# **Piecewise Potentials II**

Lecture 13

Physics 342 Quantum Mechanics I

Monday, February 25th, 2008

We have seen a few different types of behavior for the stationary states of piecewise potentials – we can have oscillatory solutions on one or both sides of a potential discontinuity, we can also have growing and decaying exponentials. In general, we will select between the oscillatory and decaying exponential by choosing an energy scale for the stationary state.

Our final pass at this subject will begin with a finite step, where we set up some matrix machinery to avoid the tedious algebra that accompanies boundary matching. Aside from the result, the important observation is that the matrix form we develop is independent of the potential, so that we can apply this type of approach to any potential, provided it does not extend to infinity.

Remember the process we are going through over and over (and over): Given a potential, find the stationary states, use those to form the general solution to Schrödinger's equation by appending the appropriate temporal factor  $(e^{-i\frac{Et}{\hbar}})$ , and exploit completeness to decompose some initial  $\bar{\psi}(x)$  waveform. In practice, as should be evident from our studies so far, this program is sensible but difficult. The initial distribution of choice, a Gaussian, has unwieldy decomposition in bases other than  $e^{ikx}$  (the natural, Fourier set) – is there another/easier way to get a basic idea of what an initial Gaussian distribution does when evolved in time under the influence of a potential? Yes, and we discuss the simplest possible numerical solution at the end.

## **13.1** Finite Step Potential

Take, as our potential, the finite step:

$$V(x) = \begin{cases} 0 & x < 0\\ V_0 & 0 < x < a\\ 0 & x > a \end{cases}$$
(13.1)

Now the spatial solution is naturally partitioned into three regions – we'll make the usual ansatz:

$$\psi_I(x) = A e^{i k x} + B e^{-i k x}$$
  

$$\psi_{II}(x) = C e^{\bar{k} x} + D e^{-\bar{k} x}$$
  

$$\psi_{III}(x) = F e^{i k x} + G e^{-i k x},$$
  
(13.2)

with  $k \equiv \sqrt{\frac{2mE}{\hbar^2}}$ ,  $\bar{k} \equiv \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$  so that  $\bar{k}$  is real for  $E < V_0$ , and imaginary for  $E > V_0$ .

The continuity equations, working from the left, read:

$$A + B = C + D \quad i k (A - B) = \bar{k} (C - D), \tag{13.3}$$

and on the right, we have

$$C e^{\bar{k}a} + D e^{-\bar{k}a} = F e^{ika} + G e^{-ika}$$
  
$$\bar{k} \left( C e^{\bar{k}a} - D e^{-\bar{k}a} \right) = i k \left( F e^{ika} - G e^{-ika} \right)$$
(13.4)

There are a few different ways to make the required connections. Thinking of the typical "scattering" problem (wave is incident from the left, gives rise to reflected wave and transmitted wave, etc.), we would typically set G = 0, and attempt to find B and F for the waves on the left and right. That suggests that we set up the following matrix equations:

$$\underbrace{\begin{pmatrix} 1 & 1\\ i\,k & -i\,k \end{pmatrix}}_{\equiv \mathbb{M}_1} \begin{pmatrix} A\\ B \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 1\\ \bar{k} & -\bar{k} \end{pmatrix}}_{\equiv \mathbb{M}_2} \begin{pmatrix} C\\ D \end{pmatrix}$$
(13.5)

and

$$\underbrace{\begin{pmatrix} e^{\bar{k}a} & e^{-\bar{k}a} \\ \bar{k}e^{\bar{k}a} & -\bar{k}e^{-\bar{k}a} \end{pmatrix}}_{\equiv \mathbb{M}_3} \begin{pmatrix} C \\ D \end{pmatrix} = \underbrace{\begin{pmatrix} e^{ika} & e^{-ika} \\ ike^{ika} & -ike^{-ika} \end{pmatrix}}_{\equiv \mathbb{M}_4} \begin{pmatrix} F \\ G \end{pmatrix}. (13.6)$$

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Then we can solve for F and G in terms of A and B:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \underbrace{\mathbb{M}_1^{-1} \mathbb{M}_2 \mathbb{M}_3^{-1} \mathbb{M}_4}_{\equiv \mathbb{M}} \begin{pmatrix} F \\ G \end{pmatrix}.$$
(13.7)

Since we want to find B and F given A and G = 0, we can rewrite the above, once we know the matrix elements:

$$F = \frac{1}{M_{11}}A \qquad B = \frac{M_{21}}{M_{11}}A.$$
 (13.8)

Computing  $\mathbb{M}$ , I find that:

$$M_{11} = \frac{e^{a(ik-k)}}{4k\bar{k}} \left[ i\left(-1+e^{2a\bar{k}}\right)(\bar{k}^2-k^2) + 2\left(1+e^{2a\bar{k}}\right)k\bar{k} \right]$$

$$M_{12} = \frac{ie^{-a(ik+\bar{k})}}{4k\bar{k}} \left[ \left(-1+e^{2a\bar{k}}\right)(k^2+\bar{k}^2) \right]$$

$$M_{21} = (M_{12})^*$$

$$M_{22} = (M_{11})^*.$$
(13.9)

It is interesting that we now have a direct relation between the left and right coefficients that makes no explicit reference to the intermediate region where the potential acts. This suggests that the structure of  $\mathbb{M}$  contains all the physics – both boundary conditions and potential (through  $\bar{k}$ ). Now that we have the above matrix elements, we are ready to do some test-cases.

#### **13.1.1** Scattering for $V_0 > 0$

If we take  $V_0 > 0$  (a step), then we can consider the two obvious cases:  $E < V_0$  (but greater than zero, of course) and  $E > V_0$ .

#### $E < V_0$

When  $E < V_0$ , we have  $\bar{k}$  real, and our setup was adapted to this case (our choice to use  $e^{\bar{k}x}$  for example). Then the solution inside the potential is growing and decaying exponentials. We can set G = 0, and employ the

trigonometric relations to get (via (13.8)):

$$F = \frac{2 k \bar{k} e^{-i a k} A}{2 k \bar{k} \cosh(a \bar{k}) - i (k^2 - \bar{k}^2) \sinh(a \bar{k})}$$
  

$$B = -\frac{i (k^2 + \bar{k}^2) \sinh(a \bar{k}) A}{2 k \bar{k} \cosh(a \bar{k}) - i (k^2 - \bar{k}^2) \sinh(a \bar{k})}.$$
(13.10)

The reflection and transmission coefficients can be defined "as usual" here, since in the left and right-hand regions, we have the same k. The transmissions coefficient, written in unitless  $z \equiv \sqrt{\frac{2 m E}{\hbar^2}} a$  notation is:

$$T \equiv \frac{|F|^2}{|A|^2} = \frac{8 z^2 (z^2 - z_0^2)}{8 z^4 - 8 z^2 z_0^2 - 2 z_0^4 \sinh^2\left(\sqrt{z_0^2 - z^2}\right)}$$
(13.11)

with  $z_0 \equiv \sqrt{\frac{2 m V_0}{\hbar^2}} a$ . The transmission coefficient, as a function of z is shown in Figure 13.1.



Figure 13.1: Transmission coefficient from (13.11) for  $z_0 = 1$ .

We can recover the C and D coefficients from (13.5), either set will do. In this case, we have

$$C = -\frac{A e^{-a\bar{k}} k (k - i\bar{k})}{2 i k \bar{k} \cosh(a\bar{k}) + (k^2 - \bar{k}^2) \sinh(a\bar{k})}$$

$$D = \frac{A e^{a\bar{k}} k (k + i\bar{k})}{2 i k \bar{k} \cosh(a\bar{k}) + (k^2 - \bar{k}^2) \sinh(a\bar{k})}.$$
(13.12)

An example wave-function is shown in Figure 13.2 – the potential is non-zero in the range  $x \in (0, 1)$ .



Figure 13.2: A wave function with plane wave input – the real part is shown, there are oscillatory portions on the left and right of the potential step, with "tunneling" through the step.

 $E > V_0$ 

For energy greater than the potential, we can take our results from above directly, and replace  $\bar{k} = i K$  for K real. That amounts to setting:

$$K = \sqrt{\frac{2\,m\,|V_0 - E|}{\hbar^2}}.$$
(13.13)

Making this replacement<sup>1</sup> to find the transmission coefficient, for example, we have

$$T = \frac{1}{\cos^2(a\,K) + \frac{(k^2 + K^2)^2 \,\sin^2(a\,K)}{4\,k^2\,K^2}},\tag{13.14}$$

or, using our nondimensionalized form (compare with (13.11))

$$T = \frac{8 z^2 (z^2 - z_0^2)}{8 z^4 - 8 z^2 z_0^2 + 2 z_0^2 \sin^2(\sqrt{z^2 - z_0^2})},$$
(13.15)

and this is shown in Figure 13.3.

Notice the tantalizing possibility presented by (13.15), and shown clearly in the figure: Periodically (no pun intended), the transmission is perfect (T = 1). This happens whenever

$$2\sqrt{z^2 - z_0^2} = 2\,m\,\pi,\tag{13.16}$$

<sup>&</sup>lt;sup>1</sup>Note that  $\cosh(ix) = \cos(x)$  for x real, and  $\sinh(ix) = i \sin(x)$ , these follow directly from the exponential representation of cosine and sine.



Figure 13.3: Transmission coefficient (13.15) as a function of "energy" z for the  $E > V_0$  potential step.

for integer m. In terms of E and  $V_0$ , the requirement is

$$\sqrt{2m(E-V_0)} = \frac{\hbar m \pi}{a}.$$
 (13.17)

The quantization of energy (relative to  $V_0$ ) is occuring here because of the "resonance" inside the potential – it is possible to tune the energy so that the solution inside the potential step is oscillatory at (an integer multiple of) the fundamental wavelength of the potential itself, a standing wave inside the step.

Some example wavefunctions are shown pieced together in Figure 13.4

We have exhausted the energy relations (except for  $E = V_0$ , which requires a very different sort of analysis) for  $V_0 > 0$ . The finite potential well has very similar solutions, we can study the scattering case ( $V_0 < 0, E > 0$ ) by sending  $V_0 \rightarrow -V_0$  in our current setup. But for the finite well, we also have a new possibility: Bound states.

### **13.1.2** Bound States of the Finite Well $(V_0 < 0)$

For  $V_0 < 0$ , we can have E < 0. The solutions to the left and right of the well will now be growing and decaying exponentials, while the solution inside the well will be oscillatory. In a sense, we are reversing the case  $V_0 > 0$ with  $E < V_0$ , where we had oscillation outside the step, and exponentials inside. The big difference for  $V_0 < 0$ , E < 0 is that now, our demand that the wavefunction vanish at infinity means that we can have only decaying exponentials on either side of the well.

Referring to (13.2), we can see the modifications clearly. Now  $k = \sqrt{\frac{2 m E}{\hbar^2}}$  is



Figure 13.4: Example  $E > V_0$  wavefunctions. For the top plot, we have  $z_0 = 1, z = 2$ . The bottom plot shows a resonance at  $2\sqrt{z^2 - z_0^2} = 2m\pi$  for m = 4.

imaginary, since E < 0, so set k = i K, and then we have to kill the growing exponential on the left: A = 0, and on the right: G = 0. That means we need to return to (13.7) – we must have  $B = M_{21} F$  and  $M_{11} = 0$  before we can sensibly discuss the interior solution. Thinking about  $\bar{k} = \sqrt{-\frac{2 m (|V_0| - |E|)}{\hbar^2}}$ , we see that  $\bar{k}$  is imaginary, so set  $\bar{k} \equiv i \bar{K}$ . Then from (13.9), we have

$$M_{11} = \frac{e^{a\left(-K-i\bar{K}\right)}}{-4\,K\,\bar{K}} \left[i\left(-1+e^{i\,2\,a\,\bar{K}}\right)\,\left(K^2-\bar{K}^2\right) - 2\left(1+e^{i\,2\,a\,\bar{K}}\right)\,K\,\bar{K}\right].$$
(13.18)

To get  $M_{11} = 0$ , we solve the above for K:

$$K = \bar{K} \tan\left(\frac{1}{2} a \bar{K}\right), \qquad (13.19)$$

and now going to dimensionless:  $z \equiv \bar{K}a = \sqrt{\frac{2 m (|V_0| - |E|)}{\hbar^2}} a$ , with  $z_0 = \sqrt{\frac{2 m |V_0|}{\hbar^2}} a$ , so that  $Ka = \sqrt{\frac{2 m |E|}{\hbar^2}} a = \sqrt{z_0^2 - z^2}$  and the above can be written:

$$\sqrt{z_0^2 - z^2} = z \, \tan\left(\frac{1}{2}\,z\right) \longrightarrow \left[ \tan\left(\frac{1}{2}\,z\right) = \sqrt{-1 + \frac{z_0^2}{z^2}} \right]$$
(13.20)

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Evidently, for a bound state to exist (meaning that it decays to zero at positive and negative infinity), we must have a very particular (quantized) relation between the energy of the particle and the potential. The transcendental roots are shown in Figure 13.5 – we have set  $z_0 = 8\pi$  there, and plotted the left and right-hand sides of (13.20).



Figure 13.5: The  $\tan(z/2)$  vs.  $\sqrt{-1 + \frac{z_0^2}{z^2}}$  for  $z_0 = 8\pi$ . The cross-over points represent the allowed energies for bound solutions to the finite potential well.

Taking the solution  $z \sim 14.4799678$  and  $z \sim 20.1329987$  (obtained by numerical root-finding), the third and fourth circled points in Figure 13.5, we can construct the complete wavefunction here – the result is shown in Figure 13.6.

## 13.2 Limit

We should be able to recover the bound state of the Dirac delta function potential (well):  $V_0 = -\alpha \, \delta(x)$  with  $\alpha$  positive. Take our condition (13.20), and input  $z, z_0$ :

$$\tan\left(\frac{a\sqrt{m\left(|V_0| - |E|\right)}}{2\hbar^2}\right) = \sqrt{-1 + \frac{|V_0|}{|V_0| - |E|}}$$
(13.21)



Figure 13.6: Third and fourth bound state for finite well.

We can approximate the delta function in one dimension as a box of height  $\frac{1}{a}$  in the limit  $a \to 0^2$ , inputting  $|V_0| = \frac{\alpha}{a}$  gives

$$\tan\left(\sqrt{\frac{m\,a\,(\alpha-|E|\,a)}{2\,\hbar^2}}\right) = \sqrt{-1 + \frac{1}{1-\frac{a}{\alpha}\,|E|}}.$$
(13.22)

Now Taylor expand both sides to get the small a behavior – using  $\tan(z) \sim z$  for small z,

$$\sqrt{\frac{m \, a \, \alpha}{2 \, \hbar^2}} = \sqrt{\frac{a \, |E|}{\alpha}} \tag{13.23}$$

to order  $\sqrt{a}$ . We can solve this for |E| to recover the usual relation for the bound state energy of the delta well:

$$E = -\frac{m\,\alpha^2}{2\,\hbar^2},\tag{13.24}$$

where we have assumed throughout that E < 0.

<sup>&</sup>lt;sup>2</sup>That provides the defining feature  $\int_{-\infty}^{\infty} \delta(x) dx = 1$  for all values of *a*.

# **13.3** Numerical Solution

There are a variety of ways to solve Schrödinger's equation numerically. Any method will require spatial discretization, and there is a well-defined way to turn differential operators like  $\frac{d^2}{dx^2}$  into matrices. The basic idea is to approximate:

$$\frac{d^2 f(x)}{dx^2} \sim \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2}$$
(13.25)

on a grid of evenly spaced points, say,  $x_j = j \Delta x$ . Then we can form a vector of f(x) evaluated at the grid points:  $f_j \equiv f(x_j)$ , and a matrix that repeats the above stencil for each grid point. Call this operator  $\mathbb{H}$  – then Schrödinger's equation can be written as:

$$i\,\hbar\,\dot{\Psi} = \mathbb{H}\,\Psi \tag{13.26}$$

as a matrix-vector equation (with the elements of  $\Psi$  defined to be  $\psi_j \equiv \psi(x_j)$ ).

#### 13.3.1 Discrete Eigenvalues

Since the grid is discrete, and  $\mathbb{H} = \mathbb{H}^T$ , we can calculate the numerical eigenvalues and eigenvectors associated with  $\mathbb{H}$ , define:

$$\mathbb{H}\,\boldsymbol{\psi}_n = \lambda_n\,\boldsymbol{\psi}_n,\tag{13.27}$$

then the solution to (13.26) is given, for each of the eigenvectors, as

$$i\hbar\dot{\Psi}_n = \lambda_n\Psi_n \longrightarrow \Psi_n = \alpha \,e^{-i\frac{\lambda_n}{\hbar}t}\,\psi_n,\tag{13.28}$$

for any overall  $\alpha$ . This is a vector, remember, and we can construct a general solution by decomposing some initial waveform given at t = 0 – the general solution is:

$$\Psi = \sum_{j=1}^{N} \alpha_j \, e^{-i \frac{\lambda_n}{\hbar} t} \, \psi_n \tag{13.29}$$

where N is the number of gridpoints (hence the number of eigenvectors). Given  $\Psi(t = 0)$ , we just decompose as usual:

$$\alpha_j = \boldsymbol{\psi}_j \cdot \boldsymbol{\Psi}(0) \tag{13.30}$$

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and use these  $\alpha_j$ 's in our full solution (13.29). It's a nice idea, especially since it exactly parallels what we have been doing with continuous functions. There are a few difficulties, though – even for the simplest Gaussian wavepacket, we expect nontrivial dependence on all eigenvectors, and these eigenvectors are finite – while we can perfectly represent a wave packet on the grid, there is no way to ensure that the wavepacket travels smoothly. Effectively, we need too large of a grid to ensure enough eigenvectors to correctly decompose the packet as it moves along the grid. The result of too few eigenvectors is a solution plagued by "Gibbs' phenomena", ringing from unresolved modes that travel at inexact speeds (remember, our spectrum for a matrix is finite, at some level a poor approximation to the infinite spectrum we expect).

#### 13.3.2 Implicit Differencing

Rather than use the separated form of Schrödinger's equation, we can work directly from (13.26) by introducing a finite temporal "grid", and approximating the time derivative of the solution vector as:

$$\dot{\boldsymbol{\Psi}}(x,t) \sim \frac{\boldsymbol{\Psi}(x,t+\Delta t) - \boldsymbol{\Psi}(x,t)}{\Delta t},$$
(13.31)

so that if we let  $\Psi^n$  represent the vector (on the finite spatial grid) solution at time  $t^n \equiv n \Delta t$ , our method is defined by:

$$\Psi^{n+1} = \left( \mathbb{I} + \frac{\Delta t}{i\hbar} \mathbb{H} \right) \Psi^n.$$
(13.32)

We could start with a known initial waveform at t = 0 (a Gaussian, for example), and propagate the solution vector forward in time using the above. But it is easy to show that repeated multiplication by a matrix has the property that any initial vector rotates into the direction of the matrix's maximum eigenvector (that is, the eigenvector associated with the largest eigenvalue), and this property, for maximum eigenvalue > 1 will artificially spoil the numerical solution allowing the wavefunction, in this case, to grow exponentially with time. The matrix in (13.32) has maximum (absolute value) eigenvalue greater than one, and the resulting numerical method is known to be unstable.

The fix is relatively simple – we want an approximation equivalent to the above, but one with a matrix whose iterated multiplication will not artificially favor its maximum eigenvector – that is, a matrix that has largest

eigenvalue < 1, but yields the same approximation. We can form such a matrix via:

$$i\hbar \frac{\Psi^{n+1} - \Psi^n}{\Delta t} = \mathbb{H}\Psi^{n+1}, \qquad (13.33)$$

that is, replace the vector evaluation on the right with the updated vector. Now rearranging, we have:

$$\Psi^{n+1} = \underbrace{\left(\mathbb{I} - \frac{\Delta t}{i\hbar} \mathbb{H}\right)^{-1}}_{\equiv \mathbb{P}} \Psi^n, \qquad (13.34)$$

and while we now have to invert a matrix, it is the case that  $\mathbb{P}$  has largest eigenvalue with unit magnitude. This "implicit" method is stable, and works well with our one-dimensional scattering problems.

## 13.4 Examples

To check the method, we'll start with a Gaussian bump with some initial momentum p and expected value for position b – so our initial wave-function is

$$\psi(x,0) = \left(\frac{2a}{\pi}\right)^{1/4} e^{ipx} e^{-a(x-b)^2}.$$
(13.35)

The time evolution of this initial waveform is shown in Figure 13.7.

We can introduce a potential barrier, then the behavior of the wavefunction depends on the magnitude of the barrier height. For a "large" barrier, we get essentially reflective decomposition, shown in Figure 13.8

Finally, we can use a moderate-sized barrier, one for which the maximum energy modes of the initial Gaussian are both bigger and smaller than the height of the barrier. Now the probability density spreads out over the entire domain after some time has passed. The temporal evolution is shown in Figure 13.9.

#### Homework

Reading: Griffiths, pp. 78-83.



Figure 13.7: The temporal evolution of a Gaussian bump initial waveform (13.35). We are plotting probability density for the one-dimensional grid in each pane.



Figure 13.8: Time evolution of a Gaussian wavepacket under the influence of a large potential barrier centered at the origin.



Figure 13.9: Probability density evolution under the influence of a medium sized finite barrier.

#### Problem 13.1

For the delta function potential,  $V(x) = \alpha \, \delta(x)$ :

a. Write the solution ansatz to the left and the right of the barrier in terms of: 1. A plane wave traveling to the right with amplitude A and one traveling to the left with amplitude B in the region x < 0 and 2. A plane wave traveling to the left with amplitude G and one traveling to the right with amplitude F in x > 0.

Using the boundary conditions appropriate to the delta potential, find the matrix connecting (A, B) and (F, G),  $\mathbb{M}$  below:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \mathbb{M} \begin{pmatrix} F \\ G \end{pmatrix}.$$
(13.36)

b. From this matrix, and using the "standard" setup where we have an incoming and reflected wave in x < 0 and a transmitted wave in x > 0, find the reflection and transmission coefficients for  $\alpha > 0$  (scattering for a positive delta spike). Show that these sum to one. Do they look familiar?

c. Now take  $\alpha < 0$ , and show that  $M_{11} = 0$  leads to the energy

constraint for the bound state of the delta well (so take E < 0, and show that  $M_{11} = 0$  gives back the single energy:  $E = -\frac{m \alpha^2}{2 \hbar^2}$ ).

## Problem 13.2

Griffiths 2.27. Here you are finding the bound state(s) of a pair of delta wells.