Physics 428: Quantum Mechanics III
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Practice Problems 1

Problem 1

A particle in free space in one dimension is initially in a wave packet described by

$$\psi(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

a) What is the probability that its momentum is in the range $(p, p + dp)$? (Hint: remember the Fourier transform relation between position and momentum space).

The probability that the particle has momentum in this range is $|\phi(p)|^2 dp$, where $\phi(p)$ is the Fourier transform of $\psi(x)$,

$$\phi(p) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{\infty} dx\ \psi(x) e^{-ipx/\hbar} = (2\pi\hbar)^{-1/2} \int_{-\infty}^{\infty} dx\ \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2} e^{-ipx/\hbar}$$

To do the integral, complete the square in the exponent,

$$\frac{\alpha x^2}{2} + \frac{ipx}{\hbar} = \frac{\alpha}{2}\left(x + \frac{ip}{\alpha\hbar}\right)^2 + \frac{\alpha}{2}\frac{p^2}{\alpha^2\hbar^2}$$

Thus

$$\phi(p) = (2\pi\hbar)^{-1/2} \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{p2}{2\alpha\hbar^2}} \int_{-\infty}^{\infty} dx\ e^{-\frac{\alpha}{2}(x+ip/\alpha\hbar)^2}$$

The substitution $u = \sqrt{\alpha/2}(x + ip/\alpha\hbar), du = dx\sqrt{\alpha/2}$ yields a simple integral over a Guassian, and we obtain

$$\phi(p) = \frac{1}{\sqrt{\hbar\sqrt{\alpha\pi}}} e^{-p^2/2\alpha\hbar^2}$$

so the probability is

$$|\phi(p)|^2 dp = \frac{1}{\hbar\sqrt{\alpha\pi}} e^{-p^2/\alpha\hbar^2} dp$$

b) What is the expectation value of the energy? Can you give a rough argument, based on the "size" of the wave function and the uncertainty principle, for why the answer should be roughly what it is?

$$\langle E \rangle \ = \ \langle \psi | H | \psi \rangle = \int_{-\infty}^{\infty} dx\ \psi^* H \psi \qquad (1)$$

$$= \int_{-\infty}^{\infty} dx \ \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2} \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right] \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2} \quad (2)$$

$$= \frac{\alpha\hbar^2}{2m}\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} du \ (1-u^2)e^{-u^2} \quad (3)$$

$$= \frac{\hbar^2\alpha}{4m} \quad (4)$$

where we make the substitution $u = \sqrt{\alpha}x$ in the third line (look up these integrals if you don't understand the result!).

The uncertainty principle is $\Delta p \Delta x \geq \hbar/2$. The width of the wave packet is $\Delta x \sim 1/\sqrt{\alpha}$, $\langle p \rangle = 0$ and since $\Delta p \equiv \langle p^2 \rangle - \langle p \rangle^2$, the energy must be of order

$$\langle E \rangle \sim \frac{\langle p^2 \rangle}{2m} \sim \frac{(\Delta p)^2}{2m} \sim \frac{1}{2m}\left(\frac{\hbar}{2}\right)^2 \alpha = \frac{\hbar^2\alpha}{8m}$$

which is within a factor of 2 of the exact result.

Problem 2

Consider a free particle of mass m in one dimension with periodic boundary conditions:

$$\psi(x+L) = \psi(x)$$

a) Write down the complete set of normalized energy eigenfunctions and eigenvalues.

The solution to the Schrödinger equation for a free particle defined on a interval of length L is simply

$$\psi_k(x) = \frac{1}{\sqrt{L}}e^{ikx}$$

But the condition $\psi(x+L) = \psi(x)$ constrains the allowed values of k, because we require $e^{ikx} = e^{ik(x+L)} = e^{ikx}e^{ikL}$ or $e^{ikL} = 1$, which implies $kL = 2n\pi$ with $n = 0, \pm 1, \pm 2, ...$ Thus the allowed solutions are

$$\psi_n(x) = \frac{1}{\sqrt{L}}e^{ik_n x}$$

with

$$k_n = \frac{2\pi}{L}n, n = 0, \pm 1, \pm 2...$$

where the classical ground state $n = 0$ is not allowed.

These solutions are clearly eigenfunctions of both H and p,

$$\hat{H}\psi_n(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left[\frac{1}{\sqrt{L}}e^{ik_n x}\right] = \frac{\hbar^2 k_n^2}{2m}\psi_n(x)$$

Thus, the eigenvalue for the nth eigenstate is

$$\frac{\hbar^2 k_n^2}{2m} = \frac{2\pi^2\hbar^2}{mL^2} n^2$$

Similarly,

$$\hat{p}\psi_n(x) = -i\hbar \frac{\partial}{\partial x}\left[\frac{1}{\sqrt{L}} e^{ik_n x}\right] = \hbar k_n \psi_n(x)$$

Thus, these are also eigenfunctions of momentum, with eigenvalues

$$\hbar k_n = \frac{2\pi\hbar}{L} n$$

b) Show that any two of these eigenfunctions corresponding to different eigenvalues are orthonormal; that is

$$\int_0^L dx\ \psi_m^*(x)\psi_n(x) = \delta_{nm}$$

Plugging in the solution above,

$$\int_0^L dx\ \psi_m^*(x)\psi_n(x) = \frac{1}{L}\int_0^L dx\ e^{i(k_n - k_m)}$$

If $m = n$, the integral is trivially equal to 1. For $m \neq n$,

$$\int_0^L dx\ e^{i(k_n + k + m)} = \frac{1}{i(k_n - k_m)}\left[e^{i\frac{2\pi}{L}(n-m)x}\right]_0^L = 0$$

Therefore,

$$\int_0^L dx\ \psi_m^*(x)\psi_n(x) = \delta_{nm}$$

Problem 3

A particle of mass m moves in the potential

$$V(x) = \begin{cases} \frac{1}{2}kx^2 & x > 0 \\ \infty & x \leq 0 \end{cases}$$

What are the energy levels and eigenfunctions for the this system? (Hint: compare this problem to that of the simple harmonic oscillator.)

This potential is a semi-infinite harmonic oscillator. For $x > 0$, the potential is identical to that of the S.H.O. The infinite potential at $x = 0$ requires the eigenfunctions to be zero at $x = 0$. This is what all the anti-symmetric (odd) eigenfunctions of the S.H.O.

do. Thus, the eigenfunctions of this problem are proportional to the anti-symmetric eigenfunctions of the S.H.O., with different normalization,

$$1 = \int_0^\infty dx\ \psi^*(x)\psi(x)$$

instead of

$$1 = \int_\infty^\infty dx\ \psi^*(x)\psi(x) = 2\int_0^\infty dx\ \psi^*(x)\psi(x)$$

The eigenfunctions are therefore

$$\psi_n(x) = \begin{pmatrix} \sqrt{2}u_n(x) & n = 1,3,5,... & x > 0 \\ 0 & & x \leq 0 \end{pmatrix}$$

where the $u_n(x)$ are the S.H.O. eigenfunctions. In terms of the variable $y = x\sqrt{m\omega/\hbar}$, the eigenfunctions are

$$\psi_n(y) = \frac{1}{\sqrt{2^{n-1}n!\sqrt{\pi}}}e^{-y^2}H_n(y)$$

where the $H_n(y)$ are Hermite polynomials. The energy levels are

$$E_n = (n + 1/2)\hbar\omega, n = 1,3,5,...$$

Problem 4

In three-dimensional space, rotation of a vector about the $z-$axis is performed by the matrix

$$R(\phi) = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

What are the eigenvalues of this matrix? What is their magnitude?

The eigenvalue equation is

$$\begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \lambda\begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

which is solved by computing the determinant

$$\begin{vmatrix} \cos\phi - \lambda & \sin\phi & 0 \\ -\sin\phi & \cos\phi - \lambda & 0 \\ 0 & 0 & 1 - \lambda \end{vmatrix} = 0$$

and finding the roots $\lambda_1 = 1$, $\lambda_{2,3} = e^{\pm i\phi}$. The magnitude of all the eigenvalues is $|\lambda| = 1$.

Problem 5

Consider the matrix

$$Q = \begin{pmatrix} 1 & i & 1 \\ -i & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

a) Is Q Hermitian?

Yes. Complex conjugate all the matrix elements and reverse the indices and you get the same matrix ($Q^\dagger = Q$).

b) What are the eigenvalues of Q?

As in problem 4, the eigenvalues are found by computing the determinant

$$\begin{vmatrix} 1-\lambda & i & 1 \\ -i & -\lambda & 0 \\ 1 & 0 & \lambda \end{vmatrix} = 0$$

and finding the roots of the resulting polynomial. The eigenvalues are $\lambda = 0, -1, 2$.

Problem 6

Consider the angular momentum matrices in the basis of spherical harmonic eigenfunctions. That is, the matrix elements of L^2 are given by

$$\langle Y_{l'm'}|L^2|Y_{lm}\rangle$$

and the matrix elements of L_z are given by

$$\langle Y_{l'm'}|L_z|Y_{lm}\rangle$$

Notice that the full matrix can be decomposed into *submatrices* (corresponding to angular momentum of dimension $2l+1$): a 1×1 submatrix for $l = 0$, a 3×3 submatrix for $l = 1$, etc.

Write out the matrices for L^2 and L_z up to and including $l = 2$ in this representation. Indicate the submatrices by dashed lines.

Recall $L^2 Y_{lm} = l(l+1)\hbar^2 Y_{lm}$ and the orthonormality of the spherical harmonics, which yields

$$\langle Y_{l'm'}|L^2|Y_{lm}\rangle = l(l+1)\hbar^2 \delta_{ll'}\delta_{mm'}$$

Similarly, $L_z Y_{lm} = m\hbar Y_{lm}$ yields

$$\langle Y_{l'm'}|L_z|Y_{lm}\rangle = m\hbar^2 \delta_{ll'}\delta_{mm'}$$

Therefore, the L^2 matrix is

$$L^2 = \begin{pmatrix} 0 &&&&&&&&& \\ & 2\hbar^2 &&&&&&&& \\ && 2\hbar^2 &&&&&&& \\ &&& 2\hbar^2 &&&&&& \\ &&&& 6\hbar^2 &&&&& \\ &&&&& 6\hbar^2 &&&& \\ &&&&&& 6\hbar^2 &&& \\ &&&&&&& 6\hbar^2 && \\ &&&&&&&& 6\hbar^2 & \\ &&&&&&&&& ... \end{pmatrix}$$

and the L_z matrix is

$$L_z = \begin{pmatrix} 0 &&&&&&&&& \\ & \hbar &&&&&&&& \\ && 0 &&&&&&& \\ &&& -\hbar &&&&&& \\ &&&& 2\hbar &&&&& \\ &&&&& \hbar &&&& \\ &&&&&& 0 &&& \\ &&&&&&& \hbar && \\ &&&&&&&& 2\hbar & \\ &&&&&&&&& ... \end{pmatrix}$$