Homework H21 Solution

1. In the previous lecture, Hilbert spaces were introduced with an example where you define the axes as $\psi_1(x) = \cos x$ and $\psi_2(x) = \sin x$. Then, according to the notation for basis functions, what are $\frac{\partial}{\partial x}|1\rangle$ and $\frac{\partial}{\partial x}|2\rangle$?

Solution:
In Hilbert space, the unit vectors are replaced by basis functions. In this example the basis functions are $|1\rangle = \cos x$ and $|2\rangle = \sin x$.

$$\frac{\partial}{\partial x}|1\rangle = \frac{\partial}{\partial x}\cos x = -\sin x = -|2\rangle$$

$$\frac{\partial}{\partial x}|2\rangle = \frac{\partial}{\partial x}\sin x = \cos x = |1\rangle$$

2. By using the analogy between Dirac and conventional integral notation, prove that $\langle n|\psi\rangle = (\langle\psi|n\rangle)^*$. [Hint: write down the analogous integral expression, and then remember that $a^*b = (ab^*)^*$.]

Solution:

$$\langle n|\psi\rangle = \int dx\ \psi_n^*(x)\psi(x)$$

$$(\langle\psi|n\rangle)^* = \left(\int dx\ \psi^*(x)\psi_n(x)\right)^*$$

$$= \int dx\ (\psi^*(x)\psi_n(x))^*$$

$$= \int dx\ \ \psi_n^*(x)\psi(x)$$

$$= \langle n|\psi\rangle \quad \text{[Since } (ab)^* = b^*a^*\text{]}$$

3. **Turn in** Postulate 5 states that $P(A = a_n) = \left|\int_{-\infty}^{\infty} dx\ \psi_n{}^*\psi\right|^2 = |\langle n|\psi\rangle|^2$, where the states $|n\rangle$ are the eigenfunctions of the operator A with eigenvalues a_n. Use the identity operator expressed in bracket notation and your result from problem (2) to prove that the average value of A, written as $\langle A\rangle$, is equal to $\langle\psi|A|\psi\rangle$. [Hint: remember $\langle A\rangle = \Sigma\ a_n\ P(A=a_n)$.]
The average value is also called the "expectation value" in quantum mechanics.

Solution:
Remember that $\hat{A}$ is an operator with eigenfunctions ψ_n, with eigenvalues a_n.

Now the average of any quantity is defined as all the allowed values of that quantity, weighted by the probability of occurrence of that value.

$$\langle A \rangle = \sum_n a_n P(A = a_n)$$

$$= \sum_n a_n |\langle n|\psi\rangle|^2$$

$$= \sum_n a_n \langle n|\psi\rangle\langle\psi|n\rangle$$

$$= \sum_n a_n \langle\psi|n\rangle\langle n|\psi\rangle$$

$$= \sum_n \langle\psi|a_n|n\rangle\langle n|\psi\rangle$$

$$= \sum_n \langle\psi|\hat{A}|n\rangle\langle n|\psi\rangle$$

$$= \langle\psi|\hat{A}\sum_n |n\rangle\langle n|\,\psi\rangle = \langle\psi|\hat{A}|\psi\rangle$$

Note that $\langle\psi|n\rangle$ and $\langle n|\psi\rangle$ are just numbers, so their orders can be interchanged, and any other number may as well be inserted (a_n) within them. Also, in the 2nd-last step we have used the eigenvalue equation for the operator A, that is we replaced $a_n|n\rangle$ by $\hat{A}|n\rangle$. In the last step, we removed the identity operator.

The formula <A> = $\langle\psi|\hat{A}|\psi\rangle$ when the molecule is in state ψ is one of the most important in quantum mechanics. It allows you to calculate on average the result you expect to get by repeating many independent measurements. Of course each individual measurement will give you an eigenvalue a_n of operator $\hat{A}$.

Note: in the next problem, a tilde "~" denotes a matrix.

4. The technique of finding the eigenvalues and eigenvectors of an operator in matrix form is termed as "diagonalization". In this problem, you will diagonalize the matrix

$$\widetilde{M} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

The starting point is the equation $(\widetilde{M} - \tilde{\Lambda}) * \mathbf{v} = 0$, where $\widetilde{M}$ is your non-diagonal matrix, $\tilde{\Lambda}$ is the corresponding diagonal eigenvalue matrix, obtained by $\tilde{\Lambda} = \lambda.\tilde{I}$, with λ being any of the eigenvalues, and v is one of the eigenvectors, a column vector. In order to obtain a non-trivial solution, we need the condition $\det\|\tilde{M} - \tilde{\Lambda}\| = 0$.

Solution:

a) We start with multiplying out the determinant equation

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

to obtain

$$\lambda^2 + 1 = 0$$

Solving the quadratic eigenvalue equation gives the eigenvalues $\lambda = \pm i$

b) To begin, let us first prove that any multiple of **v** is also an eigenvector. Lets represent the multiple of **v** as N**v** where N is some constant. Substituting this expression into the eigenvector equation for **v** we have

$$(\tilde{M} - \tilde{\Lambda}) * N\mathbf{v} = 0$$

and since N is just a constant, we see that the above equation is satisfied, thus indicating that any multiple of **v** is also an eigenvector.

In order to find the eigenvectors (up to an unknown constant) plug each eigenvalue into the equation $(\tilde{M} - \tilde{\Lambda}) * \mathbf{v} = 0$ and solve for **v**:

$\boldsymbol{\lambda = -i}$ **:**

$$\begin{pmatrix} i & 1 \\ -1 & i \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0$$

We get two equations:

$$ic_1 + c_2 = 0$$
$$-c_1 + ic_2 = 0$$

The equation only determines c_1 *in terms of* c_2 *or vice-versa*, not both. To get both, we also need to invoke normalization, or $c_1^2+c_2^2=1$. A simple trick is to *assign* a value to either c_1 or c_2, and then solve for the other. It is by far the easiest course of action to set one of the constants equal to unity and solve for the other, and that is what shall be done here. Setting $c_1 = 1$ we have

$$i + c_2 = 0$$

and

$$-1 + ic_2 = 0$$

Both equations confirm that c_2 must equal $-i$ (BECAUSE we set $c_1 = 1$). Thus the eigenvector corresponding to $\lambda = +i$ is given by

$$\mathbf{v}_{-i} = \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

The eigenvector is of course not normalized since we arbitrarily picked c_1=1.

$\boldsymbol{\lambda = +i}$ **:**

$$\begin{pmatrix} -i & 1 \\ -1 & -i \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0$$

The two equations are:

$$-ic_1 + c_2 = 0$$
$$-c_1 - ic_2 = 0$$

Again letting $c_1 = 1$ yields

$$-i + c_2 = 0$$

and

$$-1 - ic_2 = 0$$

Both equations confirm that c_2 must equal $+i$ (BECAUSE we set $c_1 = 1$). Thus the eigenvector corresponding to $\lambda = -i$ is given by

$$\mathbf{v}_{+i} = \begin{pmatrix} 1 \\ i \end{pmatrix}$$

c) Normalizing $\mathbf{v}_{-i}$ we write

$$\mathbf{v}_{-i}{}^{\dagger}\ \mathbf{v}_{-i} = (1 \quad i) \begin{pmatrix} 1 \\ -i \end{pmatrix} = 1 - i^2 = 2$$

Dividing $\mathbf{v}_{+i}$ by $\sqrt{2}$ gives the normalized eigenvector

$$\mathbf{v}_{-i} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

Normalizing $\mathbf{v}_{+i}$ we write

$$\mathbf{v}_{+i}{}^{\dagger}\ \mathbf{v}_{+i} = (1 \quad -i) \begin{pmatrix} 1 \\ i \end{pmatrix} = 1 - i^2 = 2$$

Dividing $\mathbf{v}_{-i}$ by $\sqrt{2}$ gives the normalized eigenvector

$$\mathbf{v}_{+i} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

d) In order to check that $\widetilde{M}\mathbf{v} = \lambda\mathbf{v}$ is satisfied, simply plug and chug:

$$\widetilde{M}\ \mathbf{v}_{-i} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 - i \\ -1 \quad 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ -1 \end{pmatrix}$$

Factoring out – i gives

$$\widetilde{M}\ \mathbf{v}_{-i} = \frac{-i}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} = -i * \mathbf{v}_{-i} = \lambda\, \mathbf{v}_{-i}$$

Similarly for the other eigenvector. Next, to prove that the eigenvectors are orthogonal,

$$\mathbf{v}_{-i}{}^{\dagger}\ \mathbf{v}_{+i} = \frac{1}{2}\,(1 \quad i) \begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{1}{2}(1 + i^2) = 0$$

Done!