Assignment #3 solutions

Physics 322

1. In order to show that $M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$ can be written as a linear combination of the matrices $\{I, \sigma_x, \sigma_y, \sigma_z\}$, we note that the diagonal terms m_{11}, m_{22} can only be written as the sum of the identity I and σ_z. We can write

$$\begin{pmatrix} m_{11} & 0 \\ 0 & 0 \end{pmatrix} = \frac{m_{11}}{2}\left\{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\} = \frac{m_{11}}{2}(I + \sigma_z)$$

and

$$\begin{pmatrix} m_{22} & 0 \\ 0 & 0 \end{pmatrix} = \frac{m_{22}}{2}\left\{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\} = \frac{m_{22}}{2}(I - \sigma_z)$$

Similarly, the off-diagonal terms must be combinations of σ_x and σ_y:

$$\begin{pmatrix} 0 & m_{12} \\ 0 & 0 \end{pmatrix} = \frac{m_{12}}{2}\left\{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\right\} = \frac{m_{12}}{2}(\sigma_x + i\sigma_y)$$

and

$$\begin{pmatrix} 0 & 0 \\ m_{21} & 0 \end{pmatrix} = \frac{m_{21}}{2}\left\{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\right\} = \frac{m_{21}}{2}(\sigma_x - i\sigma_y)$$

So, the matrix M is just the sum of these four expressions:

$$M = \frac{m_{11}}{2}(I + \sigma_z) + \frac{m_{22}}{2}(I - \sigma_z) + \frac{m_{12}}{2}(\sigma_x + i\sigma_y) + \frac{m_{21}}{2}(\sigma_x - i\sigma_y)$$

which we can rearrange in terms of each matrix to read:

$$\boxed{M = \left(\frac{m_{11}+m_{22}}{2}\right) I + \left(\frac{m_{12}+m_{21}}{2}\right)\sigma_x + i\left(\frac{m_{12}-m_{21}}{2}\right)\sigma_y + \left(\frac{m_{11}-m_{22}}{2}\right)\sigma_z}$$

and thus we confirm that $\{I, \sigma_x, \sigma_y, \sigma_z\}$ form a basis for the space of 2×2 matrices.

2. (a) The hydrogen wavefunctions are $\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)Y_{lm}(\theta, \phi)$, where $R_{nl}(r) = \langle r|nl\rangle$ are the radial wavefunctions. The expected energies can be calculated as

$$\langle H\rangle = \langle nlm|H|nlm\rangle \int_0^{\pi}\int_{-\pi/2}^{\pi/2}\int_0^{\infty} \langle nlm|r, \theta, \phi\rangle\langle r, \theta, \phi|H|nlm\rangle \; r^2 \sin\theta \; dr \; d\theta \; d\phi$$

This integral is just

$$\langle H\rangle = \int_0^{\pi}\int_{-\pi/2}^{\pi/2}\int_0^{\infty} \psi^*_{nlm}(r, \theta, \phi)\left[-\frac{\hbar^2}{2\mu r}\frac{d^2}{dr^2}r + \frac{l(l+1)}{2\mu r^2} - \frac{e^2}{r}\right]\psi_{nlm}(r, \theta, \phi)\, r^2 \sin\theta \; dr \; d\theta \; d\phi$$

By separation of variables, we can independently evaluate the angular integral, which by orthogonality is

$$\int_0^{\pi} \int_{-\pi/2}^{\pi/2} Y^*_{lm}(\theta,\phi) Y_{lm}(\theta,\phi) \ \sin\theta \ d\theta \ d\phi = 1$$

So, the only integral left to evaluate is the radial one:

$$\langle H \rangle = \int_0^{\infty} R_{nl}(r) \left[-\frac{\hbar^2}{2\mu r} \frac{d^2}{dr^2} r + \frac{l(l+1)}{2\mu r^2} - \frac{e^2}{r} \right] R_{nl}(r) \ r^2 \ dr$$

We are interested in the states $(n,l) = (1,0),(2,0),(3,0)$, which are the 1s, 2s, and 3s states. In this case, $l = 0$, so the middle term in the above integral is omitted.

See Maple worksheet for the rest!

(b) When we consider the 2p and 3p states, the Hamiltonian now must include the middle angular momentum term. This will shift the energy levels (see Maple).

3. (a) A spin state in a magnetic field $\mathbf{B} = B_0 cos(\omega t) \ \hat{\mathbf{z}}$ has as its Hamiltonian

$$\boxed{H = g\mathbf{S}\cdot\mathbf{B} = \tfrac{\hbar g B_0 \cos\omega t}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

(b) We can write the time-dependent state vector as $|\psi(t)\rangle = a(t)|+\rangle + b(t)|-\rangle = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$, with the initial condition $a(0) = \frac{1}{\sqrt{2}}, b(0) = frac1\sqrt{2}$, since we are told that the initial spin state is $|+\rangle_x$. We can solve for the coefficients for $t > 0$ using the time-dependent Schrödinger equation,

$$\begin{aligned} i\hbar \frac{d}{dt}|\psi(t) &= H|\psi(t)\rangle \\ i\hbar \frac{d}{dt} \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} &= \frac{\hbar g B_0 \cos\omega t}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} \\ \begin{pmatrix} \dot{a}(t) \\ \dot{b}(t) \end{pmatrix} &= \frac{g B_0 \cos\omega t}{2i} \begin{pmatrix} a(t) & 0 \\ 0 & -1 \end{pmatrix} \end{aligned} \quad (1)$$

These have solution (using Maple):

$$\boxed{a(t) = \tfrac{1}{\sqrt{2}} \exp\left(-\tfrac{igB_0 \sin(\omega t)}{2\omega}\right) \quad , \quad b(t) = \tfrac{1}{\sqrt{2}} \exp\left(+\tfrac{igB_0 \sin(\omega t)}{2\omega}\right)}$$

(c) In order to measure a spin value of $-\hbar/2$, we evaluate the probability $|_x\langle -|\psi(t)\rangle|^2$, where the amplitude is

$$_x\langle -|\psi(t)\rangle = \frac{1}{\sqrt{2}} [\ \langle +| - \langle -|\ ] \left[a(t)|+\rangle + b(t)|-\rangle \right]$$

$$= \frac{1}{\sqrt{2}} (a(t) - b(t))$$

The probability is thus

$$\begin{aligned} |_x\langle -|\psi(t)\rangle|^2 &= \frac{1}{2}|a(t) - b(t)|^2 \\ &= \frac{1}{2}(a^*(t) - b^*(t))(a(t) - b(t)) \\ &= \frac{1}{2}\left[1 - \cos\left(\frac{gB_0 \sin(\omega t)}{\omega}\right)\right] \end{aligned}$$

which by a trigonometric identity is simply $\boxed{\sin^2\left(\frac{gB_0 \sin(\omega t)}{2\omega}\right)}$.

(d) To completely flip its state (*i.e.* yield $-\hbar/2$ with 100% probability), we require the above probability to be 1. Thus, the argument of the sine function must be $\pi/2$, which means we can solve for B_0 accordingly: $\frac{\pi}{2} = \frac{gB_0 \sin(\omega t)}{2\omega}$ $\boxed{\implies \quad B_0 = \frac{\pi\omega}{g \sin(\omega t)}}$

4. For the particle in the state

$$|+\rangle_u = \cos\frac{\theta}{2} e^{-i\frac{\phi}{2}}|+\rangle + cos\frac{\theta}{2} e^{-i\frac{\phi}{2}}|-\rangle$$

we can evaluate each expectation value by noting the action of S_x, S_y, and S_z on the eigenstates $|+\rangle$ and $|-\rangle$. This is best done by writing the states as vectors:

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad ; \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

In this case, the action of S_x on the vectors can be determined:

$$S_x|+\rangle = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar}{2}|-\rangle$$

$$S_x|-\rangle = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}|+\rangle$$

Hey! That makes things much easier! We can similarly show that

$$S_y|+\rangle = \frac{-i\hbar}{2}|-\rangle = \frac{\hbar}{2i}|-\rangle \quad ; \quad S_y = -\frac{\hbar}{2i}|+\rangle$$

Since $|\pm\rangle$ are eigenvectors of S_z, we already know what happens in that case. So, evaluating the expectation values becomes much simpler now!

We find:

$$\begin{aligned}
\langle S_x\rangle &= {}_u\langle +|S_x|+\rangle_u \\
&= \left(\cos\frac{\theta}{2}\ e^{+i\phi/2}\langle +| + \sin\frac{\theta}{2}\ e^{-i\phi/2}\langle -|\right) S_x \left(\cos\frac{\theta}{2}\ e^{-i\phi/2}|+\rangle + sin\frac{\theta}{2}\ e^{+i\phi/2}|-\rangle\right) \\
&= \frac{\hbar}{2}\left(\cos\frac{\theta}{2}\ e^{+i\phi/2}\langle +| + \sin\frac{\theta}{2}\ e^{-i\phi/2}\langle -|\right)\left(\cos\frac{\theta}{2}\ e^{-i\phi/2}|-\rangle + sin\frac{\theta}{2}\ e^{+i\phi/2}|+\rangle\right)
\end{aligned}$$

Now, we simply keep all the $\langle +|+\rangle$ and $\langle -|-\rangle$ terms, since the others vanish by orthogonality:

$$\begin{aligned}
&= \frac{\hbar}{2}\left(\sin\frac{\theta}{2}\cos\frac{\theta}{2}\ e^{+i\phi} + \sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-i\phi}\right) \\
&= \frac{\hbar}{2}\frac{\sin\theta}{2}(e^{i\phi} + e^{-i\phi}) \\
\langle S_x\rangle &= \frac{\hbar}{2}\sin\theta\cos\phi
\end{aligned}$$

since we can use the identities $\sin\theta = 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}$, and $\cos\phi = \frac{e^{i\phi}+e^{-i\phi}}{2}$.

Similarly, we have

$$\begin{aligned}
\langle S_y\rangle &= {}_u\langle +|S_y|+\rangle_u \\
&= \left(\cos\frac{\theta}{2}\ e^{+i\phi/2}\langle +| + \sin\frac{\theta}{2}\ e^{-i\phi/2}\langle -|\right) S_y \left(\cos\frac{\theta}{2}\ e^{-i\phi/2}|+\rangle + sin\frac{\theta}{2}\ e^{+i\phi/2}|-\rangle\right) \\
&= \frac{\hbar}{2i}\left(\cos\frac{\theta}{2}\ e^{+i\phi/2}\langle +| + \sin\frac{\theta}{2}\ e^{-i\phi/2}\langle -|\right)\left(\cos\frac{\theta}{2}\ e^{-i\phi/2}|-\rangle - \sin\frac{\theta}{2}\ e^{+i\phi/2}|+\rangle\right) \\
&= \frac{\hbar}{2i}\left(\sin\frac{\theta}{2}\cos\frac{\theta}{2}\ e^{+i\phi} - \sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-i\phi}\right) \\
&= \frac{\hbar}{2i}\frac{\sin\theta}{2}(e^{i\phi} - e^{-i\phi}) \\
\langle S_y\rangle &= \frac{\hbar}{2}\sin\theta\sin\phi
\end{aligned}$$

where in this case we use the identify $\sin\phi = \frac{e^{i\phi}-e^{-i\phi}}{2i}$.

Finally, the easiest one to show is $\langle S_z\rangle$, since we know that $S_z|\pm\rangle = \pm\frac{\hbar}{2}|\pm\rangle$ (because they are eigenvectors of S_z!):

$$\begin{aligned}
\langle S_z\rangle &= {}_u\langle +|S_z|+\rangle_u \\
&= \left(\cos\frac{\theta}{2}\ e^{+i\phi/2}\langle +| + \sin\frac{\theta}{2}\ e^{-i\phi/2}\langle -|\right) S_z \left(\cos\frac{\theta}{2}\ e^{-i\phi/2}|+\rangle + sin\frac{\theta}{2}\ e^{+i\phi/2}|-\rangle\right) \\
&= \frac{\hbar}{2}\left(\cos\frac{\theta}{2}\ e^{+i\phi/2}\langle +| + \sin\frac{\theta}{2}\ e^{-i\phi/2}\langle -|\right)\left(\cos\frac{\theta}{2}\ e^{-i\phi/2}|+\rangle - \sin\frac{\theta}{2}\ e^{+i\phi/2}|-\rangle\right)
\end{aligned}$$

$$
\begin{aligned}
&= \frac{\hbar}{2}\left(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}\right) \\
\langle S_y \rangle &= \frac{\hbar}{2}\cos\theta
\end{aligned}
$$

where we have used yet another identity.

And so, voilá! The expectation values are simply the components of the classical angular momentum vector.