

Energy and Free Particles

Lecture 11

Physics 342
Quantum Mechanics I

Wednesday, February 17th, 2010

We begin with a partition of energies – classically, we can have particles “bound” together in a potential well formed by their interaction, or we can have particles that “scatter” off of one another. For a generic potential, both behaviors are allowed, and the total energy of the particle selects one or the other. This is also true for quantum mechanics, and we will discuss the basic physical ideas that allow us to predict scattering or bound states on the quantum side. This idea is tied up with normalizability, and provides a venue for discussing plane wave solutions and their physical characterization.

11.1 Classical Energetics

We are used to looking at potentials in one dimension, and specifying physical behavior based on a particle’s energy. For example, the potential shown in Figure 11.1 is not necessarily connected to a physical process. Yet, for the energies shown, we can predict the basic motion of a particle.

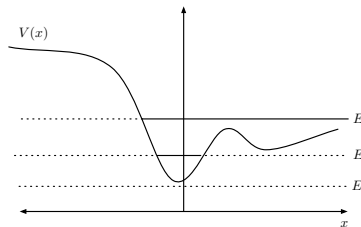


Figure 11.1: A potential with three energy regimes shown. The dotted portion of the energy lines are the inaccessible regimes.

A particle with energy E_a cannot exist under this potential, at least not in the usual sense, since $E_a = V(x) + \frac{1}{2} m v^2$ is a constant of the motion, if $E < V(x)$, then $E_a - V(x) = \frac{1}{2} m v^2 < 0$, implying a complex velocity, so we do not expect valid solutions for any energy $E < \min(V(x))$. The E_b energy is allowed, and the potential in that region can be well-approximated by a parabola, so we have simple harmonic motion (roughly). The energy E_c is also allowed, and here we expect scattering – that is, particle comes in with some velocity, reaches a location x_c for which $E_c = V(x_c)$ (i.e. all the energy is potential, so the particle is at rest), turns around and goes back out.

We have seen the “bound” case for quantum mechanics – both the infinite square well and the harmonic oscillator have bound solutions, the analogue of E_b in the above picture. We have also excluded solutions that have $E < \min(V(x))$, when we introduced the idea of ψ_0 for the harmonic oscillator – there, the minimum of the potential is $V_{min} = 0$ (at $x = 0$), and we argued that negative energy solutions could not exist, so that $a_- \psi_0 = 0$ was a way out. An energy below some potential minimum is invalid quantum mechanically because any resulting wavefunction would not be normalizable. To see this, take the one-dimensional time-independent Schrödinger equation, written as

$$-\frac{\hbar^2}{2m} \psi''(x) = (E - V(x)) \psi(x) \longrightarrow \psi''(x) = \alpha(x) \psi(x) \quad (11.1)$$

$$\alpha(x) \equiv \frac{2m}{\hbar^2} (V(x) - E).$$

If $V(x) > E$ for all x , then $\alpha(x) > 0$ for all x . If we multiply both sides of this equation by $\psi(x)$ and integrate from $-\infty \rightarrow \infty$, then

$$\int_{-\infty}^{\infty} \psi''(x) \psi(x) dx = \int_{-\infty}^{\infty} \alpha(x) \psi(x)^2 dx \quad (11.2)$$

$$- \int_{-\infty}^{\infty} \psi'(x)^2 dx = \int_{-\infty}^{\infty} \alpha \psi(x)^2 dx$$

where we used integration by parts on the left-hand-side (so we have assumed that the wavefunction vanishes at spatial infinity). But now the left hand side is strictly negative, the right-hand side, strictly positive, we cannot find such a $\psi(x)$. This is the quantum version of the classical argument from above.

What about the “scattering” states? As we shall see, the hallmark of scattering in quantum mechanics is a continuum of allowed energies. Our bound

state work has all ended up with quantized energy, this comes about mathematically from boundary conditions and normalizability.

11.2 Free Particle

The simplest “scattering” solution is a free particle – it scatters off of nothing, of course, just as a classical free particle doesn’t scatter (traveling forever in a straight line) – but the basic idea, a continuum of energies, is there. We have already encountered the solution – when we studied the infinite square well, so we know that the time-independent Schrödinger equation with zero potential has solutions:

$$-\frac{\hbar^2}{2m} \psi''(x) = E \psi(x) \longrightarrow \psi(x) = A e^{i \sqrt{\frac{2mE}{\hbar^2}} x} + B e^{-i \sqrt{\frac{2mE}{\hbar^2}} x}. \quad (11.3)$$

With no boundary conditions to impose, we have no restriction on E , so any E is allowed. The full solution is just $\Psi(x, t) = e^{-iEt/\hbar} \psi(x)$ as usual, so

$$\Psi(x, t) = A e^{i \left(\sqrt{\frac{2mE}{\hbar^2}} x - \frac{Et}{\hbar} \right)} + B e^{-i \left(\sqrt{\frac{2mE}{\hbar^2}} x + \frac{Et}{\hbar} \right)}. \quad (11.4)$$

If we define $k \equiv \sqrt{\frac{2mE}{\hbar^2}}$, then we can write this as

$$\Psi(x, t) = A e^{i \left(kx - \frac{\hbar k^2}{2m} t \right)} + B e^{-i \left(kx + \frac{\hbar k^2}{2m} t \right)}. \quad (11.5)$$

This solution represents left and right traveling plane waves. The general solution to the wave equation with fundamental velocity v

$$-\frac{1}{v} \frac{\partial^2 f(x, t)}{\partial t^2} + \frac{\partial^2 f(x, t)}{\partial x^2} = 0 \quad (11.6)$$

is $f(x, t) = \phi(x \pm vt)$, and what we have above is precisely this with $\phi(y) = e^{iky}$ and $v = \frac{\hbar k}{2m}$. That these represent monochromatic plane waves is familiar from electrodynamics. There, we usually take just the real part of the solution, so what we have is a cosine wave in space that travels to the left or right with constant speed.

Here, for our statistical interpretation, we take the full, complex $\Psi(x, t)$ – an individual solution cannot represent any particular physics – these wavefunctions are *not* normalizable, we cannot make $\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx =$

1. Nevertheless, we *can* build solutions out of them. Take just the right-traveling form (that's all we need anyway)

$$\Psi_k(x, t) = A e^{i(kx - \frac{\hbar k^2}{2m} t)} \quad (11.7)$$

where we allow k to be positive or negative to cover both terms of the full solution. Consider a valid initial waveform, $\bar{\psi}(x)$ (valid meaning that $\int_{-\infty}^{\infty} \bar{\psi}(x)^* \bar{\psi}(x) dx = 1$), then the question is: Can we build $\bar{\psi}$ out of combinations of $\Psi(x, t = 0)$? That is the procedure we have followed in both cases so far – take the spatial solutions and use them to construct some desired initial state. That we could do so was guaranteed by the completeness of the sine series for the square well, and the completeness of the Hermite polynomials for the harmonic potential. Here, even though the individual $\Psi(x, t = 0)$ are not square-integrable, we know from Fourier transformation that we can build (most) functions out of them.

11.2.1 Fourier Transform

Given a function $f(x)$, define the symmetric Fourier transform via

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \quad (11.8)$$

then the inverse transform is

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} dk. \quad (11.9)$$

Incidentally, from these definitions, we can find the Fourier transform of the Dirac delta function:

$$\text{FT}(\delta(x - a)) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x - a) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} e^{-ika} \quad (11.10)$$

and the useful relation for the inverse:

$$\text{FT}(e^{-ika}) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-ika} e^{ikx} dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-a)} dk \quad (11.11)$$

but since the Fourier transform of the Fourier transform is the original function, we have a nice integral representation for the delta function:

$$\delta(x - a) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-a)} dk \quad (11.12)$$

The utility is clear – if we are given an initial waveform $\bar{\psi}(x)$, then we can compute its Fourier transform to get $\tilde{\psi}(k) \equiv \phi(k)$, and then the initial waveform itself is

$$\bar{\psi}(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} dk \quad (11.13)$$

The generic solution is, then,

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} e^{-i\frac{\hbar k^2}{2m}t} dk \quad (11.14)$$

with

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \bar{\psi}(x) dx. \quad (11.15)$$

This should remind you of the general solutions we studied in the harmonic oscillator and infinite square well cases. There, we had:

$$\Psi(x, t) = \sum_{j=1}^{\infty} A_j \psi_j(x) e^{-i\frac{E_j}{\hbar}t}, \quad (11.16)$$

the analogue of (11.14), where $\{A_j\}_{j=1}^{\infty}$ is the discrete set of coefficients corresponding to the continuous function $\phi(k)$, while $\psi_j(x)$ is playing the role of the free particle solution e^{ikx} – finally, E_j is some relation between the index j and the energy associated with the stationary state (for the harmonic oscillator, $E_j = (j + \frac{1}{2}) \hbar\omega$, for the infinite square well, $E_j = \frac{j^2 \pi^2 \hbar^2}{2ma^2}$) while for the free particle, $E(k) = \frac{\hbar^2 k^2}{2m}$, a continuous function of k .

For the oscillator and infinite square well, we use the initial condition $\Psi(x, 0) = \bar{\psi}(x)$ (with $\bar{\psi}(x)$ provided), together with the completeness and orthonormality of the eigenfunctions $\{\psi_j(x)\}_{j=1}^{\infty}$ to find the coefficients via:

$$A_j = \int_{-\infty}^{\infty} \psi_j^*(x) \bar{\psi}(x) dx. \quad (11.17)$$

This is the discrete analogue of (11.15) (note there that $(e^{ikx})^* = e^{-ikx}$ as always) – the index j is an integer, while the variable k in $\phi(k)$ is a continuous “index”.

11.3 A Gaussian Wave Packet

Suppose we start with a wavefunction that is a Gaussian with mean 0 (meant to represent a particle sitting at the origin initially within experimental

accuracy) – properly normalized, we have

$$\bar{\psi}(x) = \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2} \quad (11.18)$$

and the variance here is $\frac{1}{4a}$, so that a large value for a means a more sharply peaked distribution, smaller a corresponds to a broader distribution.

We must find $\phi(k)$ associated with this initial $\bar{\psi}(x)$. From the Fourier transform, we have

$$\begin{aligned} \phi(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{2a}{\pi}\right)^{1/4} e^{-ikx - ax^2} dx \\ &= \frac{1}{\sqrt{2\pi}} \left(\frac{2a}{\pi}\right)^{1/4} \sqrt{\frac{\pi}{a}} e^{-\frac{k^2}{4a}} \\ &= \left(\frac{1}{2\pi a}\right)^{1/4} e^{-\frac{k^2}{4a}}, \end{aligned} \quad (11.19)$$

and then the full wavefunction with time dependence is

$$\begin{aligned} \Psi(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{1}{2\pi a}\right)^{1/4} e^{ikx - \frac{\hbar k^2}{2m} t - \frac{k^2}{4a}} dk \\ &= \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2\pi a}\right)^{1/4} \left(2\sqrt{\pi} e^{-\frac{amx^2}{m+2ia\hbar t}}\right) \left(\sqrt{\frac{1}{a} + \frac{2i\hbar t}{m}}\right)^{-1} \\ &= \left(\frac{2}{\pi a}\right)^{1/4} \frac{e^{-\frac{amx^2}{m+2ia\hbar t}}}{\sqrt{\frac{1}{a} + \frac{2i\hbar t}{m}}}. \end{aligned} \quad (11.20)$$

What happens here? We start with probability density peaked about $x = 0$, the density itself takes the form

$$|\Psi(x, t)|^2 = e^{-\frac{2am^2x^2}{m^2+4a^2\hbar^2t^2}} \sqrt{\frac{2am^2}{\pi(m^2+4a^2\hbar^2t^2)}} \quad (11.21)$$

which is again Gaussian with mean zero and variance

$$\sigma_x^2 = \langle x^2 \rangle - 0 = \int_{-\infty}^{\infty} \Psi^*(x, t) x^2 \Psi(x, t) dx = \frac{1}{4a} + \frac{a\hbar^2 t^2}{m^2}. \quad (11.22)$$

So as time goes on, the Gaussian spreads – the probability that the particle is in a small region near the origin drops. In fact, if we calculate the energy of the configuration (it is a constant, of course) via $\langle H \rangle$, then

$$\langle H \rangle \equiv E = \frac{a \hbar^2}{2m} \quad \sigma_x^2 = \frac{1}{4a} + 2 \frac{E}{m} t^2, \quad (11.23)$$

so the initial spread of the Gaussian determines the energy of the configuration, and the larger the energy, the faster the Gaussian spread decays over time. A sharply peaked Gaussian spreads out *faster* than a less localized initial distribution.

It is difficult to make a direct comparison of the classical density, as we have been doing for the stationary bound states of the infinite square well and the harmonic oscillator. Most of the basic features of a set of classical experiments are evident in the above. If we prepared a swarm of particles with the same velocity, starting at the origin, then we would expect to get average velocity zero (the particles can travel to the left or right with the same speed), and zero expectation for position.

The biggest difference comes in the observation that the classical variance in momentum would be zero, or some small quantity that depended on our velocity-measuring apparatus. In particular, you would think it was crazy to claim that the variance in the momentum, the error associated with our momentum measurements, depended on the error associated with our initial position measurements. And yet, if we take our Gaussian, above, and calculate $\langle p^2 \rangle$, we will get

$$\langle p^2 \rangle = 2m \langle H \rangle = 2mE = a \hbar^2 \quad (11.24)$$

where a is related to the initial position variance of the distribution. Evidently, the quantum mechanical variances for position and momentum are somehow locked together in a way that our classical ones are not (no reason to expect the sensitivity of a position measuring machine to have anything to do with the sensitivity of the momentum-measuring machine.).

Homework

Reading: Griffiths, pp. 59–67.

Problem 11.1

For the classical probability density,

$$\rho(x) = \frac{1}{\pi \sqrt{x_0^2 - x^2}} \quad (11.25)$$

governing the harmonic oscillator with $x(t) = x_0 \cos(\omega t)$:

- a. find the probability that the particle is within one standard deviation of its average value – note that we already know that $\langle x \rangle = 0$ and $\langle x^2 \rangle = \frac{1}{2} x_0^2$.
- b. Find the probability that the particle is between $\frac{9x_0}{10}$ and x_0 .

Problem 11.2

What is the Fourier transform of $f(x) = f_0 \cos(qx)$, where q is a real number?

Problem 11.3

Griffiths 2.21. Finding the decomposition of a specific initial wavefunction in terms of plane waves (i.e. the Fourier transform).