it and out the entire barrier ($t_1p \cdot r_2pt'_1$). These terms also may contain any number, possibly zero, of ricochets between the two barriers (r_2pr_1p). Organized this way, the sum becomes

$$\begin{aligned} R &= r_1 + t_1p \cdot r_2pt'_1 + t_1p \cdot (r_2pr'_1p) \cdot r_2pt'_1 + t_1p \cdot (r_2pr'_1p)^2 \cdot r_2pt'_1 + \dots \\ &= r_1 + t_1p \cdot (1 + (r_2pr'_1p) + (r_2pr'_1p)^2 + \dots) \cdot r_2pt'_1 \\ &= r_1 + \frac{t_1pr_2pt'_1}{1 - (r_2pr'_1p)}. \end{aligned} \quad (22)$$

4.1 Analysis of the results: resonant scattering

The results (21) and (22) are general for any two scatterers. In the the special case where the two scatters are mirror images of one another and separated by a propagating region, we find a very beautiful phenomena known as resonance, in which at an infinite sequence of discrete incoming energies, the transmission probability becomes exactly one, *regardless of the form of the individual barriers*. This means for instance, that although the probability for a macroscopic object quantum tunneling through a wall may be very low, the probability for tunneling across a double wall becomes one for a whole series of special incoming energies. To prove this we need only the result (21) and the general scattering relations $t_1 = t_2$, $r'_1 = r_2$ from Section 3.2.

Because the t 's and r 's are equal, let us define

$$t \equiv \sqrt{P_t}e^{i\phi_t} \equiv t_1 = t_2$$

and

$$r \equiv \sqrt{P_r}e^{i\phi_r} \equiv r'_1 = r_2$$

where $P_t = 1 - P_r$ are the probabilities for transmission and reflection across the individual barriers (which are direction independent), ϕ'_t/v_{cl} gives the time delay for transmission across the barriers, and ϕ'_r/v_{cl} gives the time delay crossing the barriers from the inside, where v_{cl} is the appropriate classical velocity.

The transmission probability across both barriers is then

$$\begin{aligned}
P_T &\equiv |T|^2 \\
&= \left| \frac{tp}{1 - (prpr)} \right|^2 \\
&= \frac{|t^2 p|^2}{(1 - r^2 p^2)^*(1 - r^2 p^2)} \\
&= \frac{P_t^2}{1 - ((r^*)^2 (p^*)^2 + r^2 p^2) + P_r^2} \\
&= \frac{P_t^2}{1 - 2\Re(r^2 p^2) + P_r^2} \\
&= \frac{P_t^2}{1 - 2\Re(P_r e^{2i(\phi_r + k_c L)}) + P_r^2} \\
&= \frac{P_t^2}{1 - 2P_r \cos 2(\phi_r + k_c L) + P_r^2} \\
&= \frac{P_t^2}{1 - 2P_r(\cos 2(\phi_r + k_c L) - 1) - 2P_r + P_r^2} \\
&= \frac{P_t^2}{(1 - P_r)^2 - 2P_r(-2 \sin^2(\phi_r + k_c L))} \\
&= \frac{P_t^2}{P_t^2 + 4P_r \sin^2(\phi_r + k_c L)} \\
&\rightarrow \\
P_T &= \frac{1}{1 + 4\frac{P_r}{P_t^2} \sin^2(\phi_r + k_c L)} \tag{23}
\end{aligned}$$

Thus, whenever $\phi_r + k_c L = n\pi$ where $n = \dots, -1, 0, 1, \dots$, the transmission probability goes to one. Generally, ϕ_r does not vary very rapidly with the incoming energy, so that this condition is met for an infinite series of special values of k_c at spacing $\Delta k_c \approx n/L$.

4.2 Specific results for the barrier potential

As a specific example of resonance, consider the simple barrier potential of Figure 1 with which we started. In this case the spacing between the barriers is $L = a$. From (15), the phase of r is π and the transmission and reflection probabilities are

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

respectively. According to (23) the final transmission probability is then

$$P_T = \frac{1}{1 + \frac{1}{4} \frac{(k^2 - k_c^2)^2}{k_c^2 k^2} \sin^2(k_c a)} \tag{24}$$

And, this is precisely what we would find by direct solution of the Time Independent Schrödinger Equation (TISE)!

In Figure 16, we plot the transmission amplitude P_T as a function of the momentum k_c of the particle as it crosses the collision region, for various values of the height of the potential step V_o . In the figure, T_o , the kinetic energy of a particle bound in an infinite square well potential of length a , sets the energy scale. Perhaps the most striking result in the figure is that precisely at the values $k_c = n\pi/a$, we find perfect probability for transmission, $P_T = 1$. Also as expected, when k_c becomes

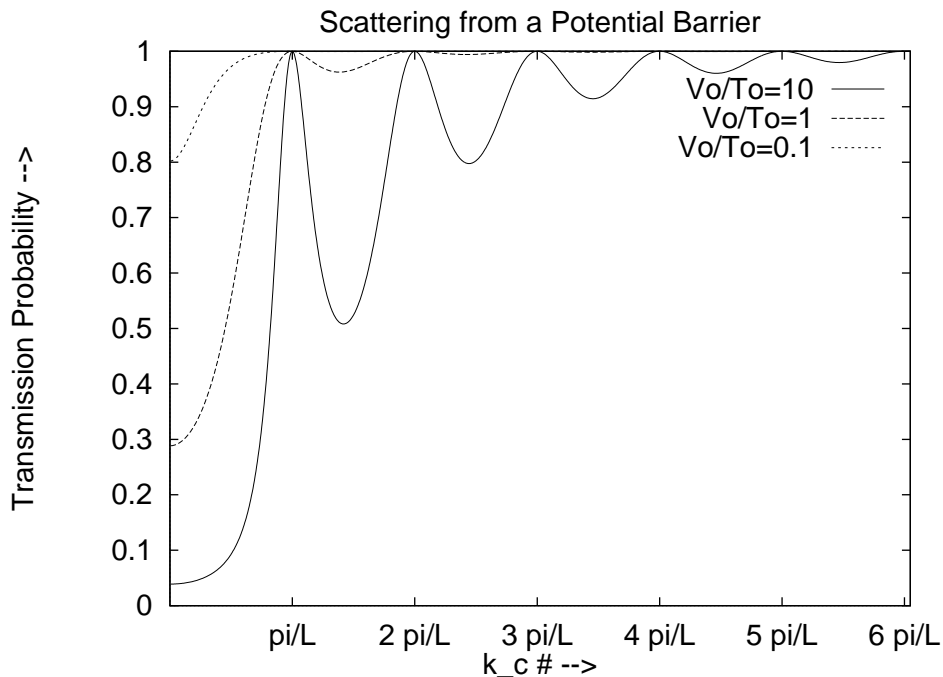


Figure 16: Transmission Probabilities across a square potential barrier

very large, the presence of the barrier becomes less and less significant, so that the transmission probability approaches unity at large k_c regardless of whether k_c is at one of the resonances. As we increase the height of the barrier, as we would expect, the transmission probability for low values of k_c decreases rapidly. As a consequence, the resonances become very narrow, as seen in the figure.

5 Three Nobel Ideas: Renormalization, Renormalization Group, Anderson Localization

5.1 Renormalization: Three scattering centers

Let us now consider scattering from a potential with three disturbances, such as the three δ -functions of strength D in Figure 17. The scattering amplitudes for a potential $V(x) = D\delta(x)$, as determined from solution of the TISE, are

$$\begin{aligned} r &= \frac{q}{ik - q} \\ t &= \frac{ik}{ik - q}, \end{aligned} \tag{25}$$

where $q \equiv mD/\hbar^2$. Because the δ -function is symmetric, the scattering amplitudes are identical for both left- and right- incidence. Figure 17 shows four diagrams for transmission which illustrate the far richer variety of diagrams which we now face. Although there is a much richer variety, the number of these diagrams is still countable as they were in Figure 13. The meaning of the thick lines in the diagram will be explained presently.

Again, we seek a physical principle to organize the Feynman sum. The result will be a general form which is independent of the nature of the three scattering centers, and for which we may generate specific results by substituting in particular values for the quantum amplitudes.

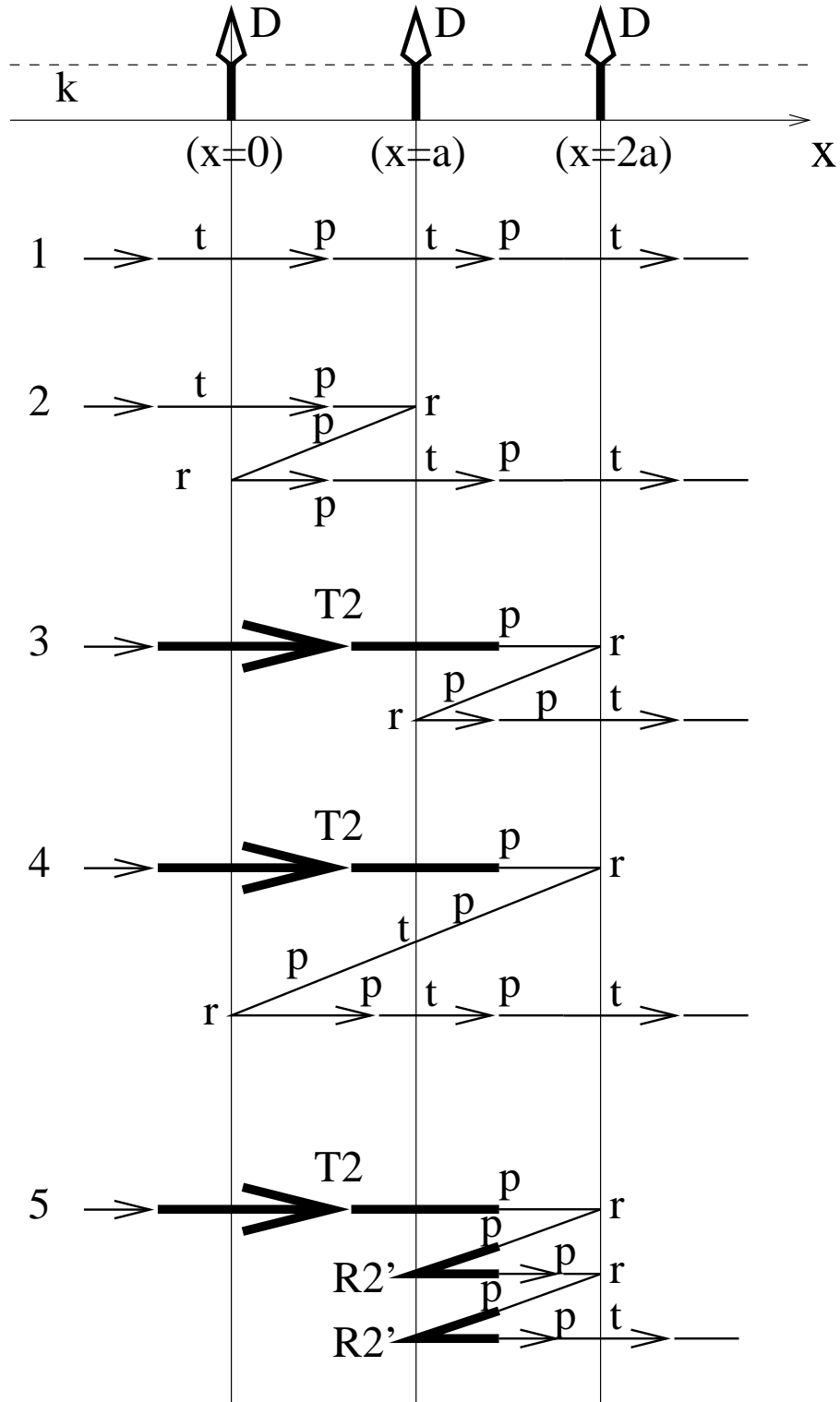


Figure 17: Transmission diagrams from a triple scatterer

The first two diagrams shown are part of an infinite subsequence of diagrams where the particle ricochets an arbitrary number of times between the first two barriers and then travels directly across to and through the third barrier. The sum of this subset of diagrams is

$$\begin{aligned}
[T]_1 &= tptpt + t(prpr)ptpt + t(prpr)^2ptpt + \dots \\
&= (tpt + t(prpr)pt + t(prpr)^2pt + \dots) pt \\
&\equiv T_2pt,
\end{aligned}$$

where the T_2 factor we recognize as the complete Feynman sum for transmission across the first two barriers. The physical reason why we were able to factor this term out is that all processes which lead to transmission across the three barriers, no matter how complicated, begin with a sequence which carries the particle across the first two barriers. The sum of all of these beginning parts, T_2 , is clearly the sum of all ways in which we may cross the first two barriers and therefore must be the Feynman amplitude for transmission across the two first two barriers viewed as an isolated unit, hence the notation T_2 . All that we are doing is changing our view of the system and its fundamental processes. We are now beginning to consider the potential as consisting of two scatterers, the first being the first two δ -functions taken as a unit and the second being the third δ -function.

In the third and fourth diagrams of Figure 17, the complete processes of all possible ways to transmit across the first two barriers as a unit is indicated by a very thick line. Such a notation is sometimes referred to as a *dressed interaction* in many-body physics. By using this notation, the diagrams in Figures 17.3 and 17.4 now serve to represent two different infinite subsets of diagrams. The total quantum amplitudes of these two subsets are given by the product of the labels in the diagram, $T_2prp \cdot r \cdot pt$ and $T_2prp \cdot tprpt \cdot pt$, respectively.

The idea of summing together an infinite subset of diagrams into a unit to produce a new fundamental process with its own quantum amplitude and diagram is known as *renormalization*. As we shall see, renormalization is a very powerful tool in organizing infinite sets of diagrams. This idea is used to deal with certain infinities which arise in quantum electrodynamics, the theory for which Feynman shared the Nobel prize with Schwinger and Tomonaga in 1965.

The the third and fourth diagrams in 17 begin another sequence of diagrams which we must consider. In this sequence, after somehow managing to penetrate through the first two δ -functions, the particle reflects once off of the third δ -function, then reflects from the unit consisting of the first two δ -functions, after some number of ricochets, and then finally travels directly across to and through the third barrier. The sum of this infinite collection diagrams clearly involves R'_2 , the amplitude for reflection from the right from the renormalized two δ -function unit. Algebraically, this part of the sum is

$$\begin{aligned}
[T]_2 &= T_2prp \cdot r \cdot pt + T_2prp \cdot tprpt \cdot pt + \dots \\
&= T_2prp \cdot (r + tprpt + \dots) \cdot pt \\
&\equiv T_2prpR'_2pt.
\end{aligned}$$

We may now combine the renormalized left-transmission T_2 with our new renormalized right-reflection R'_2 from the double δ -unit to describe *all* of the transmission diagrams for the triple δ -potential. So far, we have dealt with direct transmission $[T]_1 = T_2pt$ and transmission after one ricochet between the third δ and our renormalized δ -function pair, $[T] = T_2prpR'_2pt$. The final diagram in Figure 17 gives the next set of terms in this renormalized sequence. In Figure 17.5 there are two ricochets between the renormalized double- δ unit and the isolated third δ function. Continuing in this way, now simply generated the general sequence of scattering between two barriers shown in Figure 15 but where where the nature of the two scatterers is different.

This completes the renormalization process. We now have a new, simpler set of Feynman rules for the problem at hand. The new set of rules now has a different set of fundamental processes, namely reflection and transmission across the first two δ -functions as a renormalized unit, transmission and reflection from the third δ -function, and propagation between them. The fact that the Feynman formulation is not specific about the form of the fundamental processes is what makes the renormalization process possible. Renormalization represents a change in what is considers to be

the fundamental processes. The condition on what may be renormalized is that any history must be able to be sequenced unambiguously into the new fundamental processes. Grouping the first two δ -functions together as a unit clearly satisfies this condition, because a scattering event from the third δ -function can never be interleaved with the ricocheting between the first two δ -functions. One could not, for instance, renormalize the outer two δ -functions into a single unit, because then scattering processes within our “fundamental process” of scattering between the outer δ -functions could be interrupted by scattering processes from the central δ -function.

The final transmission amplitude across the three scatterers has now been reduced to a scattering problem between two scatterers, a renormalized unit made from the first two and the third “bare” scatterer. We may therefore use the result (21) with five substitutions. First, the propagation amplitude between the two barrier now becomes the transmission amplitude between the renormalized unit and the bare scatterer, $p \rightarrow p$. The transmission across the first barrier now becomes transmission across the renormalized unit, $t_1 \rightarrow T_2$. Reflection off of the first barrier from the right now becomes reflection from the renormalized unit, $r'_1 \rightarrow R'_2$. Finally, the reflection and transmission amplitudes from the second barrier become the reflection and transmission amplitudes from the isolated bare scatterer, $r_2 \rightarrow r$ and $t_2 \rightarrow t$, respectively.

Alternately, we get precisely the same result by performing the Feynman sum corresponding to Figure 18,

$$\begin{aligned} T_3 &= T_2 \cdot pt + T_2 \cdot prpR'_2 \cdot pt + T_2 \cdot (prpR'_2)^2 \cdot pt + \dots \\ &= \frac{T_2pt}{1 - (prpR'_2)}. \end{aligned} \quad (26)$$

As we have used no special properties of the amplitudes, this result is general. As we saw in Section 3.2, the transmission amplitudes in both directions are equal for any potential so that the amplitude for right-incident transmission is the same, $T'_3 = T_3$.

Reflections from three general scatterers may be handled in the same way. We apply (22), where again $p \rightarrow p$, $t_1 \rightarrow T_2$, $r'_1 \rightarrow R'_2$, and $r_2 \rightarrow r$, but now we need also reflection from the first barrier to become reflection from the renormalized unit $r_1 \rightarrow R_2$ and transmission from the right from the first unit to become transmission from the right through the renormalized unit, $t'_1 \rightarrow T'_2 = T_2$, where the equality follows from the discussion in Section 3.2.2. This gives,

$$R_3 = R_2 + \frac{T_2prpT'_2}{1 - (rpR'_2p)}. \quad (27)$$

Again, one could obtain the same result by drawing and summing the appropriate renormalized Feynman diagrams.

Because the reflection amplitudes from the left and right need not be equal, to maintain generality we must give also the right-incident reflection amplitude R'_3 . Again we use (22) where now $p \rightarrow p$, transmission across the first barrier into the scattering region is right- transmission through the bare scatterer $t_1 \rightarrow t'$, reflection from the second barrier is right-reflection from the renormalized unit $r_2 \rightarrow R'_2$, direct reflection from the first barrier is right-reflection from the bare unit $r_1 \rightarrow r'$, the ricochet reflections from the first barrier are left-reflection from the bare scatterer $r'_1 \rightarrow r$ and final transmission through the first barrier is left-transmission through the bare unit $t'_1 \rightarrow t$. The final result is then

$$R'_3 = r' + \frac{t'pR'_2pt}{1 - (R'_2prp)}. \quad (28)$$

Again, one could obtain the same result by drawing and summing the appropriate renormalized Feynman diagrams.

To complete the computation of the scattering amplitudes For the specific case of the three δ -functions in Figure 17, we take $p = \exp(ika)$ and $r = r'$ and $t = t'$ from (25). In terms of these amplitudes, the specific values for T_2 and R'_2 come directly from (21) and (22),

$$\begin{aligned} T_2 &= \frac{tpt}{1 - (prpr)} \\ R'_2 &= r + \frac{tprpt}{1 - (prpr)}. \end{aligned}$$

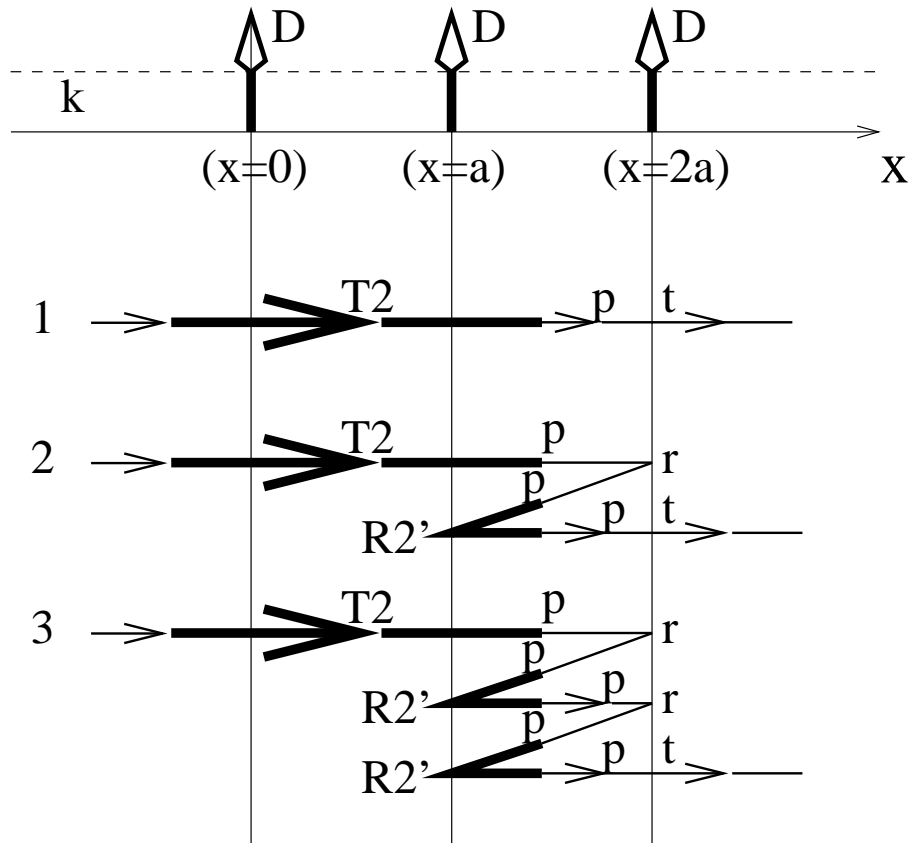


Figure 18: Complete set of renormalized transmission diagrams from a triple scatterer

5.2 Renormalization Group and Summing Uncountably Infinite Diagrams: An infinite crystal

In Section 5.1 we showed how *renormalization*, redefinition of fundamental processes into larger units, allowed us to organize and perform the Feynman sum for a three scatterers. In this section, we take the idea to the next level in order to analyze scattering from a infinite perfectly periodic array of scatterers, corresponding to the physics of electrons moving through a crystal. (A crystal is a perfectly regular array of identical atoms, each of which, by renormalization into a single unit, may be viewed as a single scatterer.) For concreteness we will consider an infinite array of δ -functions but, again the Feynman approach will allow us to derive general formulae which differ from system to system only in the specific values assigned to the scattering amplitudes of the fundamental units.

Figure 19 illustrates the potential which we consider. The infinite variety of Feynman diagrams describing electrons which are transmitted into the crystal and never return is so large that they are no longer countable, there are in fact as many of these diagrams as there are real numbers. We must be very clever in organizing the sum of these diagrams.

Our strategy here is to apply the idea of renormalization over and over and study the behavior of the system in the limit of an infinite number of renormalizations. Figure 19 illustrates how this process allows us to study an infinite crystal. Our strategy is to build upon the results of Section 5.1. We now take the quantum amplitudes for the first three scatterers taken together as a renormalized unit and combine this unit with the fourth scatterer to find the quantum amplitudes for the first four scatterers as a renormalized unit. We then combine this quadruple unit with the fifth scatterer in the sequence to produce the transmission amplitude for the first five. We continue the process to build up the amplitudes for an infinite crystal. The idea of applying successive renormalizations like this is known as the *Renormalization Group*. It represents the intellectual content of Ken Wilson's Nobel prize in 1982.

Specifically, at each step in the process, we take the scattering amplitudes for the first n units $T_n = T'_n, R_n, R'_n$ and combine them with the quantum amplitudes for the next bare scatterer in the sequence $t_{n+1} = t'_{n+1}, r_{n+1}, r'_{n+1}$ and the propagation factor separating these two units p_{n+1} . The mathematics of this is precisely the same as we followed to produce $T_3 = T'_3, R_3, R'_3$ from $T_2 = T'_2, R_2, R'_2$ in (26,27,28). The general result is

$$\begin{aligned} T_{n+1} &= \frac{T_n p_{n+1} t_{n+1}}{1 - (p_{n+1} r_{n+1} p_{n+1} R'_n)} \\ R_{n+1} &= R_n + \frac{T_n p_{n+1} r_{n+1} p_{n+1} T'_n}{1 - (r_{n+1} p_{n+1} R'_n p_{n+1})} \\ R'_{n+1} &= r'_{n+1} + \frac{t'_{n+1} p_{n+1} R'_n p_{n+1} t_{n+1}}{1 - (R'_n p_{n+1} r_{n+1} p_{n+1})}, \end{aligned} \quad (29)$$

where the initial case is that $T_1, R_1, R'_1 = t_1, r_1, r'_1$ as indicated in Figure 19.

The behavior of a single physical quantity, such as the transmission coefficient, as a function of the number of times the renormalization is carried through is known as the *renormalization flow* of the quantity. Figure 20.1 shows the renormalization flow of T_n in the complex plane for a small value of the incoming energy. The first of the connected points on the plot, approximately $0.45 - 0.2i$, shows the value (25) for the transmission amplitude across one δ -function at this energy. The transmission probability across one δ -function at this energy is therefore approximately $P_{t_1} \approx 0.24$. The successive points on the plot show the transmission amplitudes T_n across n δ -functions at this energy as computed according to (29) with a very simple computer program. The plot shows that as $n \rightarrow \infty$, $T_n \rightarrow 0$ and therefore these electrons do not have enough energy to propagate through the crystal.

Figure 20.2 shows the flow at a slightly higher value of the energy. Now something interesting happens. As n increases, the transmission amplitudes do not approach a limit. They cycle around in the complex plane in a figure-eight pattern and never approach the origin. These electrons may therefore propagate through the crystal without returning. The fact that the transmission amplitudes do not settle down to a single point indicates that the electronic wave function is sensitive

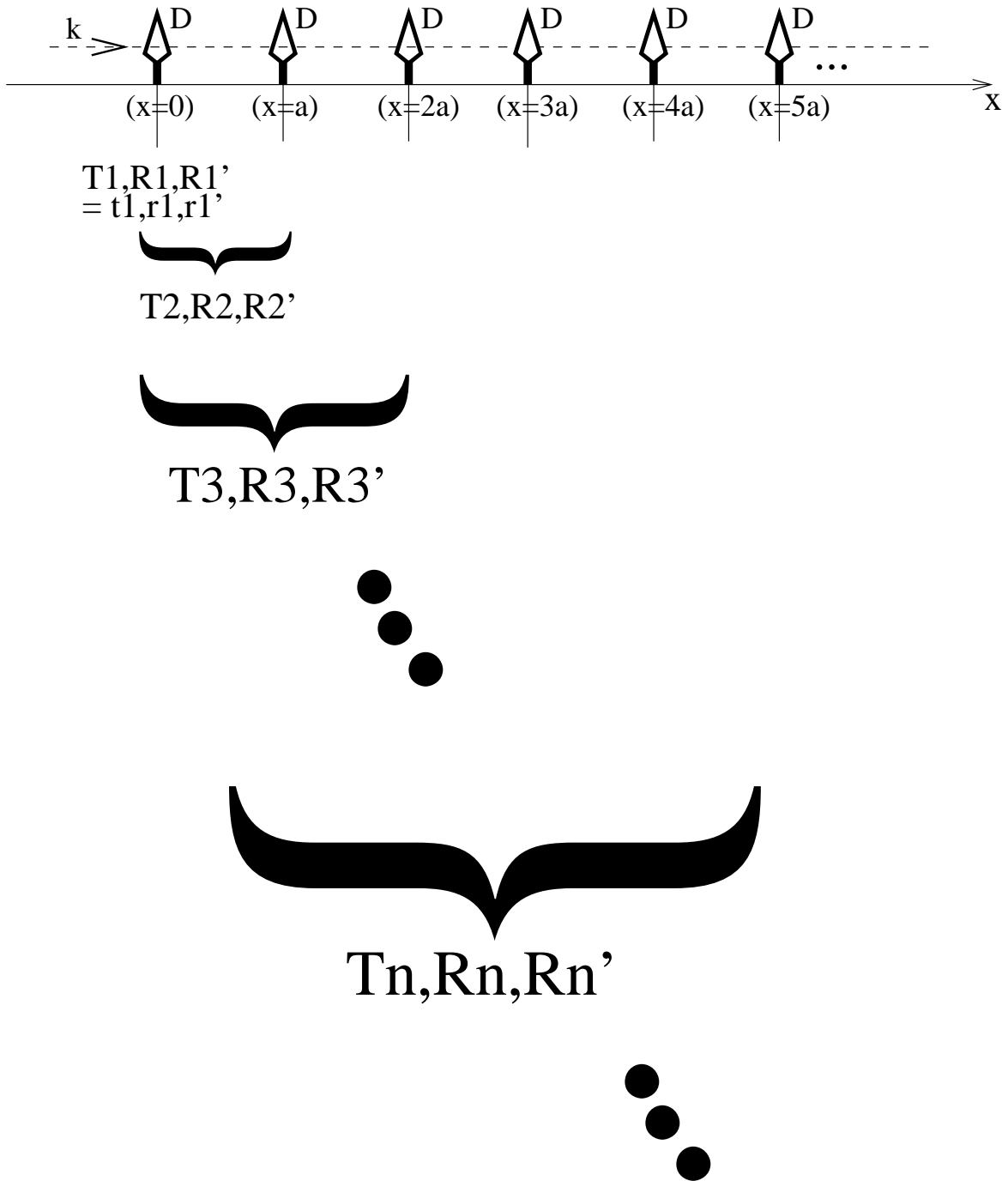


Figure 19: Renormalization Group Calculation of Propagation Through a Crystal

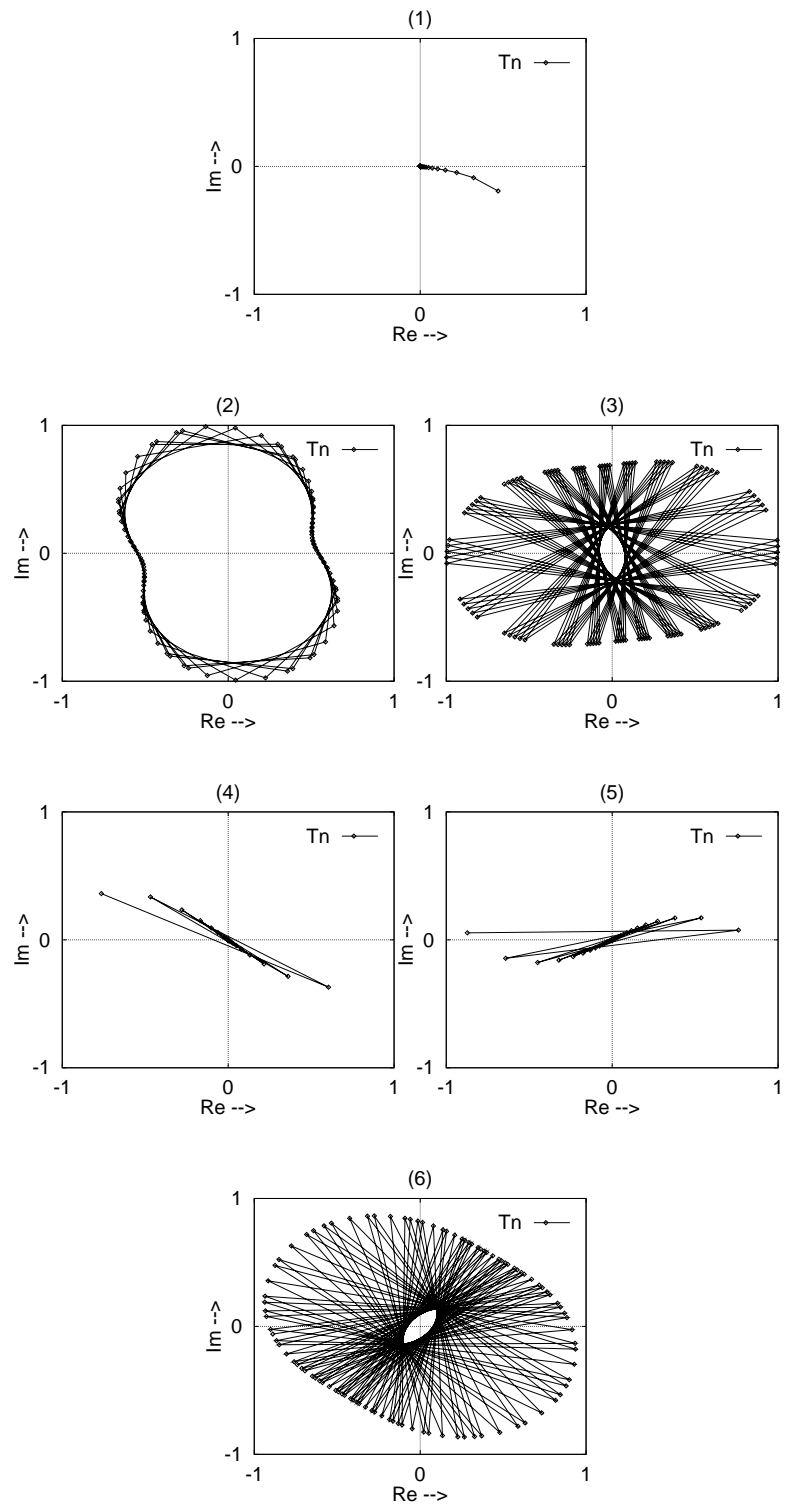


Figure 20: Renormalization Flows of Transmission Through a Perfect Crystal

to the placement of the next atom in the crystal, another indicator that the wave function for the electron spreads throughout the entire crystal. As the energy is further increased we see a continuous series of such patterns; one of the highest energy ones appears in Figure 20.3. Such a continuous range of energies where electrons may propagate in a crystal is called an allowed *band* in solid state physics. Note that for this state near the top of the band, the successive T_n now appear on nearly opposite sides of the origin. This indicates that the phase going through successive δ -functions is approaching -1 .

As we continue to increase the energy we find the flow of Figure 20.4. The phases from successive scatterers are now sufficiently close to -1 that the successive reflections in the crystal no longer interfere sufficiently constructively to allow the electrons to propagate forward in the crystal. This continues as we increase the energy through that of Figure 20.5. A range like this where no states propagate through the crystal is known in solid state physics as a *gap* or *band gap*. Finally, Figure 20.6 shows that with a little more energy, we begin another *band* of energies where propagation occurs. This alternation between *bands* and *gaps* continues as we increase the energy of the electrons.

5.3 Anderson Localization: Introduction of disorder

Once it is understood that in special bands of energy electrons may propagate through an infinite crystal, it is natural to inquire as to what happens in a more realistic situation when there is disorder in the crystal, for instance when the spacing between the atoms is slightly irregular with small, random perturbations. Phil Anderson won the Nobel prize in 1977 for his investigations into this very issue.

Our renormalization approach to crystal propagation makes such studies easy to carry out. We now compute the renormalization flows according to (29) with a simple computer program which generates slightly random displacements between the atoms and therefore slightly different p_n for each n . Figures 21.1-21.6 show the renormalization flows of the transmission amplitude for a random crystal (with atomic locations varying by $\pm 15\%$) at precisely corresponding energies to those in Figure 20.

Figures 21.1,4,5 show the typical behavior in the *gap*. There is still a rapid approach to the origin, although now the approach is a little random. The electrons still cannot propagate at these energies in the gaps.

Figures 21.2,3,6 show that with disorder, even electrons in the allowed energy bands cannot propagate in the crystal. The flows cycle around the origin as before, but all eventually spiral into it. By studying how quickly these flows “fall” into the origin, one may determine the typical maximum distance which an electron may travel in the crystal. These results show that all electrons become localized in this random crystal, a phenomena known as Anderson localization.

The Anderson localization teaches us an important lesson about propagation in the crystal. The classical result for the transmission probability through a crystal of scatterers is that the final probability is the product of all of the probabilities of crossing the barriers. So long as the probability of crossing each scatterer is not exactly one, classical thinking predicts that in an infinite crystal the final transmission probability will be zero. What is different in the quantum analysis is that we now must sum complex amplitudes over all histories. In this sum in perfect crystals, at those energies in the allowed *bands*, there is enough constructive interference in the forward direction to allow the propagation to continue. By introducing randomness into the crystal, we disturb this constructive interference sufficiently to localize the electrons.

6 Scattering from Smooth Potentials: WKB approximation

We conclude with a beautifully simple derivation of a very famous approximation due to Wentzel, Kramers and Brillouin for the form of the electronic wave function in a very smooth potential. The basis for our approach is that a smooth potential may be well approximated as a series of very small steps of width Δ , as Figure 22 shows. So long as we avoid regions such as $b < x < c$ where the step heights become comparable to the difference between the the potential and total energies, then the

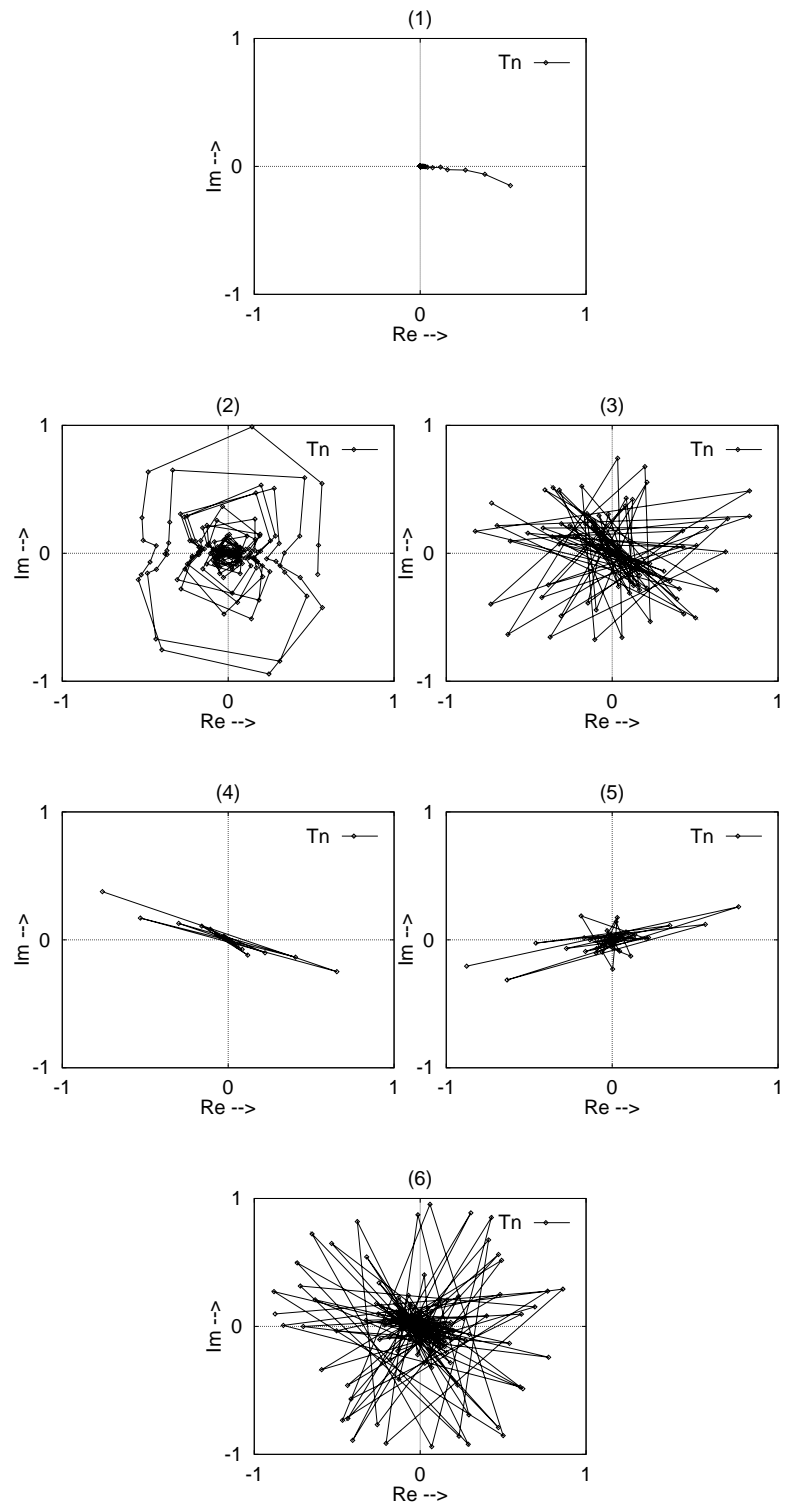


Figure 21: Renormalization Flows of Transmission Through Disordered Crystal

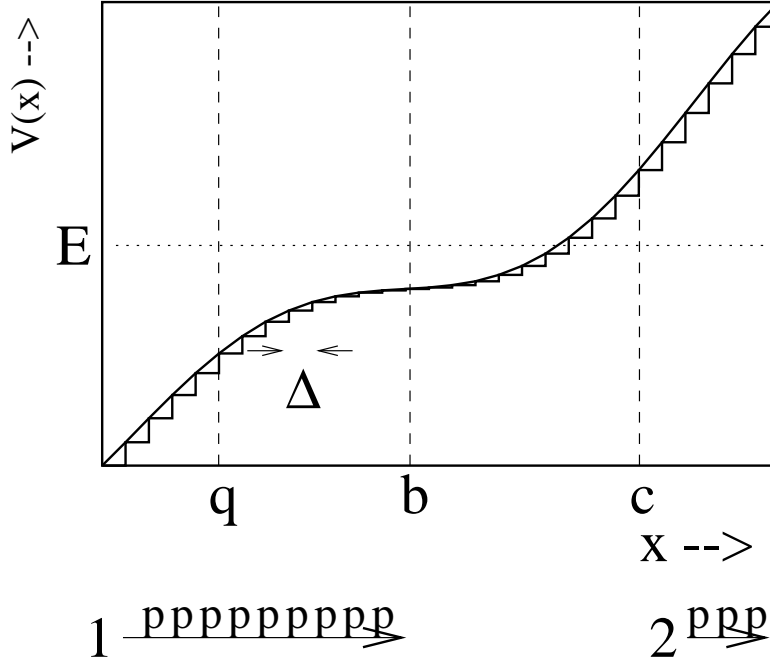


Figure 22: Smooth Potential Viewed as a series of small steps

reflection coefficients such as (14) and its forbidden analogue in Section 3.6 will be very small and the stepped potential acts like the smooth potential which it is supposed to mimic.

Because the reflection amplitudes are small within these regions, we may ignore diagrams involving reflections because they give negligible contributions to the final result. The entire Feynman sum for the propagating wave function then reduces to a single diagram progressing to the right. Figure 22 gives two such examples, one in a classically allowed region and the other in a classically forbidden region.

Corresponding to the small reflection amplitudes, the transmission amplitudes across the steps in allowed and forbidden regions are almost exactly one. These amplitudes are the ratio of the geometric to the algebraic mean of the wave vectors or decay constants before and after each step, $\sqrt{k_1 k_2} / (\frac{1}{2}(k_1 + k_2))$ and $\sqrt{\alpha_1 \alpha_2} / (\frac{1}{2}(\alpha_1 + \alpha_2))$, respectively. So long as the step size is small, $k_1 \approx k_2$ or $\alpha_1 \approx \alpha_2$, these amplitudes approach unity. Because all of the transmission factors are nearly one, we do not even need to list them explicitly in the amplitude for the history. The entire Feynman sum for a smooth potential is thus approximated by a simple product of either propagating or penetrating factors.

In the classically allowed case we then find for transmission between two points q_1 and q_2 the following amplitude

$$\begin{aligned}
 T^{(a)} &= p_1 p_2 \dots p_n & (30) \\
 &= e^{i k_1 \Delta} e^{i k_2 \Delta} \dots e^{i k_N \Delta} \\
 &= e^{i(k_1 \Delta + k_2 \Delta + \dots + k_N \Delta)} \\
 &\rightarrow e^{i \int_{q_1}^{q_2} k(x) dx},
 \end{aligned}$$

where in the last step we have noted that in the limit of infinitely narrow steps, the exponent just become the Riemann sum for the integral of $k(x) \equiv \sqrt{2m(E - V(x))}/\hbar$. The classically forbidden case follows a similar logic,

$$T^{(f)} = p_1 p_2 \dots p_n \quad (31)$$

$$\begin{aligned}
&= e^{-\alpha_1 \Delta} e^{-\alpha_2 \Delta} \dots e^{-\alpha_N \Delta} \\
&= e^{-(\alpha_1 \Delta + \alpha_2 \Delta + \dots + \alpha_N \Delta)} \\
&\rightarrow e^{-\int_{q_1}^{q_2} \alpha(x) dx},
\end{aligned}$$

where $\alpha(x) \equiv \sqrt{2m(V(x) - E)}/\hbar$. The fact the wave progresses as an integral of the local wave vector $k(x)$ or decay constant $\alpha(x)$ is the heart of the WKB approximation.

The WKB approximation actually goes one step further, and it is easy for us to obtain the full expression. The usual expression for the WKB approximation gives the value of the wave function as a function of x . In our Feynman formulation the wave function in the region just after the step at point q is the quantum amplitude at that point $T^{(a)}(q)$ at point q time the corresponding, appropriately centered unit current,

$$\psi_q(x) = T^{(a)} \frac{e^{ik(q)(x-q)}}{\sqrt{\hbar k(q)/m}}.$$

The wave of the wave function at the point $x = q$ is therefore

$$\psi(q) = T^{(a)} \frac{1}{\sqrt{\hbar k(q)/m}}.$$

Combining this with (30) gives the value of the wave function in a smoothly varying classically allowed region as

$$\psi^{(a)}(q) \propto \frac{e^{i \int^q k(x) dx}}{\sqrt{k(q)}}.$$

As we discussed in Section 3.6, the unit transmitted beam in forbidden regions is given by $\exp(-\alpha)/\sqrt{\hbar \alpha}/m$. Therefore in classically forbidden regions we find

$$\psi^{(f)}(q) \propto \frac{e^{-\int^q \alpha(x) dx}}{\sqrt{\alpha(q)}},$$

These last two results are the complete WKB approximation derived as just the first Feynman diagram in scattering theory!!!