CHEM 120A Midterm 1 Solutions

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1. (a) An operator $\hat{O}$ is said to be linear if for any pair of function f and g and scalar c_1 and c_2, it satisfies

$$\hat{O}(c_1 f + c_2 g) = c_1 \hat{O}(f) + c_2 \hat{O}(g)$$

Use this condition to check if $\hat{A}$, $\hat{B}$ and $\hat{C}$ are linear operator:

$$\begin{aligned}\hat{A}\big(c_1 f(x) + c_2 g(x)\big) &= \cos(x)\big(c_1 f(x) + c_2 g(x)\big) \\ &= c_1 \cos(x) f(x) + c_2 \cos(x) g(x) \\ &= c_1 \hat{A}\big(f(x)\big) + c_1 \hat{A}\big(g(x)\big)\end{aligned}$$

So we know that $\hat{A}$ is a linear operator.

$$\begin{aligned}\hat{B}\big(c_1 f(x) + c_2 g(x)\big) &= (c_1 f(x) + c_2 g(x)) \frac{\partial(c_1 f(x) + c_2 g(x))}{\partial x} \\ &= c_1^2 f(x)\frac{\partial f(x)}{\partial x} + c_2^2 g(x)\frac{\partial g(x)}{\partial x} + c_1 c_2 f(x)\frac{\partial g(x)}{\partial x} + c_1 c_2 g(x)\frac{\partial f(x)}{\partial x} \\ &\neq c_1 \hat{B}\big(f(x)\big) + c_2 \hat{B}\big(g(x)\big)\end{aligned}$$

Thus $\hat{B}$ is not a linear operator.

$$\begin{aligned}\hat{C}\big(c_1 f(x) + c_2 g(x)\big) &= -i\hbar \frac{\partial\big(c_1 f(x) + c_2 g(x)\big)}{\partial x} \\ &= c_1(-i\hbar)\frac{\partial\big(f(x)\big)}{\partial x} + c_2(-i\hbar)\frac{\partial g(x)}{\partial x} \\ &= c_1 \hat{C}\big(f(x)\big) + c_1 \hat{C}\big(g(x)\big)\end{aligned}$$

Thus $\hat{C}$ is a linear operator.

(b) In order for the observables of $\hat{A}$ and $\hat{C}$ to be known simultaneously, $\hat{A}$ and $\hat{C}$ must share the same eigenvectors, which means the commutator $[\hat{A}, \hat{C}] = 0$. To evaluate the commutator, we should have $[\hat{A}, \hat{C}]$, which is also an operator, act on an arbitary function $f(x)$, and check if $[\hat{A}, \hat{C}]f(x) = 0$. We have

$$\hat{A}\hat{C}f(x) = \hat{A}\big(-i\hbar\frac{\partial f(x)}{\partial x}\big) = -i\hbar\cos(x)\frac{\partial f(x)}{\partial x}$$

$$\hat{C}\hat{A}f(x) = \hat{C}\big(\cos(x)f(x)\big) = -i\hbar\frac{\partial \cos(x) f(x)}{\partial x} = i\hbar\sin(x)f(x) - i\hbar\cos(x)\frac{\partial f(x)}{\partial x}$$

so

$$[\hat{A},\hat{C}]f(x) = (\hat{A}\hat{C} - \hat{C}\hat{A})f(x) = -i\hbar\sin(x)f(x) \neq 0$$

We get a non-zero result indicated that $[\hat{A},\hat{C}] \neq 0$, this means we cannot know the observable of $\hat{A}$ and $\hat{C}$ simultaneously.

2. (a) Using $|u\rangle$ and $|d\rangle$ as our basis, the matrix representation of $\hat{H}$ is given by:

$$H_{11} = \langle u|\hat{H}|u\rangle = 1 \qquad H_{12} = \langle u|\hat{H}|d\rangle = 2$$
$$H_{21} = \langle d|\hat{H}|u\rangle = 2 \qquad H_{22} = \langle d|\hat{H}|d\rangle = -2$$

Note that to determine H_{21}, we have used the fact that $\hat{H}$ is a Hermitian, so that $H_{21} = H_{12}^* = 2$. Next we can check that $|a\rangle$ and $|b\rangle$ are eigenvectors of $\hat{H}$ by doing

$$\begin{pmatrix} 1 & 2 \\ 2 & -2 \end{pmatrix}\begin{pmatrix} \frac{2}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} \end{pmatrix} = 2\begin{pmatrix} \frac{2}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} \end{pmatrix}$$
$$\begin{pmatrix} 1 & 2 \\ 2 & -2 \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{5}} \\ -\frac{2}{\sqrt{5}} \end{pmatrix} = -3\begin{pmatrix} \frac{1}{\sqrt{5}} \\ \frac{-2}{\sqrt{5}} \end{pmatrix}$$

So $|a\rangle$ is eigenvector of $\hat{H}$ with eigenvalue $E_a = 2$, and $|b\rangle$ is eigenvector of $\hat{H}$ with eigenvalue $E_b = -3$.

(b) We want to write $|u\rangle$ in the form of $|u\rangle = c_a|a\rangle + c_b|b\rangle$, and the expansion coefficient is given by $c_a = \langle a|u\rangle$, and $c_b = \langle b|u\rangle$. From the expansion of $|a\rangle$ and $|b\rangle$ in terms of $|u\rangle$ and $|d\rangle$, we can easily find out that

$$\langle u|a\rangle = \frac{2}{\sqrt{5}} = c_a^* \qquad \langle b|u\rangle = \frac{1}{\sqrt{5}} = c_b^*$$

Thus

$$|u\rangle = \frac{2}{\sqrt{5}}|a\rangle + \frac{1}{\sqrt{5}}|b\rangle.$$

(c) We know that at $t = 0$, the system is in state $|u\rangle$, i.e,

$$|\psi(0)\rangle = |u\rangle = \frac{2}{\sqrt{5}}|a\rangle + \frac{1}{\sqrt{5}}|b\rangle$$

Now that $|a\rangle$ and $|b\rangle$ are eigenvectors of $\hat{H}$, the time propagation is straight forward:

$$|\psi(t)\rangle = \frac{2}{\sqrt{5}}e^{-2it}|a\rangle + \frac{1}{\sqrt{5}}e^{3it}|b\rangle$$

At time t, the probability of winning, i.e, the probability of observe the system in state $|w\rangle$ is given by

$$P = |\langle w|\psi(t)\rangle|^2$$

Since $|w\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle$, we have

$$\langle w|\psi(t)\rangle = \frac{2}{\sqrt{5}}e^{-2it}\Big(\frac{1}{\sqrt{2}}\langle u|a\rangle + \frac{1}{\sqrt{2}}\langle d|a\rangle\Big) + \frac{1}{\sqrt{5}}e^{3it}\Big(\frac{1}{\sqrt{2}}\langle u|b\rangle + \frac{1}{\sqrt{2}}\langle d|b\rangle\Big)$$

Plug in $\langle u|a\rangle = 2/\sqrt{5}$, $\langle d|a\rangle = 1/\sqrt{5}$, $\langle u|b\rangle = 1/\sqrt{5}$, $\langle d|b\rangle = -2/\sqrt{5}$, we find

$$\langle w|\psi(t)\rangle = \frac{3\sqrt{2}}{5}e^{-2it} - \frac{1}{5\sqrt{2}}e^{3it}$$
$$P = |\langle w|\psi(t)\rangle|^2 = \frac{18}{25} + \frac{1}{50} - \frac{3}{25}(e^{5it} + e^{-5it}) = \frac{37}{50} - \frac{6}{25}\cos(5t)$$

When $\cos 5t = -1$, we will have the maximum chance of winning, so we should wait for $t = \pi/5$.

3. In this question, we want evaluate $\frac{\partial\langle\hat{A}\rangle}{\partial t} = \frac{\partial\langle\psi|}{\partial t}|\hat{A}|\psi\rangle + \langle\psi|\hat{A}|\frac{\partial|\psi\rangle}{\partial t}$. To proceed, we can use the time-dependent S.E:

$$\hat{H}|\psi\rangle = i\hbar\frac{\partial|\psi\rangle}{\partial t} \qquad \langle\psi|\hat{H} = -i\hbar\frac{\partial\langle\psi|}{\partial t}$$

plug in these two equation, we have

$$\frac{\partial\langle\hat{A}\rangle}{\partial t} = -\frac{1}{i\hbar}\langle\psi|\hat{H}\hat{A}|\psi\rangle + \frac{1}{i\hbar}\langle\psi|\hat{A}\hat{H}|\psi\rangle = \frac{1}{i\hbar}\langle\psi|[\hat{A},\hat{H}]|\psi\rangle$$

We also know that the commutator is related to the uncertainty by

$$\Delta A\Delta H \geq \frac{1}{2}\left|\langle[\hat{A},\hat{H}]\rangle\right|$$

Thus

$$\frac{\Delta A}{\left|\frac{\partial\langle\hat{A}\rangle}{\partial t}\right|} = \frac{\Delta A}{\left|\frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle\right|} \geq \frac{\hbar\Delta A}{2\Delta A\Delta H} = \frac{\hbar}{2\Delta H}$$