

# Problem Set

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## Section I (Oct. 4)

1. Consider two kets  $|\alpha\rangle$  and  $|\beta\rangle$ . Let  $|i\rangle$  be a complete set of basis ket states. Suppose  $\langle i|\alpha\rangle$  and  $\langle i|\beta\rangle$  are known for all basis states  $|i\rangle$ . Find the matrix representation of the operator  $|\alpha\rangle\langle\beta|$  in that basis.
2. We now consider a qubit system and let  $|\alpha\rangle = |\sigma^z = +1\rangle$  and  $|\beta\rangle = |\sigma^x = +1\rangle$ . Write down the explicit square matrix that corresponds to  $|\alpha\rangle\langle\beta|$  in the  $\sigma^z$  basis.
3. Construct the state  $|\mathbf{n} \cdot \boldsymbol{\sigma} = +1\rangle$  such that

$$\mathbf{n} \cdot \boldsymbol{\sigma} |\mathbf{n} \cdot \boldsymbol{\sigma} = +1\rangle = (+1) |\mathbf{n} \cdot \boldsymbol{\sigma} = +1\rangle, \quad (1)$$

where  $\mathbf{n} = (n_x, n_y, n_z)$  is a unit vector.

- $\mathbf{n} \cdot \boldsymbol{\sigma}$  is an *operator*

$$\mathbf{n} \cdot \boldsymbol{\sigma} = n_x \sigma^x + n_y \sigma^y + n_z \sigma^z. \quad (2)$$

- $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$  is a *vector* of *operators*, i.e. each component of the vector  $\boldsymbol{\sigma}$  is an operator.

If we treat the qubit as a spin, the spin operators are related by

$$\mathbf{S} = \frac{\hbar}{2} \boldsymbol{\sigma}. \quad (3)$$

4. A beam of electrons goes through a series of Stern-Gerlach measurements as follows: (a) the first measurement accepts  $s_z = \hbar/2$  atoms and rejects  $s_z = -\hbar/2$  atoms; (b) the second measurement accepts  $s_n = \hbar/2$  atoms and rejects  $s_n = -\hbar/2$  atoms, where  $s_n$  is the eigenvalue of the operator  $\mathbf{n} \cdot \mathbf{S}$ ; (c) the third measurement accepts  $s_z = -\hbar/2$  atoms and rejects  $s_z = \hbar/2$  atoms. What is the intensity of the final  $s_z = -\hbar/2$  beam when the  $s_z = \hbar/2$  beam surviving the first measurement is normalized to unity? How must we orient the second measuring apparatus if we are to maximizing the intensity of the final  $s_z = -\hbar/2$  beam?

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## Section II (Oct. 11)

1. An operator (or matrix)  $\hat{A}$  is normal if it satisfies the condition  $[\hat{A}, \hat{A}^\dagger] = 0$ .
  - (a) Show that real symmetric, hermitian, real orthogonal and unitary operators are normal
  - (b) Show that any operator can be written as  $\hat{A} = \hat{H} + i\hat{G}$ , where  $\hat{H}$  and  $\hat{G}$  are Hermitian. [Hint: consider the combinations  $\hat{A} + \hat{A}^\dagger$ ,  $\hat{A} - \hat{A}^\dagger$ ]. Show that  $\hat{A}$  is normal if and only if  $[\hat{H}, \hat{G}] = 0$ .
  - (c) Show that a normal operator  $\hat{A}$  admits a spectral representation

$$\hat{A} = \sum_{i=1}^N \lambda_i \hat{P}_i \quad (4)$$

for a set of projectors  $\hat{P}_i$  and complex numbers  $\lambda_i$ .

**2.** Recall the trace of an operator  $\text{Tr}[A] = \sum_i \langle i | A | i \rangle$  for some basis  $\{|i\rangle\}$

(a) Prove that this definition is independent of basis. This implies if  $A$  is diagonalizable with eigenvalues  $\lambda_i$  that  $\text{Tr}[A] = \sum_i \lambda_i$ .

(b) Prove the cycle property:  $\text{Tr}[ABC] = \text{Tr}[BCA] = \text{Tr}[CAB]$

(c) Consider an operator  $A$ . Show the following identity

$$\det e^A = e^{\text{Tr}[A]} \quad (5)$$

**3.** Clock and shift operators

Consider an  $N$ -dimensional Hilbert space, with orthonormal basis  $\{|n\rangle\}$ . Consider operators  $T$  and  $U$  which act on this  $N$ -state system by

$$T|n\rangle = |n+1\rangle, \quad U|n\rangle = e^{\frac{2\pi i n}{N}} |n\rangle. \quad (6)$$

In the definition of  $T$ , the label on the ket should be understood as its value modulo  $N$ .

(a) Find the matrix representations of  $T$  and  $U$  in the basis  $\{|n\rangle\}$ .

(b) What are the eigenvalues of  $U$ ? What are the eigenvalues of its adjoint  $U^\dagger$ ?

(c) Show that

$$U T = e^{\frac{2\pi i}{N}} T U \quad (7)$$

(d) From the definition of adjoint, how does  $T^\dagger$  act?

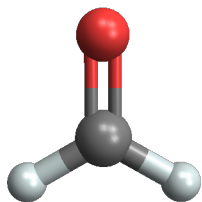
(e) Show that the clock operator  $T$  is normal.

(f) Find the eigenvalues and eigenvectors of  $T$ . [Hint: consider states of the form  $\frac{1}{\sqrt{N}} \sum_n e^{i k n} |n\rangle$ ].

## Section III (Oct. 18)

**1.** Formaldehyde (From Shauna Kravec)

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



There are two  $\pi$ -electrons associated with the double bond between carbon and oxygen. The Hilbert space of single  $\pi$ -electron is  $\mathcal{H} = \text{span}\{ \begin{matrix} \text{ } \end{matrix} \}$ , where these represent occupation on either the carbon or oxygen.

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

$$H = E_O |O\rangle \langle O| + E_C |C\rangle \langle C| - A(|C\rangle \langle O| + |O\rangle \langle C|) \quad (8)$$

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

(b) Calculate the eigenvalues and eigenvectors associated with (8). Sketch how this would look in the position space. Assume the system is in its ground state.

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

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

## 2. Single Qubit Gate (From Nielsen-Chuang)

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

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} \quad (9)$$

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

(b) Prove the following identities

$$H X H = Z, \quad H Y H = -Y, \quad H Z H = X \quad (10)$$

(c) Show that  $T = U_z(\frac{\pi}{4})$  and  $H T H = U_x(\frac{\pi}{4})$ , where  $U_n(\theta) = e^{\frac{-i}{2} \theta \hat{n} \cdot \vec{\sigma}}$ .

## 3. Quantum resonance in qubit system.

Let's consider a qubit system, say a trapped electron, whose energy gap is  $\Delta$ . We use a microwave with frequency  $\omega$  to couple that system. In classical mechanics, we know that if the driving force has the same frequency with inertial frequency of the system, we will observe enhanced oscillation, which we call it resonance. Here, we try to see the same thing for the simplest quantum system.

(a) Derive or convince yourself the Hamiltonian is

$$H(t) = \begin{pmatrix} \frac{\Delta}{2} & \epsilon e^{-i\omega t} \\ \epsilon e^{i\omega t} & -\frac{\Delta}{2} \end{pmatrix}. \quad (11)$$

(b) Derive the time propagator.

$$U(t) = \cos(\kappa t) \hat{I} - i \sin(\kappa t) \left[ \frac{\omega - \Delta}{2\kappa} \sigma_z + \frac{\epsilon}{\kappa} \sigma_x \right], \quad (12)$$

where  $\kappa = \sqrt{\epsilon^2 + (\omega - \Delta)^2} / 2$ . Or alternatively, we could solve the Schrödinger Equation.

(c) Try two limit: 1) Off-resonance limit  $|\omega - \Delta| \gg |\epsilon|$ , 2) resonance limit  $|\omega - \Delta| \ll |\epsilon|$ . Observe what will happen.

## Section IV(Oct.25)

### 1. Quantum resonance in qubit system.

Let's consider a qubit system, say a trapped electron, whose energy gap is  $\Delta$ . We use a microwave with frequency  $\omega$  to couple that system. In classical mechanics, we know that if the driving force has the same frequency with inertial frequency of the system, we will observe enhanced oscillation, which we call it resonance. Here, we try to see the same thing for the simplest quantum system.

(a) Derive or convince yourself the Hamiltonian is

$$H(t) = \begin{pmatrix} \frac{\Delta}{2} & \epsilon e^{-i\omega t} \\ \epsilon e^{i\omega t} & -\frac{\Delta}{2} \end{pmatrix}. \quad (13)$$

(b) Derive the time propagator.

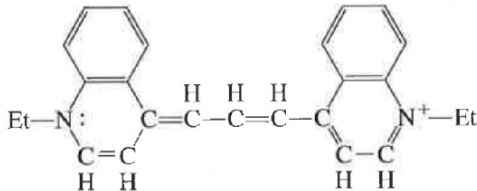
$$U(t) = \cos(\kappa t) \hat{I} - i \sin(\kappa t) \left[ \frac{\omega - \Delta}{2\kappa} \sigma_z + \frac{\epsilon}{\kappa} \sigma_x \right], \quad (14)$$

where  $\kappa = \sqrt{\epsilon^2 + (\omega - \Delta)^2} / 2$ . Or alternatively, we could solve the Schrödinger Equation.

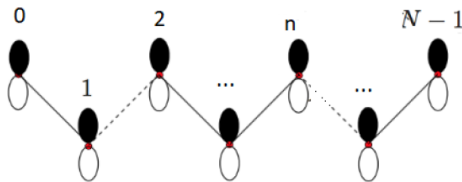
(c) Try two limit: 1) Off-resonance limit  $|\omega - \Delta| \gg |\epsilon|$ , 2) resonance limit  $|\omega - \Delta| \ll |\epsilon|$ . Observe what will happen.

### 2. Linear Polyenes

Polyenes are molecules with chains of alternating single/double carbon bonds. For example, this cyanine dyes:



We'll focus exclusively on the  $\pi$ -electrons that compose the carbon bonds. We can then model this as a finite length chain composed of  $N$  sites.



The difference between this and the cyclic chain is that we no longer have translation symmetry, and the chain have two ends. A trick is to introduce a fictious site, which connects the two ends, and then impose the boundary condition that the wavefunction must vanish there.

(a) Write the hopping Hamiltonian, as before, but including this fictious site. Use the form of the

translation generators  $T = |n+1\rangle\langle n|$ .

- (b) Write the eigenvectors and eigenvalue of the operator  $T^\dagger + T$  which satisfy the boundary condition.
- (c) Write down the spectrum of the Hamiltonian as before. Is there any degeneracy?
- (d) Assume that for N-carbons there are N many  $\pi$ -electrons. What is the gap between the “highest occupied molecular orbital” and “lowest unoccupied molecular orbital”?
- (e) The absorption peak for cryptocyanine is  $\lambda=648\text{nm}$ . How does this compare to the model with N=9 carbons? The hopping parameter is  $\beta=3.1\text{eV}$ .