Free Particle Comparison

Lecture 10

Physics 342
Quantum Mechanics I

Monday, February 18th, 2008

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:

$$\psi_k(x) = A\,e^{\pm i\,k\,x} \quad k^2 \equiv \frac{2\,m\,E}{\hbar^2} \tag{10.1}$$

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:

$$\psi_k(x) = \frac{1}{\sqrt{2\,\pi}}\,e^{i\,k\,x}. \tag{10.2}$$

When the stationary states are discrete, we have:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\,\psi_n(x)\,e^{-i\,\frac{E_n}{\hbar}\,t} \tag{10.3}$$

and use orthogonormality to set

$$c_m = \psi_m(x) \cdot \bar{\psi}(x) \equiv \int_{-\infty}^{\infty} \psi_m^*(x)\, \bar{\psi}(x)\, dx \tag{10.4}$$

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

When the stationary states are "indexed" by a continuous variable k, the sum in (10.3) becomes an integral (over k)

$$\Psi(x,t) = \int_{-\infty}^{\infty} \phi(k)\, \psi_k(x)\, e^{-i\frac{E_k}{\hbar}t}\, dk \quad E_k = \frac{\hbar^2\, k^2}{2\, m} \tag{10.5}$$

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 $\bar{\psi}(x)$:

$$\phi(k) = \psi_k(x) \cdot \bar{\psi}(x) = \int_{-\infty}^{\infty} \psi_k^*(x)\, \bar{\psi}(x)\, dx = \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} e^{-i\,k\,x}\, \bar{\psi}(x)\, dx, \tag{10.6}$$

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.

10.1 Gaussian Integrals

In studying Gaussian initial wavefunctions, which is relevant given experiment, we often encounter integrals of the form:

$$\int_{-\infty}^{\infty} e^{-\left(A\,x^2 + B\,x + C\right)}\, dx, \tag{10.7}$$

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

$$\int_{-\infty}^{\infty} e^{-y^2}\, dy = \sqrt{\pi}. \tag{10.8}$$

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

$$\left(\sqrt{A}\,x + F\right)^2 = A\,x^2 + 2\sqrt{A}\,F\,x + F^2, \tag{10.9}$$

and notice that if we were to set:

$$2\sqrt{A}\,F\,x = B\,x \longrightarrow F = \frac{B}{2\sqrt{A}}, \tag{10.10}$$

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

$$y^2 - F^2 = A\,x^2 + B\,x \longrightarrow y^2 - \frac{B^2}{4\,A} = A\,x^2 + B\,x, \tag{10.11}$$

so that our integral becomes:

$$\int_{-\infty}^{\infty} e^{-\left(A\,x^2 + B\,x + C\right)}\,dx = e^{-C}\int_{-\infty}^{\infty} e^{-\left(y^2 - \frac{B^2}{4\,A}\right)}\,\frac{dy}{\sqrt{A}}$$

$$= \frac{e^{-C + \frac{B^2}{4\,A}}}{\sqrt{A}}\int_{-\infty}^{\infty} e^{-y^2}\,dy \tag{10.12}$$

$$= \sqrt{\frac{\pi}{A}}\,e^{-C + \frac{B^2}{4\,A}}.$$

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.

Homework

Reading: Griffiths, pp. 59–66.

Problem 10.1

Verify that $\Psi(x,t)$ from (9.18) does indeed solve Schrödinger's equation.

Problem 10.2

The Gaussian wave-packet solution from (9.18) has $\langle x \rangle = 0$, so its "center" doesn't move. Suppose we wanted to develop a wavefunction $\Psi(x,t)$ that had:

$$\bar{\psi}(x) = \left(\frac{1}{2\,\pi\,a}\right)^{\frac{1}{4}} e^{-a\,x^2} \tag{10.13}$$

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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 $\psi(x) = e^{i\, f(x)}$ leads to the same initial density as $\bar{\psi}(x)$ in (10.13).

b.   Find the simplest function $f(x)$ that gives a constant $\langle p \rangle$.

c.   Using your modified initial wavefunction $\psi(x)$, find the complete solution for the wave equation.