

Piecewise Potentials II

Lecture 15

Physics 342
Quantum Mechanics I

Friday, February 26th, 2010

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.

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 ($e^{-i\frac{E}{\hbar}t}$), 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.

15.1 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:

$$\frac{d^2 f(x)}{dx^2} \sim \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2} \quad (15.1)$$

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:

$$i \hbar \dot{\Psi} = \mathbb{H} \Psi \quad (15.2)$$

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

15.1.1 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:

$$\mathbb{H} \psi_n = \lambda_n \psi_n, \quad (15.3)$$

then the solution to (15.2) is given, for each of the eigenvectors, as

$$i \hbar \dot{\Psi}_n = \lambda_n \Psi_n \longrightarrow \Psi_n = \alpha e^{-i \frac{\lambda_n}{\hbar} t} \psi_n, \quad (15.4)$$

for any overall α . 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:

$$\Psi = \sum_{j=1}^N \alpha_j e^{-i \frac{\lambda_j}{\hbar} t} \psi_j \quad (15.5)$$

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

$$\alpha_j = \psi_j \cdot \Psi(0) \quad (15.6)$$

and use these α_j ’s in our full solution (15.5). 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).

15.1.2 Implicit Differencing

Rather than use the separated form of Schrödinger's equation, we can work directly from (15.2) by introducing a finite temporal “grid”, and approximating the time derivative of the solution vector as:

$$\dot{\Psi}(x, t) \sim \frac{\Psi(x, t + \Delta t) - \Psi(x, t)}{\Delta t}, \quad (15.7)$$

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

$$\Psi^{n+1} = \left(\mathbb{I} + \frac{\Delta t}{i \hbar} \mathbb{H} \right) \Psi^n. \quad (15.8)$$

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 (15.8) 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:

$$i \hbar \frac{\Psi^{n+1} - \Psi^n}{\Delta t} = \mathbb{H} \Psi^{n+1}, \quad (15.9)$$

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

$$\Psi^{n+1} = \underbrace{\left(\mathbb{I} - \frac{\Delta t}{i \hbar} \mathbb{H} \right)^{-1}}_{\equiv \mathbb{P}} \Psi^n, \quad (15.10)$$

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, however

it implies a decrease in the “normalization” of the wave function – i.e. we lose probability artificially. As it turns out, an “average” of the explicit and implicit methods gives a numerical method that, like Schrödinger’s equation itself, preserves the initial normalization of the wavefunction.

15.2 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

$$\psi(x, 0) = \left(\frac{2a}{\pi}\right)^{1/4} e^{ipx} e^{-a(x-b)^2}. \quad (15.11)$$

The time evolution of this initial waveform is shown in Figure 15.1.

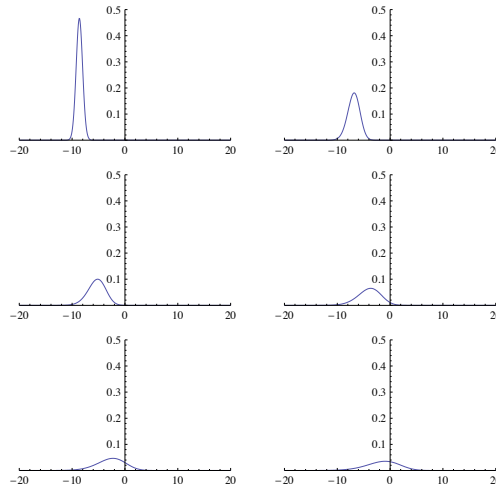


Figure 15.1: The temporal evolution of a Gaussian bump initial waveform (15.11). We are plotting probability density for the one-dimensional grid in each pane.

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 15.2

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

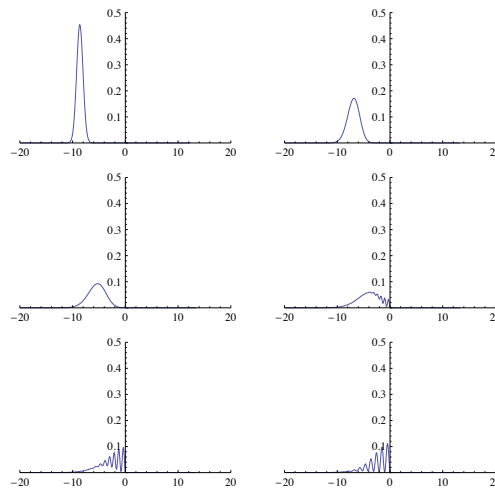


Figure 15.2: Time evolution of a Gaussian wavepacket under the influence of a large potential barrier centered at the origin.

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 15.3.

Homework

Reading: Griffiths, pp. 78–83.

Problem 15.1

Find the scattering states, reflection and transmission coefficients for a delta potential: $V(x) = \alpha \delta(x)$, with $\alpha > 0$ this time.

Problem 15.2

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

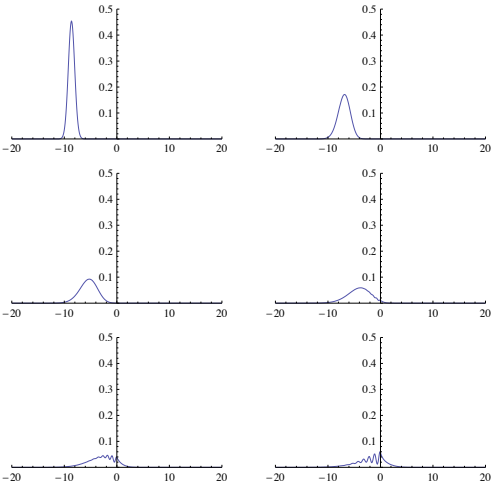


Figure 15.3: Probability density evolution under the influence of a medium sized finite barrier.