Physics 130B Midterm Solutions Fall 2011

Version 5: Small clarifications.

1. A spin-1/2 particle has a definite value of spin "up" along an axis tilted 20 deg from the +z axis, toward the +x axis.

(a 5pt) What is the probability of measuring the spin up along the z-axis?

$$|\chi\rangle = \begin{pmatrix} \cos\left(20^o/2\right) \\ \sin\left(20^o/2\right)e^{i0} \end{pmatrix} = \begin{pmatrix} \cos 10^o \\ \sin 10^o \end{pmatrix}$$

$$\Pr\left(measuring\ |z+\rangle\right) = \left|\langle z+|\chi\rangle\right|^2 = \left|[1\ \ 0]\begin{pmatrix} \cos 10^o \\ \sin 10^o \end{pmatrix}\right|^2 = \cos^2 10^o$$

(b 5) What is the probability of measuring the spin down along the z-axis?

$$\Pr\left(measuring\ |z-\rangle\right) = 1 - \Pr\left(|z+\rangle\right) = 1 - \cos^2 10^o \qquad or$$

$$\Pr\left(measuring\ |z-\rangle\right) = \left|\langle z-|\chi\rangle\right|^2 = \left|[0\ \ 1]\begin{pmatrix} \cos 10^o \\ \sin 10^o \end{pmatrix}\right|^2 = \sin^2 10^o$$

Note that Pr(|z+>) + Pr(|z–>) = 1

(c 5) What is the average (over many particles) z-component of spin?

$$\langle s_z\rangle = \frac{\hbar}{2}\Pr\left(|z+\rangle\right) - \frac{\hbar}{2}\Pr\left(|z-\rangle\right) = \frac{\hbar}{2}\left(\cos^2 10^o - \sin^2 10^o\right) = \frac{\hbar}{2}\cos 20^o$$

$$or \qquad \langle s_z\rangle = \langle\chi|\hat{s}_z|\chi\rangle = \left[\cos^* 10^o, \sin^* 10^o\right]\begin{pmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{pmatrix}\begin{pmatrix} \cos 10^o \\ \sin 10^o \end{pmatrix}$$

$$= \frac{\hbar}{2}\left[\cos 10^o, \sin 10^o\right]\begin{pmatrix} \cos 10^o \\ -\sin 10^o \end{pmatrix} = \frac{\hbar}{2}\left(\cos^2 10^o - \sin^2 10^o\right) = \frac{\hbar}{2}\cos 20^o$$

(d 5) What is the classical z-component of spin for the given particle?

$s_{z(classical)} = \frac{\hbar}{2}\cos 20^o$, which must equal the quantum average, since the classical result is the average of billions of quantized results.

(e 5) If the particle is tilted 20 deg toward +y (instead of +x), what is the probability of measuring spin up along the z-axis?

By axial symmetry about the z-axis, this is the same as part (a)

2. In computational quantum chemistry, the local energy of a trial wave-function is computed numerically, to provide adjustments to the wave-function, which is then the starting point for a new iteration. Given a trial wave-function:

$$\psi(x) = N\frac{1}{x^2+1}, \qquad N \equiv \text{normalization constant}$$

(a 10) The potential is everywhere 0. Find the local energy, $E(x)$.

$$E(x) \equiv \frac{\hat{E}\psi(x)}{\psi(x)} = \frac{1}{2m}\frac{\hat{p}^2\psi(x)}{\psi(x)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)},$$ N cancels, so we drop it:

$$\psi' = -\left(x^2+1\right)^{-2}\cdot 2x = -2x\left(x^2+1\right)^{-2}$$

$$\psi'' = -2\left[x(-2)\left(x^2+1\right)^{-3}\cdot 2x + \left(x^2+1\right)^{-2}\right]$$

$$\psi''/\psi = -2\left[-4x^2\left(x^2+1\right)^{-2} + \left(x^2+1\right)^{-1}\right]$$

$$E(x) = -\frac{\hbar^2}{2m}\cdot -2\left[-4x^2\left(x^2+1\right)^{-2} + \left(x^2+1\right)^{-1}\right] = \frac{\hbar^2}{m}\cdot\left[\frac{-3x^2+1}{\left(x^2+1\right)^2}\right]$$

(b 5) Is the total energy for this particle finite, or infinite? Justify your answer.

$$E = \int_{-\infty}^{\infty} E(x)\left|\psi(x)\right|^2\,dx$$

Since both terms in $E(x)$ drop off faster than $1/x^2$, and integral $1/x^2$ is finite, and $|\psi|^2$ is bounded, the total energy is finite.

(c 10) What is the average momentum of this state?

By symmetry of $\psi(x)$ about $x = 0$, $\langle p \rangle = 0$.

Or, $$\langle p\rangle = \langle\psi|\hat{p}|\psi\rangle = \int_{-\infty}^{\infty}\psi^*\frac{\hbar}{i}\frac{\partial}{\partial x}\psi\,dx = \frac{\hbar}{i}\int_{-\infty}^{\infty}\psi^*\frac{\partial}{\partial x}\psi\,dx, \textit{ but this must be real.}$$

$$\textit{Since } \psi \textit{ is real, the only way to get rid of the 'i' is if the integral} = 0$$

Note this is true for any real function $\psi(x)$.

Or, For any real $\psi(x)$, we can evaluate the integral by parts:

$$\int_{-\infty}^{\infty}\psi\psi'\,dx = \cancel{\left[\psi\psi\right]_{-\infty}^{\infty}} - \int_{-\infty}^{\infty}\psi'\psi\,dx \qquad \text{Using } \int UV'\,dx = [UV] - \int U'V\,dx$$

$$\Rightarrow \qquad \int_{-\infty}^{\infty}\psi\psi'\,dx = 0$$

Or, $$\langle p\rangle = \langle\psi|\hat{p}|\psi\rangle = \int_{-\infty}^{\infty}\psi^*\frac{\hbar}{i}\frac{\partial}{\partial x}\psi\,dx = \frac{\hbar}{i}\int_{-\infty}^{\infty}\left(x^2+1\right)^{-1}\cdot(-1)\left(x^2+1\right)^{-2}(2x)\,dx,$$

but the integrand is odd, and we integrate over a symmetric interval, so the left and right halves (about 0) cancel. Thus, $\langle p \rangle = 0$.

3. Consider a simple harmonic oscillator, in standard notation.

(a 5) What is $\langle x \rangle$ in the state $|0\rangle$?

By symmetry of $|\psi(x)|^2$ about $x = 0$, $\langle x \rangle = 0$.

(b 5) What is $\langle x \rangle$ in the state $|1\rangle$?

Ditto. Note that $\psi(x)$ is anti-symmetric about $x = 0$.

(c 5) What is $\langle x \rangle$ in the state $\frac{1}{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle$?

$$\langle x\rangle = \langle\psi|x|\psi\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle\psi|\left(a^\dagger + a\right)|\psi\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{1}{2}\frac{\sqrt{3}}{2}\langle 0|a|1\rangle + \frac{\sqrt{3}}{2}\frac{1}{2}\langle 1|a^\dagger|0\rangle\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{1}{2}\frac{\sqrt{3}}{2} + \frac{\sqrt{3}}{2}\frac{1}{2}\right) = \sqrt{\frac{\hbar}{2m\omega}}\cdot\frac{\sqrt{3}}{2}$$

(d 5) What is <x> in the state $\frac{1}{2}|2\rangle + \frac{\sqrt{3}}{2}|1\rangle$?

$$\langle x\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{\sqrt{3}}{2}\frac{1}{2}\langle 1|a|2\rangle + \frac{1}{2}\frac{\sqrt{3}}{2}\langle 2|a^\dagger|1\rangle\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(\frac{\sqrt{3}}{2}\frac{1}{2}\sqrt{2} + \frac{1}{2}\frac{\sqrt{3}}{2}\sqrt{2}\right) = \sqrt{\frac{\hbar}{2m\omega}}\cdot\frac{\sqrt{6}}{2}$$

(e 5) What is <x^2> in the state of (d)?

$$\left\langle x^2\right\rangle = \frac{\hbar}{2m\omega}\langle\psi|\left(a^\dagger + a\right)^2|\psi\rangle = \frac{\hbar}{2m\omega}\langle\psi|\left(a^\dagger a^\dagger + a^\dagger a + aa^\dagger + aa\right)|\psi\rangle$$

$$= \frac{\hbar}{2m\omega}\left(\frac{\sqrt{3}}{2}\frac{\sqrt{3}}{2}\langle 1|\left(a^\dagger a + aa^\dagger\right)|1\rangle + \frac{1}{2}\frac{1}{2}\langle 2|\left(a^\dagger a + aa^\dagger\right)|2\rangle\right)$$

$$= \frac{\hbar}{2m\omega}\left(\frac{3}{4}(1+2) + \frac{1}{4}(2+3)\right) = \frac{\hbar}{2m\omega}\frac{14}{4} = \frac{\hbar}{2m\omega}\frac{7}{2} = \frac{7\hbar}{4m\omega}$$

4. For $l = 1$, we have

$$\hat{L}_x = \hbar\begin{pmatrix} 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 0 \end{pmatrix}, \qquad \hat{L}_y = \hbar\begin{pmatrix} 0 & -i/\sqrt{2} & 0 \\ i/\sqrt{2} & 0 & -i/\sqrt{2} \\ 0 & i/\sqrt{2} & 0 \end{pmatrix}$$

(a 10) What is the operator for angular momentum along an axis 30 deg CCW from the +x axis?

L-hat$_\phi$ can be written as a superposition of L-hat$_x$ and L-hat$_y$, each of which projects a component onto L-hat$_\phi$:

$$\hat{L}_\phi = \cos 30^o\,\hat{L}_x + \sin 30^o\,\hat{L}_y = \cos\frac{\pi}{6}\hat{L}_x + \sin\frac{\pi}{6}\hat{L}_y$$

$$= \hbar\cos\frac{\pi}{6}\begin{pmatrix} 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 0 \end{pmatrix} + \hbar\sin\frac{\pi}{6}\begin{pmatrix} 0 & -i/\sqrt{2} & 0 \\ i/\sqrt{2} & 0 & -i/\sqrt{2} \\ 0 & i/\sqrt{2} & 0 \end{pmatrix}$$

$$= \hbar\begin{pmatrix} 0 & e^{-i\pi/6}/\sqrt{2} & 0 \\ e^{+i\pi/6}/\sqrt{2} & 0 & e^{-i\pi/6}/\sqrt{2} \\ 0 & e^{+i\pi/6}/\sqrt{2} & 0 \end{pmatrix}$$

(b 10) What are its eigenvalues?

From the isotropy of space, the eigenvalues of any $l = 1$ component measurement are $\hbar$, 0, $-\hbar$

(c 5) What is the eigenstate for measuring $+\hbar$ along this tilted axis?

Dropping the $\hbar$, so the eigenvalues reduce to +1, 0, –1, we use the eigenvector equation:

$$\hat{\mathcal{O}}|\chi\rangle = \lambda|\chi\rangle, \qquad \textit{where} \quad \lambda \text{ is the known eigenvalue. In this case:} \qquad \hat{L}_\phi \begin{pmatrix}1\\ b\\ c\end{pmatrix} = 1\begin{pmatrix}1\\ b\\ c\end{pmatrix}$$

where we have assumed we can set $a = 1$. This is justified by getting a result below. Solving:

$$\begin{pmatrix} 0 & e^{-i\pi/6}/\sqrt{2} & 0 \\ e^{+i\pi/6}/\sqrt{2} & 0 & e^{-i\pi/6}/\sqrt{2} \\ 0 & e^{+i\pi/6}/\sqrt{2} & 0 \end{pmatrix}\begin{pmatrix}1\\ b\\ c\end{pmatrix} = \begin{pmatrix}1\\ b\\ c\end{pmatrix}$$

$$\textit{From the top row}: \qquad be^{-i\pi/6}/\sqrt{2} = 1 \quad \Rightarrow \qquad b = \sqrt{2}e^{+i\pi/6}$$

$$\textit{From the 2nd row}: \qquad e^{+i\pi/6}/\sqrt{2} + ce^{-i\pi/6}/\sqrt{2} = b = \sqrt{2}e^{+i\pi/6}$$

$$e^{+i\pi/6} + ce^{-i\pi/6} = 2e^{+i\pi/6}, \; ce^{-i\pi/6} = e^{+i\pi/6}, \;\; c = e^{+i\pi/3}$$

$$\textit{eigenvector} = \begin{pmatrix}1\\ \sqrt{2}e^{+i\pi/6}\\ e^{+i\pi/3}\end{pmatrix}, \textit{Normalize}: \textit{mag}^2 = 1+2+1 = 4, \textit{ multiply by } \frac{1}{\sqrt{4}}$$

$$\textit{eigenstate} = \begin{pmatrix}1/2\\ \left(1/\sqrt{2}\right)e^{+i\pi/6}\\ \left(1/2\right)e^{+i\pi/3}\end{pmatrix}$$