MA3441 Problem Set 3

Professor Fry (typset by Mark Allen)

Issued: 17th October 2012
Due: 24th October 2012 (optional)

Disclaimer

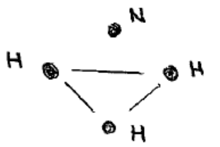
Everything I've written might be completely wrong. Check that what I wrote matches with what Prof. Fry wrote, especially if you keep getting the wrong answer.

Problems

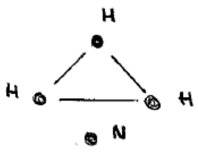
1. Two-state quantum systems.

   Examples:

   - Ammonia molecule NH^3



$|1\rangle$



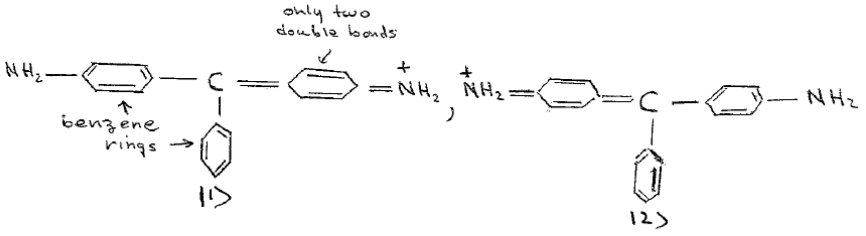
$|2\rangle$

   - Hydrogen molecular ion H_2^+

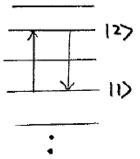
$|1\rangle$

$|2\rangle$

- Magenta dye



- System with many energy levels, confining our attention to transitions between states $|1\rangle$ and $|2\rangle$ only.



If a two-level system were not allowed to make the transition $|1\rangle \leftrightarrow |2\rangle$ its Hamiltonian operator would be

$$\begin{pmatrix} H_{11} & 0 \\ 0 & H_{22} \end{pmatrix}$$

For the first three examples above, $H_{11} = H_{22} = E_0$ by symmetry. E_0 is real. For the last example, $H_{11} = E_1$, $H_{22} = E_2$. For the rest of this problem, we consider the case $H_{11} = H_{22} = E_0$. Then eigenstates of H are

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} ,$$

and their time dependence is derived from Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |1, t\rangle = E_0 |1, t\rangle$$

$$\Longrightarrow \ |1, t\rangle = e^{-iE_0 t/\hbar} |1, 0\rangle = e^{-iE_0 t/\hbar} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

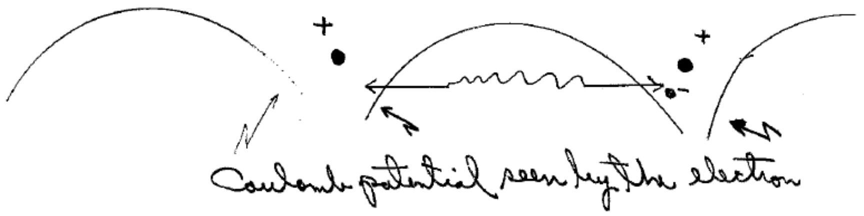
Similarily for $|2, t\rangle$. Then, once in state $|1\rangle$ or $|2\rangle$ the system remains in it forever. Now suppose we allow for the possibility of the transition $|1\rangle \leftrightarrow |2\rangle$ by introducing off-diagonal elements in H. Let

$$H_{12} = -A$$

Since $H_{12}^* = H_{21}$, $H_{21} = -A^*$. For simplicity, assume $A^* = A$. Then

$$H = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$$

A corresponds to a tunnelling process. Thus, consider the H_2^+ ion: the electron detaches itself from one proton and tunnels through the potential barrier to the other. The business of QM is to calculate A.



(a) Find the eigenvalues of H. Ans: $E_0 \pm A$.

(b) Find the normalized eigenstates of H in terms of $|1\rangle$ and $|2\rangle$.
Ans: $|\pm\rangle = \frac{1}{\sqrt{2}}(|1\rangle \mp |2\rangle)$

Conclusions:

- The N atom in NH_3 and the electron in H_2^+ are not localized. The energy difference 2A is responsible for the ammonia maser and the one-electron bond, respectively.
- The dye magenta has two energy states, neither of which is $|1\rangle$ or $|2\rangle$, but a superposition of them. This is the basis for its colour: photons with energy $\hbar\omega = 2A$ are absorbed in the optical region.
  More reading: Feynman Lectures, Vol. III, Chapters 8-10.

2. (a) Consider a spin-$\frac{1}{2}$ particle. It can have 'spin up' ($= \frac{\hbar}{2}$) or 'spin down' ($= -\frac{\hbar}{2}$) with respect to some axis in space. The following are basis states:

$$|\uparrow\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad |\uparrow\rangle_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \qquad |\uparrow\rangle_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

or or

$$|\downarrow\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad |\downarrow\rangle_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} \qquad |\downarrow\rangle_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

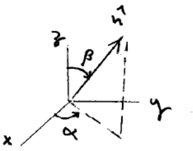
We already know that the spin angular momentum operators for the x and z directions are

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Find S_y by construction an appropriate unitary transformation.

(b) Show that $[S_x, S_y] = i\hbar S_z +$ cyclic perms of x, y, z.

3. (a) Construct the normalised spin state $|\uparrow\rangle_{\hat{n}}$ with spin $+\frac{\hbar}{2}$ in the direction $\hat{\mathbf{n}}$ (see fig.) where $\hat{\mathbf{n}}$ is a unit vector. Use the results for S_x, S_y, S_z in problem 2.



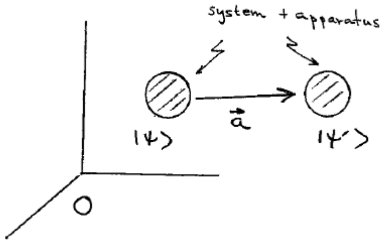
Hint: You want $\mathbf{S}\cdot\hat{\mathbf{n}}|\uparrow\rangle_{\hat{n}} = +\frac{\hbar}{2}|\uparrow\rangle_{\hat{n}}$.
Ans: $|\uparrow\rangle_{\hat{n}} = \cos\left(\frac{\beta}{2}\right)|\uparrow\rangle_z + e^{i\alpha}\sin\left(\frac{\beta}{2}\right)|\downarrow\rangle_z$

(b) Suppose S_x is measured. What is the probability for getting $+\frac{\hbar}{2}$?
Ans: $\frac{1}{2}(1 + \cos\alpha\sin\beta)$

4. One way to get the basic commutator

$$[x_i, p_j] = i\hbar\delta_{ij}, \quad i, j = 1, 2, 3.$$

Let $|\psi\rangle$ be the state of a system. Suppose the *system* is translated by $\mathbf{a}$ and that its new state is $|\psi'\rangle$.



Just as for a time translation, require norm preservation:

$$\langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle.$$

This is guaranteed if states are related by a unitary transformation U:

$$U(\mathbf{a})|\psi\rangle = |\psi'\rangle, \quad U^+ = U^{-1}.$$

For an infinitesimal translation let

$$U(\delta\mathbf{a}) = 1 - i\delta\mathbf{a}\cdot\mathbf{P}/\hbar$$

where

$$\mathbf{P}^+ = \mathbf{P}$$

and by construction $[\mathbf{P}] =$ momentum. This is probably the most basic definition of momentum: the generator of space translations.

Let $\mathbf{X}$ be the position operator. Assume that the expectation value of $\mathbf{X}$ in any state undergoes a translation $\mathbf{a}$ when the state is translated by $\mathbf{a}$. Then

$$\langle\psi'|\mathbf{X}|\psi'\rangle = \langle\psi|\mathbf{X}|\psi\rangle + \mathbf{a} \tag{*}$$

Specialise (*) to an infinitesimal translation and show that

$$[X_i, p_j] = i\hbar\delta_{ij}, \quad i, j = 1, 2, 3.$$