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Quantum Mechanics A (Physics 212A) Fall 2018
Worksheet 2 – Solutions

Problems

1. **Formaldehyde** (From Le Bellac)

   Let's consider a simple two state system motivated by the Huckel theory.

   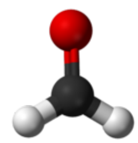

   Figure 1: Formaldehyde visualized

   There are two π-electrons associated with the double bond between carbon and oxygen. Let's consider the Hilbert space of a single π-electron as $\mathcal{H} = \text{span}\{|O\rangle, |C\rangle\}$ where these represent occupation on either the carbon or oxygen.

   (a) Give a physical motivation for the Hamiltonian to be of the form

   $$\hat{H} = E_O|O\rangle\langle O| + E_C|C\rangle\langle C| - A(|C\rangle\langle O| + |O\rangle\langle C|) \tag{1}$$

   where $E_C > E_O$ are the energies associated with being localized and A is known as the "delocalization" energy

   The oxygen is more electronegative than carbon so this translates to a lower energy for being bonded to it.

   The hopping term is the A piece which is trying to capture the kinetic energy of the electrons which naively suggests it's symmetric though maybe this could be weakened.

   The sign is important though as for $A > 0$ it determines whether the wave-function is (approximately) symmetric/anti-symmetric. The potential should be approximately symmetric so this explains the choice.

   (b) Calculate the eigenvalues and eigenvectors associated with (1). Sketch how this would look in position space.

   $\lambda_\pm = \frac{E_C+E_O}{2} \pm \sqrt{A^2+\Delta^2}$ where $\Delta \equiv \frac{E_C-E_O}{2}$

   $|+\rangle = e^{-\mathbf{i}\frac{\phi}{2}} \cos\frac{\theta}{2}|O\rangle + e^{\mathbf{i}\frac{\phi}{2}} \sin\frac{\theta}{2}|C\rangle$

   $|-\rangle = -e^{-\mathbf{i}\frac{\phi}{2}} \sin\frac{\theta}{2}|O\rangle + e^{\mathbf{i}\frac{\phi}{2}} \cos\frac{\theta}{2}|C\rangle$

   where $-\frac{A}{\sqrt{A^2+\Delta^2}} = \sin\theta\cos\phi$ and $\frac{\Delta}{\sqrt{A^2+\Delta^2}} = \cos\theta$

   Assume that the system is in its ground state.

(c) For a given π-electron, calculate the probability of finding it localized at the oxygen.

$P = \langle -|O\rangle\langle O|-\rangle = \sin^2\frac{\theta}{2} = \frac{1}{2}(1-\cos\theta)$

(d) Assume that the electric dipole moment of formaldehyde only gets contributions from the symmetric axis. Express this as a function of the bond length ℓ.

There are 8 protons on oxygen and 6 protons on carbon. There are 7 core+σ electrons associated with oxygen and 5 for carbon. The remaining two electrons are the ones we reasoned about above. The second π-electron can be placed also in the groundstate of the first under the assumption they don't interact.

The excess charge on the oxygen from the π-electrons is then $(1-2P)e$ where e is the charge of the electron. $d = (1-2P)e\ell$ choosing the carbon to be our reference point.

2. **Single Qubit Gates** (From Nielsen-Chuang)

Aside from the usual Pauli matrices there are a few common operators for a two state system. These are the Hadamard (H), the phase gate (S), and the T-gate (T). In the Z-basis these can be written as:

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} \quad S = \begin{pmatrix}1 & 0\\ 0 & \mathbf{i}\end{pmatrix} \quad T = \begin{pmatrix}1 & 0\\ 0 & e^{\mathbf{i}\frac{\pi}{4}}\end{pmatrix} \tag{2}$$

(a) Write these in terms of our original Pauli's. Note that $S = T^2$. What is the action of H on Z-eigenvectors?

$H = \frac{1}{\sqrt{2}}(X+Z)$ and $T = \frac{1}{2}(1+e^{\mathbf{i}\frac{\pi}{4}})\mathbb{1} + \frac{1}{2}(1-e^{\mathbf{i}\frac{\pi}{4}})Z$

$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

Note $H^2 = \mathbb{1}$

(b) Prove the following identities

$$HXH = Z \quad HYH = -Y \quad HZH = X \tag{3}$$

$XH = \frac{1}{\sqrt{2}}(\mathbb{1} - \mathbf{i}Y) \implies HXH = \frac{1}{\sqrt{2}}(H - \mathbf{i}HY) = \frac{1}{\sqrt{2}}[H - \frac{\mathbf{i}}{\sqrt{2}}(\mathbf{i}Z - \mathbf{i}X)] = Z$

The rest are similar.

(c) Show that[1] $T = U_z(\frac{\pi}{4})$ and $HTH = U_x(\frac{\pi}{4})$ where $U_n(\theta) \equiv e^{-\mathbf{i}\frac{\theta}{2}\hat{n}\cdot\vec{\sigma}}$

$T = e^{+\mathbf{i}\frac{\pi}{8}}\begin{pmatrix}e^{-\mathbf{i}\frac{\pi}{8}} & 0\\ 0 & e^{\mathbf{i}\frac{\pi}{8}}\end{pmatrix} = e^{+\mathbf{i}\frac{\pi}{8}}U_z(\frac{\pi}{4}) \propto \cos\frac{\pi}{8}\mathbb{1} - \mathbf{i}\sin\frac{\pi}{8}Z$

$HTH = \cos\frac{\pi}{8}\mathbb{1} - \mathbf{i}\sin\frac{\pi}{8}HZH = \cos\frac{\pi}{8}\mathbb{1} - \mathbf{i}\sin\frac{\pi}{8}X$

3. **Quis Custodiet Ipsos Custodes?** (From Jacobs)

Projective measurements lead to some weird things.

Consider a two state system with basis vectors $\{|0\rangle, |1\rangle\}$. We are going to evolve the system according the Hamiltonian $\hat{H} = \frac{\omega}{2}Y$ where Y is the Pauli matrix $\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$.

[1] Up to a global phase

(a) What is the unitary operator associated with time evolution? Given an initial prepared state of $|\psi_0\rangle = |0\rangle$. Write an expression for $|\psi(t)\rangle$.

$U = e^{-\mathbf{i}Ht} = e^{-\mathbf{i}\frac{\omega}{2}Yt}$. Recall that $Y|0\rangle = \mathbf{i}|1\rangle$ and that $e^{-\mathbf{i}\frac{\omega}{2}\vec{\sigma}.\hat{n}} = \cos\frac{\omega}{2}\mathbb{1} - \mathbf{i}\vec{\sigma}.\hat{n}\sin\frac{\omega}{2}$

This implies $|\psi(t)\rangle = \cos\frac{\omega t}{2}|0\rangle + \sin\frac{\omega t}{2}|1\rangle$

(b) What is the probability, as function of time, to measure $|0\rangle$?

$P_t[|0\rangle] = \cos^2\frac{\omega t}{2}$

(c) Suppose we study the system over the time interval $[0, T]$ where $T \gg \delta t \equiv \frac{T}{N}$. We perform a measurement, in this basis, at every time $\frac{T}{N}, \frac{2T}{N}, \cdots$ where N is large. Assuming each measurement is independent from the other, what's the probability that the spin *never* flips to $|1\rangle$?

Recall that our measurement axiom says we should 'collapse' $|\psi\rangle$ onto the pure state which we measure it to be.

This implies if we measure $|0\rangle$ at time $t = \frac{T}{N}$ then the time evolution from $\frac{T}{N} \to \frac{2T}{N}$ is the same as if starting from $t = 0$. The probability to not flip is always $\cos^2\frac{\omega T}{2N}$

The probability for the spin to never flip then is just the product of probabilities to not flip at every measurement.

$P_{never-flip} = (\cos^2\frac{\omega T}{2N})^N$

(d) Evaluate this probability in the limit of $N \to \infty$.

This is called the *quantum Zeno effect*.

A cheap and dirty way to do this is to take the series expansion at $N = \infty$ and drop all terms in $\mathcal{O}(\frac{1}{N})$. Just replace $\frac{1}{N} \equiv \eta$ and Taylor expand at $\eta = 0$.

$P_{never-flip} \approx 1 - \frac{\omega^2 T^2}{4N}$ which goes quickly to 1. In this limit the spin never flips.

More carefully you should see that it actually *exponentially* approaches 1 as $N \to \infty$; it's pretty dramatic