F2018

Problem 5: Time Evolution (10 Points)

Consider the Hamiltonian and a second observable, B, for a system that can be represented in a 3-dimensional Hilbert space using the orthonormal basis: $|e_1\rangle$, $|e_2\rangle$ and $|e_3\rangle$

with

$$|e_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |e_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |e_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

as:

$$H = \hbar\omega \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, B = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

The system at time t=0 is in the state:

$$|\Psi(0)\rangle = |e_2\rangle$$

a) Calculate the eigenvalues and normalized eigenvectors of H and B. **(2 Point)**

b) Determine $|\Psi(t)\rangle$, the wavefunction at a later time. **(1 Point)** want () in E basis

c) Determine $P_{|\Psi(t)\rangle}(b = 2)$, the probability of obtaining $b = 2$ if b is measured at an arbitrary time. **(1 Points)**

d) Is your probability in part c) time-dependent or time-independent? Discuss in detail. **(1 Point)**

e) Derive an expression for $\frac{\partial}{\partial t}\langle B\rangle$ where $\langle B\rangle = \langle\Psi(t)|B|\Psi(t)\rangle$ by explicit differentiation using the Time-Dependent Schrodinger Equation. **(2 Points)** Derive Ehrenfest theorem

f) Use your expression in part b) to find $\frac{\partial}{\partial t}\langle B\rangle$ for this system using the $|\Psi(t)\rangle$ you found in part a). **(2 Points)**

? g) Without doing further calculations describe what result you would expect for $\frac{\partial}{\partial t}\langle B\rangle$ if the initial wavefunction $|\Psi(0)\rangle = |e_2\rangle$ changes to:

$$|\Psi(0)\rangle = |e_1\rangle$$

Explain your answer in detail. **(1 Point)**

(a)

$$H = \hbar\omega \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\begin{vmatrix} 2\hbar\omega - \lambda & 0 & 0 \\ 0 & -\lambda & \hbar\omega \\ 0 & \hbar\omega & -\lambda \end{vmatrix} = 0$$

$$(2\hbar\omega - \lambda)(-\lambda)(-\lambda) - (\hbar\omega)(\hbar\omega)(2\hbar\omega - \lambda) = 0$$

$$(2\hbar\omega - \lambda)\lambda^2 - \hbar^2\omega^2(2\hbar\omega - \lambda) = 0$$

$$(2\hbar\omega - \lambda)(\lambda^2 - \hbar^2\omega^2) = 0$$

So letting $\lambda \to E$, our H eigenvalues are

$$\boxed{E_1 = 2\hbar\omega, \; E_2 = +\hbar\omega, \; E_3 = -\hbar\omega}$$

$|E_1 = 2\hbar\omega\rangle$

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & -2\hbar\omega & \hbar\omega \\ 0 & \hbar\omega & -2\hbar\omega \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

c_1 can be anything

$\Rightarrow -2\hbar\omega c_2 + \hbar\omega c_3 = 0$

$\hbar\omega c_2 - 2\hbar\omega c_3 = 0$

So we let $c_1 = 1$, and we must have $c_2 = c_3 = 0$. So

$$\boxed{|E_1 = 2\hbar\omega\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |e_1\rangle}$$

(a), cont'd...

$|E_2 = \hbar\omega\rangle$

$$\begin{pmatrix} \hbar\omega & 0 & 0 \\ 0 & -\hbar\omega & \hbar\omega \\ 0 & \hbar\omega & -\hbar\omega \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{matrix} \hbar\omega c_1 = 0 \\ -\hbar\omega c_2 + \hbar\omega c_3 = 0 \\ \hbar\omega c_2 - \hbar\omega c_3 = 0 \end{matrix}$$

So we must have $c_1 = 0$ and $c_2 = c_3$. Let $c_2 = c_3 = 1$. Then

$$\boxed{|E_2 = \hbar\omega\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}|e_2\rangle + \frac{1}{\sqrt{2}}|e_3\rangle}$$

$|E_3 = -\hbar\omega\rangle$

$$\begin{pmatrix} 3\hbar\omega & 0 & 0 \\ 0 & \hbar\omega & \hbar\omega \\ 0 & \hbar\omega & \hbar\omega \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{matrix} 3\hbar\omega c_1 = 0 \\ \hbar\omega c_2 + \hbar\omega c_3 = 0 \\ \hbar\omega c_2 + \hbar\omega c_3 = 0 \end{matrix}$$

Then we have $c_1 = 0$ and $c_3 = -c_2$. Let $c_2 = 1$ and $c_3 = -1$. Then

$$\boxed{|E_3 = -\hbar\omega\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}|e_2\rangle - \frac{1}{\sqrt{2}}|e_3\rangle}.$$

(a), cont'd...

$$B = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

$$\begin{vmatrix} 1-b & 0 & -1 \\ 0 & 2-b & 0 \\ -1 & 0 & 1-b \end{vmatrix} = 0$$

$$(1-b)(2-b)(1-b) - (-1)(2-b)(-1) = 0$$
$$(2-b)(1-b)^2 - (2-b) = 0$$
$$(2-b)\left((1-b)^2 - 1\right) = 0$$
$$(2-b)\left(1-2b+b^2-1\right) = 0$$
$$(2-b)\left(b^2-2b\right) = 0$$
$$b(2-b)(b-2) = 0$$

So

$$\boxed{b_1 = 0\,,\ b_{2,3} = 2} \text{ (doubly degenerate)}$$

$\underline{|b_1 = 0\rangle}$

$$\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{matrix} c_1 - c_3 = 0 \\ 2c_2 = 0 \\ -c_1 + c_3 = 0 \end{matrix}$$

We must have $c_2 = 0$ and $c_1 = c_3$. Let $c_1 = c_3 = 1$. Then

$$\boxed{|b_1 = 0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}|e_1\rangle + \frac{1}{\sqrt{2}}|e_3\rangle}$$

(a), cont'd

$|b_2=2\rangle$ and $|b_3=2\rangle$

We have

$$\begin{pmatrix} -1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & -1 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{array}{c} -c_1 - c_3 = 0 \\ c_2 = \text{anything} \\ -c_1 - c_3 = 0 \end{array}$$

for both $|b_2=2\rangle$ and $|b_3=2\rangle$. Then we must have $c_3 = -c_1$, so our generic eigenvector is

$$|b=2\rangle = \frac{1}{\sqrt{c_1^2+c_2^2+c_3^2}}\begin{pmatrix} c_1 \\ c_2 \\ -c_1 \end{pmatrix} = \frac{1}{\sqrt{2c_1^2+c_2^2}}\begin{pmatrix} c_1 \\ c_2 \\ -c_1 \end{pmatrix}$$

We know that we must have $\langle b_2=2|b_3=2\rangle = 0$. Let $c_2 = 0$ and $c_1 = 1 \rightarrow c_3 = -1$ for $|b_2=2\rangle$. So

$$\boxed{|b_2=2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}|e_1\rangle - \frac{1}{\sqrt{2}}|e_3\rangle}$$

Then we want to choose $c_1, c_2,$ and c_3 for $|b_3=2\rangle$. So

$$\langle b_2=2|b_3=2\rangle = \begin{pmatrix} 1/\sqrt{2} & 0 & -1/\sqrt{2} \end{pmatrix}\begin{pmatrix} c_1/\sqrt{2c_1^2+c_2^2} \\ c_2/\sqrt{2c_1^2+c_2^2} \\ -c_1/\sqrt{2c_1^2+c_2^2} \end{pmatrix} = 0$$

$$\frac{c_1}{\sqrt{4c_1^2+2c_2^2}} + \frac{c_1}{\sqrt{4c_1^2+2c_2^2}} = 0$$

(a), cont'd...

Since c_2 can be anything, let $c_2 = 1$. Then

$$\frac{c_1}{\sqrt{4c_1^2+2}} + \frac{c_1}{\sqrt{4c_1^2+2}} = 0$$

The only way this works is if $c_1 = 0$. So

$$\boxed{|b_3 = 2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = |e_2\rangle}$$

(b)

The time evolution operator is

$$U(t,t_0) = \sum_n |E_n\rangle\langle E_n| e^{-iE_nt/\hbar}$$

$$= |E_1\rangle\langle E_1| e^{-iE_1t/\hbar} + |E_2\rangle\langle E_2| e^{-iE_2t/\hbar} + |E_3\rangle\langle E_3| e^{-iE_3t/\hbar}.$$

So we want to determine

$$|\psi(t)\rangle = U(t,t_0)|\psi(0)\rangle.$$

We must first put our state $|\psi(0)\rangle$ into the E basis.
We know

$$|E_2 = \hbar\omega\rangle = \frac{1}{\sqrt{2}}\left(|e_2\rangle + |e_3\rangle\right)$$

$$|E_3 = -\hbar\omega\rangle = \frac{1}{\sqrt{2}}\left(|e_2\rangle - |e_3\rangle\right)$$

(b), cont'd...

Then

$$|E_2 = \hbar\omega\rangle + |E_3 = -\hbar\omega\rangle = \frac{2}{\sqrt{2}}|e_2\rangle$$

and so

$$|\psi(0)\rangle = |e_2\rangle = \frac{\sqrt{2}}{2}\left(|E_2\rangle + |E_3\rangle\right).$$

Then

$$|\psi(t)\rangle = \frac{\sqrt{2}}{2}|E_2\rangle e^{-iE_2t/\hbar} + \frac{\sqrt{2}}{2}|E_3\rangle e^{-iE_3t/\hbar}$$

$$\boxed{|\psi(t)\rangle = \frac{\sqrt{2}}{2}\left[|E_2\rangle e^{-iE_2t/\hbar} + |E_3\rangle e^{-iE_3t/\hbar}\right]}$$

$$= \frac{\sqrt{2}}{2}\left[\frac{1}{\sqrt{2}}\left(|e_2\rangle + |e_3\rangle\right)e^{-iE_2t/\hbar} + \frac{1}{\sqrt{2}}\left(|e_2\rangle - |e_3\rangle\right)e^{-iE_3t/\hbar}\right]$$

or $$\boxed{|\psi(t)\rangle = \frac{1}{2}\left[|e_2\rangle\left(e^{-iE_2t/\hbar} + e^{-iE_3t/\hbar}\right) + |e_3\rangle\left(e^{-iE_2t/\hbar} - e^{-iE_3t/\hbar}\right)\right]}$$

(c)

We have

$$P_{|\psi(t)\rangle}(b=2) = \left|\langle b_2 = 2|\psi(t)\rangle\right|^2 + \left|\langle b_3 = 2|\psi(t)\rangle\right|^2$$

$$= \left|-\frac{1}{2\sqrt{2}}\left(e^{-iE_2t/\hbar} - e^{-iE_3t/\hbar}\right)\right|^2 + \left|\frac{1}{2}\left(e^{-iE_2t/\hbar} + e^{-iE_3t/\hbar}\right)\right|^2$$

$$= \frac{1}{8}\left(e^{iE_2t/\hbar} - e^{iE_3t/\hbar}\right)\left(e^{-iE_2t/\hbar} - e^{-iE_3t/\hbar}\right)$$
$$+ \frac{1}{4}\left(e^{iE_2t/\hbar} + e^{iE_3t/\hbar}\right)\left(e^{-iE_2t/\hbar} + e^{-iE_3t/\hbar}\right)$$

$$= \frac{1}{8}\left(1 - e^{\frac{i(E_2-E_3)t}{\hbar}} - e^{\frac{-i(E_2-E_3)t}{\hbar}} + 1\right)$$
$$+ \frac{1}{4}\left(1 + e^{\frac{i(E_2-E_3)t}{\hbar}} + e^{\frac{-i(E_2-E_3)t}{\hbar}} + 1\right)$$

$$= \frac{1}{8}\left(2 - 2\cos\left(\frac{\omega' t}{\hbar}\right)\right) + \frac{1}{4}\left(2 + 2\cos\left(\frac{\omega' t}{\hbar}\right)\right)$$

$$= \frac{1}{4} - \frac{1}{4}\cos\left(\frac{\omega' t}{\hbar}\right) + \frac{1}{2} + \frac{1}{2}\cos\left(\frac{\omega' t}{\hbar}\right)$$

$$\boxed{P_{|\psi(t)\rangle}(b=2) = \frac{3}{4} + \frac{1}{4}\cos\left(\frac{\omega' t}{\hbar}\right)}\quad , \omega' = E_2 - E_3 .$$

(d)

Clearly, the probability is time-dependent. This makes sense because our wavefunction $|\psi(t)\rangle$ is a non-stationary state.

(e)

The TDSE is given by

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle .$$

Taking the derivative of $\langle B\rangle$,

$$\frac{\partial}{\partial t}\langle B\rangle = \frac{\partial}{\partial t}\langle\psi(t)|B|\psi(t)\rangle$$

$$= \frac{\partial}{\partial t}\int \psi^*(t)\, B\, \psi(t)\, d^3x$$

$$= \int \frac{\partial\psi^*(t)}{\partial t} B\psi(t) d^3x + \int \psi^*(t) \frac{\partial B}{\partial t}\psi(t) d^3x + \int \psi^*(t) B \frac{\partial\psi(t)}{\partial t} d^3x$$

$$= \int \frac{\partial\psi^*(t)}{\partial t} B\psi(t) d^3x + \left\langle \frac{\partial B}{\partial t}\right\rangle + \int \psi^*(t) B \frac{\partial\psi(t)}{\partial t} d^3x$$

By the TDSE,

$$\frac{\partial}{\partial t}|\psi(t)\rangle = \frac{1}{i\hbar} H|\psi(t)\rangle$$

and

$$\frac{\partial}{\partial t}\langle\psi(t)| = -\frac{1}{i\hbar}\langle\psi(t)|H$$

since $H = H^*$ because H is Hermitian.

(e), cont'd...

Then

$$\frac{\partial}{\partial t}\langle B\rangle = \int\left(-\frac{1}{i\hbar}\Psi^* H\right)B\Psi d^3x + \left\langle\frac{\partial B}{\partial t}\right\rangle + \int\Psi^* B\left(\frac{1}{i\hbar}H\Psi\right)d^3x$$

$$= -\frac{1}{i\hbar}\int\Psi^* HB\Psi d^3x + \left\langle\frac{\partial B}{\partial t}\right\rangle + \frac{1}{i\hbar}\int\Psi^* BH\Psi d^3x$$

$$= \left\langle\frac{\partial B}{\partial t}\right\rangle + \frac{1}{i\hbar}\int\Psi^*(HB-BH)\Psi d^3x$$

$$\boxed{\frac{\partial\langle B\rangle}{\partial t} = \left\langle\frac{\partial B}{\partial t}\right\rangle + \frac{1}{i\hbar}\left\langle[H,B]\right\rangle}$$

This is the generalized Ehrenfest theorem.

(f)

We know $\frac{\partial B}{\partial t}=0$. Then

$$[H,B] = HB - BH = \begin{pmatrix} 2\hbar\omega & 0 & 0 \\ 0 & 0 & \hbar\omega \\ 0 & \hbar\omega & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix}\begin{pmatrix} 2\hbar\omega & 0 & 0 \\ 0 & 0 & \hbar\omega \\ 0 & \hbar\omega & 0 \end{pmatrix}$$

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

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

(f), cont'd...

We have

$$\langle [H,B] \rangle = \langle \psi(t) | [H,B] | \psi(t) \rangle,$$

where

$$|\psi(t)\rangle = \frac{1}{2}\left[\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \left(e^{-\frac{iE_2 t}{\hbar}} + e^{-\frac{iE_3 t}{\hbar}} \right) + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \left(e^{-\frac{iE_2 t}{\hbar}} - e^{-\frac{iE_3 t}{\hbar}} \right) \right].$$

So

$$\langle [H,B] \rangle = \frac{1}{2}\left[(0\ 1\ 0)\left(e^{\frac{iE_2 t}{\hbar}} + e^{\frac{iE_3 t}{\hbar}} \right) + (0\ 0\ 1)\left(e^{\frac{iE_2 t}{\hbar}} - e^{\frac{iE_3 t}{\hbar}} \right) \right]$$

$$\cdot \begin{pmatrix} 0 & \hbar\omega & -2\hbar\omega \\ -\hbar\omega & 0 & -\hbar\omega \\ 2\hbar\omega & \hbar\omega & 0 \end{pmatrix}$$

$$\cdot \frac{1}{2}\left[\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \left(e^{-\frac{iE_2 t}{\hbar}} + e^{-\frac{iE_3 t}{\hbar}} \right) + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \left(e^{-\frac{iE_2 t}{\hbar}} - e^{-\frac{iE_3 t}{\hbar}} \right) \right]$$

$$= \frac{1}{4}\left[(0 1 0)\left(e^{\frac{iE_2 t}{\hbar}} + e^{\frac{iE_3 t}{\hbar}} \right) \begin{pmatrix} 0 & \hbar\omega & -2\hbar\omega \\ \hbar\omega & 0 & -\hbar\omega \\ 2\hbar\omega & \hbar\omega & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \left(e^{-\frac{iE_2 t}{\hbar}} + e^{-\frac{iE_3 t}{\hbar}} \right) \right.$$

$$+ (0\ 1\ 0)\left(e^{\frac{iE_2 t}{\hbar}} + e^{\frac{iE_3 t}{\hbar}} \right) \begin{pmatrix} 0 & \hbar\omega & -2\hbar\omega \\ \hbar\omega & 0 & -\hbar\omega \\ 2\hbar\omega & \hbar\omega & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \left(e^{-\frac{iE_2 t}{\hbar}} - e^{-\frac{iE_3 t}{\hbar}} \right)$$

$$+ (0\ 0\ 1)\left(e^{+\frac{iE_2 t}{\hbar}} - e^{\frac{iE_3 t}{\hbar}} \right) \begin{pmatrix} 0 & \hbar\omega & -2\hbar\omega \\ \hbar\omega & 0 & -\hbar\omega \\ 2\hbar\omega & \hbar\omega & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \left(e^{-\frac{iE_2 t}{\hbar}} + e^{-\frac{iE_3 t}{\hbar}} \right)$$

$$\left. + (0\ 0\ 1)\left(e^{\frac{iE_2 t}{\hbar}} - e^{\frac{iE_3 t}{\hbar}} \right) \begin{pmatrix} 0 & \hbar\omega & -2\hbar\omega \\ \hbar\omega & 0 & -\hbar\omega \\ 2\hbar\omega & \hbar\omega & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \left(e^{-\frac{iE_2 t}{\hbar}} - e^{-\frac{iE_3 t}{\hbar}} \right) \right]$$

(f), cont'd...

$$= \frac{1}{4}\Big[\left(2+2\cos\left(\tfrac{\omega' t}{\hbar}\right)\right)(\phi) + \left(0+2i\sin\left(\tfrac{\omega' t}{\hbar}\right)\right)(-\hbar\omega)$$
$$+ \left(0+2i\sin\left(\tfrac{\omega' t}{\hbar}\right)\right)(\hbar\omega) + \left(2-2\cos\left(\tfrac{\omega' t}{\hbar}\right)\right)(\phi)\Big]$$

$$= 0$$

So $\langle [H,B] \rangle = 0$ and $\left\langle \frac{\partial B}{\partial t} \right\rangle = 0$, and thus,

$$\boxed{\frac{\partial \langle B \rangle}{\partial t} = 0}.$$

(g) I would expect a similar result if the initial wavefunction was

$$|\Psi(0)\rangle = |e_1\rangle$$

because $|\Psi(t)\rangle$ would be a stationary state, since $|E_1\rangle = |e_1\rangle$.