Free Particle Comparison

Lecture 12

Physics 342
Quantum Mechanics I

Friday, February 19th, 2010

Here, we will compare our solutions so far (harmonic potential, infinite square well) with the free particle solution. There are three properties that we have relied upon in our approach to quantum mechanical problems involving "bound states":

- The stationary states are normalizable.
- Stationary states $\{\psi_n(x)\}$ form a complete basis and can be indexed with integers.
- The energy spectrum is (via the discrete form of ψ_n) discrete.

For a free particle, $\hat{H}\,\psi(x) = E\,\psi(x)$ has solution:

$$\psi_k(x) = A\,e^{\pm i\,k\,x} \qquad k^2 \equiv \frac{2\,m\,E}{\hbar^2} \tag{12.1}$$

and already, we notice that the stationary state here is: 1. Not normalizable, and 2. Does not lead to a discrete energy spectrum. We do have a notion of completeness, though, provided by the Fourier transform. Write our continuous solution with the arbitrary normalization and sign choice:

$$\psi_k(x) = \frac{1}{\sqrt{2\,\pi}}\,e^{i\,k\,x}. \tag{12.2}$$

When the stationary states are discrete, we have:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\,\psi_n(x)\,e^{-i\,\frac{E_n}{\hbar}\,t} \tag{12.3}$$

and use orthonormality to set

$$c_m = \psi_m(x) \cdot \bar{\psi}(x) \equiv \int_{-\infty}^{\infty} \psi_m^*(x)\, \bar{\psi}(x)\, dx \tag{12.4}$$

for some initial wavefunction $\bar{\psi}(x)$.

When the stationary states are "indexed" by a continuous variable k, the sum in (12.3) becomes an integral (over k)

$$\Psi(x,t) = \int_{-\infty}^{\infty} \phi(k)\, \psi_k(x)\, e^{-i\, \frac{E_k}{\hbar}\, t}\, dk \qquad E_k = \frac{\hbar^2\, k^2}{2\, m} \tag{12.5}$$

and the $\phi(k)$ play the role of the c_n's. As another point of similarity, we obtain the "coefficients" $\phi(k)$ from a dot product with a provided initial wavefunction $\bar{\psi}(x)$:

$$\phi(k) = \psi_k(x) \cdot \bar{\psi}(x) = \int_{-\infty}^{\infty} \psi_k^*(x)\, \bar{\psi}(x)\, dx = \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} e^{-i\,k\,x}\, \bar{\psi}(x)\, dx, \tag{12.6}$$

which tells us that $\phi(k)$ is interpretable as the Fourier transform of the initial wavefunction $\bar{\psi}(x)$.

In the end, the only major deviation is the normalizability of the stationary states – $e^{\pm i\,k\,x}$ doesn't vanish at spatial infinity, and cannot be integrated over all space. So by itself, this is not a candidate for an initial state, nor can we give $\psi_k(x)$ a statistical interpretation (except locally) – but as a basis for functions, $\psi_k(x)$ is still good.

12.1 Gaussian Integrals

In studying Gaussian initial wavefunctions, which are relevant given experiment[1], we often encounter integrals of the form:

$$\int_{-\infty}^{\infty} e^{-\left(A\,x^2 + B\,x + C\right)}\, dx, \tag{12.7}$$

and we would like to develop a method for evaluating these in terms of the fundamental Gaussian integral:

$$\int_{-\infty}^{\infty} e^{-y^2}\, dy = \sqrt{\pi}. \tag{12.8}$$

[1] after all, do we ever *really* know where a particle is? There is, at the very least, always an experimental tolerance to our apparati. Gaussian distributions encode that tolerance via a choice of width.

What we need is a factorization in terms of y, so consider the product:

$$\left(\sqrt{A}\,x + F\right)^2 = A\,x^2 + 2\sqrt{A}\,F\,x + F^2, \tag{12.9}$$

and notice that if we were to set:

$$2\sqrt{A}\,F\,x = B\,x \longrightarrow F = \frac{B}{2\sqrt{A}}, \tag{12.10}$$

then we could define $y \equiv \sqrt{A}\,x + F$, and have:

$$y^2 - F^2 = A\,x^2 + B\,x \longrightarrow y^2 - \frac{B^2}{4\,A} = A\,x^2 + B\,x, \tag{12.11}$$

so that our integral becomes:

$$\begin{aligned}\int_{-\infty}^{\infty} e^{-\left(A\,x^2 + B\,x + C\right)} dx &= e^{-C} \int_{-\infty}^{\infty} e^{-\left(y^2 - \frac{B^2}{4\,A}\right)} \frac{dy}{\sqrt{A}} \\ &= \frac{e^{-C + \frac{B^2}{4\,A}}}{\sqrt{A}} \int_{-\infty}^{\infty} e^{-y^2}\,dy \\ &= \sqrt{\frac{\pi}{A}}\, e^{-C + \frac{B^2}{4\,A}}.\end{aligned} \tag{12.12}$$

We are assuming, in the above, that the real part of A is greater than zero so that $e^{-A\,x^2}$ really does decay.

12.2 Fourier Series

I would like to connect the familiar Fourier series to the Fourier transformation in the usual way (see Arken, Boas or your favorite mathematical methods book) – this helps make the move from discrete energy with integer-labelled stationary states (like those associated with the infinite square well, or harmonic oscillator potential) to continuous states with a continuum of allowed energies.

A periodic function $f(x)$ defined on $x \in [0, a]$ has a Fourier series expansion:

$$f(x) = \sum_{m=-\infty}^{\infty} c_m\, e^{\frac{i\,2\,\pi\,m\,x}{a}} \tag{12.13}$$

if the Dirichlet conditions hold:

- The function $f(x)$ is periodic with period a (assumed in definition).
- $f(x)$ has a finite number of minima, maxima and discontinuities on $[0, a]$.
- $\int_0^a |f(x)|\, dx$ is finite.

What we mean by "has a Fourier series expansion" is: The series on the right converges to $f(x)$ at all points $x \in [0, a]$ where $f(x)$ is continuous, and converges to the midpoint of any discontinuities in $f(x)$.

When the Fourier series exists, we can access the coefficients of the expansion by exploiting:

$$\int_0^a e^{-\frac{i\,2\,\pi\,m\,x}{a}}\, e^{\frac{i\,2\,\pi\,n\,x}{a}}\, dx = a\,\delta_{mn}. \tag{12.14}$$

Then

$$c_m = \frac{1}{a}\int_0^a e^{-\frac{i\,2\,\pi\,m\,x}{a}}\, f(x)\, dx. \tag{12.15}$$

12.2.1 Example

Take the discontinuous function:

$$f(x) = \begin{cases} x & x < \frac{1}{2}\,a \\ x+1 & x > \frac{1}{2}a \end{cases}. \tag{12.16}$$

According to (12.15), we have:

$$\begin{aligned} c_m &= \frac{1}{a}\left(\int_0^{\frac{1}{2}\,a} x\, e^{-\frac{i\,2\,\pi\,m\,x}{a}}\, dx + \int_{\frac{1}{2}\,a}^a (x+1)\, e^{-\frac{i\,2\,\pi\,m\,x}{a}}\, dx\right) \\ &= \frac{1}{a}\left(\int_0^a x\, e^{-\frac{i\,2\,\pi\,m\,x}{a}} + \int_{\frac{1}{2}\,a}^a e^{-\frac{i\,2\,\pi\,m\,x}{a}}\, dx\right). \end{aligned} \tag{12.17}$$

Using integration-by-parts on the first term, and integrating the second, I get:

$$c_m = \frac{i\,a}{2\,\pi\,m} - \frac{i\,(-1 + (-1)^m)}{2\,\pi\,m}. \tag{12.18}$$

There is clearly a special case here, at $m = 0$, and this sets an overall constant for the function $f(x)$. If we define the approximate series:

$$f_n(x) = 1 + \sum_{m=-n}^{n} c_m\, e^{\frac{i\,2\,\pi\,m\,x}{a}}, \tag{12.19}$$

with $m \neq 0$, we can get a sense for the "convergence". A few values for n are shown in Figure 12.1.

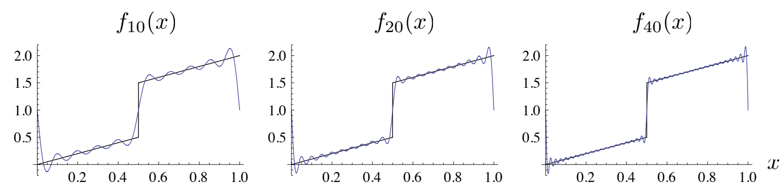

Figure 12.1: Approximate Fourier Series for the function defined in (12.16), $f(x)$ itself is shown in black.

Finally, note that we can, clumsily, introduce the c_m directly into the expansion:

$$f(x) = \sum_{n=-\infty}^{\infty} \frac{1}{a} \left(\int_0^a e^{-\frac{i\,2\,\pi\,n\,x}{a}} f(x)\,dx \right) e^{\frac{i\,2\,\pi\,n\,x}{a}} \tag{12.20}$$

12.3 Fourier Transform

One way to think of the continuous Fourier transform is to consider our function $f(x)$ to be periodic with $a \to \infty$. This allows us to make a connection with the Fourier series, but does not count as a proof of existence, uniqueness or anything else. The following is for motivation only, my goal is to give us a way to talk about the Fourier transform, not rigor (for now).

Our first move will be to symmetrize the interval – suppose we define $f(x)$ on $x \in [-a, a]$, this changes almost nothing – we can rewrite (12.20) to reflect the change:

$$f(x) = \sum_{n=-\infty}^{\infty} \frac{1}{2\,a} \left(\int_{-a}^a e^{-\frac{i\,\pi\,n\,x}{a}} f(x)\,dx \right) e^{\frac{i\,\pi\,n\,x}{a}}. \tag{12.21}$$

Let $p_n \equiv \frac{\pi\,n}{a}$, so that we can think of a "grid" of values p_n indexed by the integer n. The spacing of this grid is $p_{n+1} - p_n = \frac{\pi}{a} \equiv \Delta p$. The eventual "limit" $a \longrightarrow \infty$ will be taken by sending $\Delta p \longrightarrow 0$, giving us a continuum of values p. For now, we have

$$f(x) = \sum_{n=-\infty}^{\infty} \frac{\Delta p}{2\,\pi} \left(\int_{-\pi/\Delta p}^{\pi/\Delta p} e^{-i\,p_n\,x} f(x)\,dx \right) e^{i\,p_n\,x}. \tag{12.22}$$

Now we can think about the limit. We know that an integral can be approximated by box-sums:

$$\int_{-A}^{A} g(p)\,dp \sim \sum_{n=-N}^{N} g(p_n)\,\Delta p. \tag{12.23}$$

The right-hand side can be thought of as the starting point in the definition of the integral (without the limit). What we have, in (12.22) is precisely such an expression, with:

$$g(p_n) = \frac{e^{i\,p_n\,x}}{2\,\pi} \int_{-\pi/\Delta p}^{\pi/\Delta p} e^{-i\,p_n\,x}\,f(x)\,dx \tag{12.24}$$

and N going to infinity. This would be the source of some fancy footwork in carefully taking the limit, but we are motivating only.

Squinting, now, we take $\Delta p \longrightarrow 0$, leaving us with a continuous variable $p_n \longrightarrow p$, and an integral over p:

$$f(x) = \frac{1}{2\,\pi} \int_{-\infty}^{\infty} e^{i\,p\,x} \left[\int_{-\infty}^{\infty} e^{-i\,p\,x}\,f(x)\,dx\right] dp. \tag{12.25}$$

It is from here that we arbitrarily factor the $\frac{1}{2\,\pi}$ and define:

$$\begin{aligned}\tilde{f}(p) &= \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} e^{-i\,p\,x}\,f(x)\,dx \\ f(x) &= \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} e^{i\,p\,x}\,\tilde{f}(p)\,dp.\end{aligned} \tag{12.26}$$

The pair above encapsulates the content of (12.25), and our interpretation of $\tilde{f}(p)$ as "coefficients" in the decomposition of $f(x)$ into $e^{i\,p\,x}$ comes from the fact that they naturally inherited the role of the c_m from the Fourier series, that is where they came from.

12.4 Orthonormality

For sine and cosine series, we have an inner product defined by conjugation and integration, and with respect to that inner product, these functions are orthogonal (and can be normalized). Thinking of the infinite square well solutions: $\psi_j(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{j\,\pi\,x}{a}\right)$, we know that:

$$\int_0^a \psi_j(x)^* \, \psi_k(x) \, dx = \delta_{jk}, \tag{12.27}$$

and similarly for the harmonic oscillator case:

$$\int_{-\infty}^{\infty} \psi_j(x)^* \, \psi_k(x) \, dx = \delta_{jk} \tag{12.28}$$

for the ψ_j solving $H\,\psi_j = E_j\,\psi_j$ with H the harmonic oscillator Hamiltonian operator (with $V(x) = \frac{1}{2}\,m\,\omega^2\,x^2$).

For free particle solutions $\psi_k(x) = \frac{1}{\sqrt{2\,\pi}}\,e^{i\,k\,x}$ (I am putting the factor of $\sqrt{2\,\pi}^{-1}$ on the spatial part of the wavefunction). From (11.12), we have:

$$\int_{-\infty}^{\infty} \psi_j(x)^* \, \psi_k(x) \, dx = \frac{1}{2\,\pi} \int_{-\infty}^{\infty} e^{i\,x\,(k-j)} \, dx = \delta(k-j), \tag{12.29}$$

so our orthonormality condition has gone from the discrete Kronecker delta: δ_{jk} for integers j and k, to the continuous Dirac delta $\delta(k-j)$ where $j, k \in \mathbb{R}$.

Homework

Reading: Griffiths, pp. 59–67.

Problem 12.1

Using the free particle states to construct general solutions to Schrödinger's equation.

a. Check that:

$$\Psi(x,t) = \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} \phi(k)\,\psi_k(x)\,e^{-i\,\frac{E(k)}{\hbar}\,t} \tag{12.30}$$

with $\psi_k(x) = e^{i\,k\,x}$ and $E(k) = \frac{\hbar^2\,k^2}{2\,m}$ satisfies Schrödinger's equation for $V(x) = 0$:

$$-\frac{\hbar^2}{2\,m}\,\frac{\partial^2 \Psi(x,t)}{\partial x^2} = i\,\hbar\,\frac{\partial \Psi(x,t)}{\partial t} \tag{12.31}$$

b. Verify that $\Psi(x,t)$ from (11.20) (in Lecture 11) does indeed solve Schrödinger's equation (i.e. compute $\frac{\partial^2 \Psi(x,t)}{\partial x^2}$ and $\frac{\partial \Psi(x,t)}{\partial t}$ explicitly – have to do it once in life).

Problem 12.2

The Gaussian wave-packet solution from (11.20) has $\langle x \rangle = 0$, so its "center" doesn't move. Suppose we wanted to develop a wavefunction $\Psi(x,t)$ that had, at time $t = 0$:

$$\bar{\psi}(x) = \left(\frac{2\,a}{\pi}\right)^{\frac{1}{4}} e^{-a\,x^2} \tag{12.32}$$

but gave a time-dependent $\langle x \rangle$ moving to the right (say). This could be achieved by finding a wavefunction that had $\langle p \rangle = p_0$, a constant.

a. Show that $\tilde{\psi}(x) = e^{i\,f(x)}\,\bar{\psi}(x)$ leads to the same initial probability density as $\bar{\psi}(x)$ in (12.32).

b. Find the simplest function $f(x)$ for use in $\tilde{\psi}(x)$ that gives a constant $\langle p \rangle$ initially. (here, "simplest" means the one for which no integration is necessary).

Problem 12.3

If x has units of meters, what units must $\delta(x)$ have?