Quantum Mechanics

Assessed problem sheet 1 - to be handed to TO by Thurs 20th October 5pm.

Two isomers of a molecule are different arrangements of the atoms that constitute the molecule. They are distinct quantum states: $|1\rangle$, $|2\rangle$.

The molecule can be modeled as a two-state system. Any state of this system can be written as a linear superposition of the two orthonormal states $|1\rangle$ and $|2\rangle$:

$$|\psi\rangle = \alpha|1\rangle + \beta|2\rangle\,.$$

Equivalently you can denote such a state as

$$|\psi\rangle \equiv \begin{pmatrix} \alpha \\ \beta \end{pmatrix}\,.$$

The matrix elements of the Hamiltonian are defined as usual:

$$H_{ij} = \langle i|\hat{H}|j\rangle\,.$$

We can write the Hamiltonian in the basis $\{|1\rangle, |2\rangle\}$ as a 2×2 matrix:

$$H = \begin{pmatrix} E_1 & -\eta \\ -\eta & E_2 \end{pmatrix}\,.$$

Make sure that you use the notation in a consistent way.

1. Let us consider the state described by
$$\frac{1}{\sqrt{5}} \begin{pmatrix} 1+2i \\ 0 \end{pmatrix}$$
Is the state normalized to one? What is the probability of the system being in state $|1\rangle$? **[2]**

2. Write down the explicit expression for the diagonal elements of $\hat{H}$, and explain their physical interpretation. **[2]**

3. Expand the time-evolution operator $\exp\left[-\frac{i}{\hbar}\hat{H}t\right]$ at first order in t. Assume that the system is in the state $|2\rangle$ at time $t = 0$. Find the state of the system at time ϵ, up to terms that are $O(\epsilon^2)$. Interpret the physical meaning of η. **[4]**

4. If $E_1 = E_2 = E$, and $|\Psi(0)\rangle = |2\rangle$, find $|\Psi(t)\rangle$. **[4]**

5. Let us now consider the case where $E_1 = E + \Delta E$, and $E_2 = E - \Delta E$. Find the stationary states as linear combinations of $|1\rangle$ and $|2\rangle$. **[4]**

6. Consider the system described above in question 5. Starting from $|\Psi(0)\rangle = |1\rangle$, find the probability for the system to be in the state $|1\rangle$ at time t. **[5]**

7. Assuming $\Delta E \ll E$, discuss the limiting cases $\Delta E/\eta \ll 1$, and $\Delta E/\eta \gg 1$. **[4]**

L Del Debbio, October 2011.