Problem Set

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 σ^z basis.

3. Construct the state $|\boldsymbol{n}\cdot\boldsymbol{\sigma} = +1\rangle$ such that

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

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

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

$$\boldsymbol{n}\cdot\boldsymbol{\sigma} = n_x\,\sigma^x + n_y\,\sigma^y + n_z\,\sigma^z. \tag{2}$$

- $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ 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

$$\boldsymbol{S} = \frac{\hbar}{2}\boldsymbol{\sigma}. \tag{3}$$

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 $s_{\boldsymbol{n}} = \hbar/2$ atoms and rejects $s_{\boldsymbol{n}} = -\hbar/2$ atoms, where $s_{\boldsymbol{n}}$ is the eigenvalue of the operator $\boldsymbol{n}\cdot\boldsymbol{S}$; (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?

Section II (Oct. 11)

1. An operator (or matrix) $\hat{A}$is normal if is satisfies the condition $\left[\hat{A}, \hat{A}^\dagger\right] = 0$.

(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 $\left[\hat{H}, \hat{G}\right] = 0$.

(c) Show that a normal operator $\hat{A}$ admits a spectral representation

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

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

2. Recall the trace of an operator $\mathrm{Tr}[A] = \sum_m \langle m| A |m\rangle$ for some basis $\{|\mathtt{m}\rangle\}$

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

(b) Prove the cycle property: Tr[ABC]=Tr[BCA]=Tr[CAB]

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

$$\det e^{A} = e^{\mathrm{Tr}[A]} \tag{5}$$

3. Clock and shift operators

Consider an N-dimensional Hilbert space, with orthonormal basis $\{|n\rangle, n = 0, .., N-1\}$. Consider operators T and U which act on this N-state system by

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

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

$$U\,T \;=\; e^{\frac{2\pi i}{N}}\,T\,U \tag{7}$$

(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 $|\theta\rangle \equiv \sum_n e^{i\,n\theta}\,|n\rangle$].

Section III (Oct. 18)

1. Formaldehyde (From Shauna Kravec)

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

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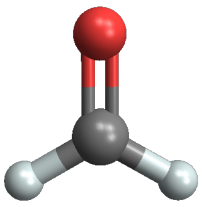


There are two π-electrons associated with the double bond between carbon and oxygen. The Hilbert space of single π-electron is $\mathcal{H} = \mathrm{span}\{|\mathtt{O}\rangle, \; |\mathtt{C}\rangle\}$, where these represent occupation on

either the carbon or oxygen.

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

$$H = E_O\,|O\rangle\langle O| + E_C\,|C\rangle\langle C| - A(|C\rangle\langle O| + |O\rangle\langle C|) \tag{8}$$

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 π-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 ℓ.

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:

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

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

(b) Prove the following identities

$$H\,X\,H = Z,\ H\,Y\,H = -Y,\ H\,Z\,H = X \tag{10}$$

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

Section IV(Oct.25)

1. Quantum resonance in qubit system.

Let's consider a qubit system, say a trapped electron, whose energy gap is Δ. We use a microwave with frequency ω 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

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

(b) Derive the time propagator.

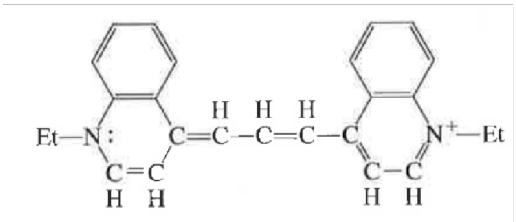
$$U(t) = \cos(\kappa t)\,\hat{I} - i\sin(\kappa t)\Big[\frac{\omega-\Delta}{2\kappa}\,\sigma_z + \frac{\epsilon}{\kappa}\,\sigma_x\Big], \tag{12}$$

where $\kappa = \sqrt{\epsilon^2 + (\omega - \Delta)^2 / 4}$. Or alternatively, we could solve the Schrödinger Equation.

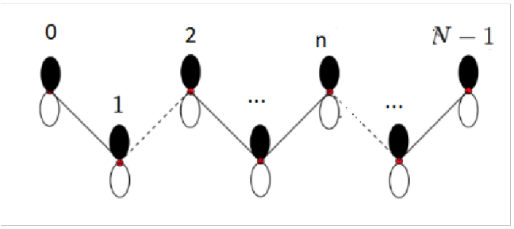
(c) Try two limit: 1) Off-resonance limit $|\omega\text{-}\Delta| \gg |\epsilon|$, 2) resonance limit $|\omega\text{-}\Delta| \ll |\epsilon|$. Observe what will happen.

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 π-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 fictional site. Use the form of the translation generators $T = |n+1\rangle\langle n|$.

(b) Write the eigenvectors and eigenvalus of the operator $T^\dagger + T$ which satisfy the boundary condition.

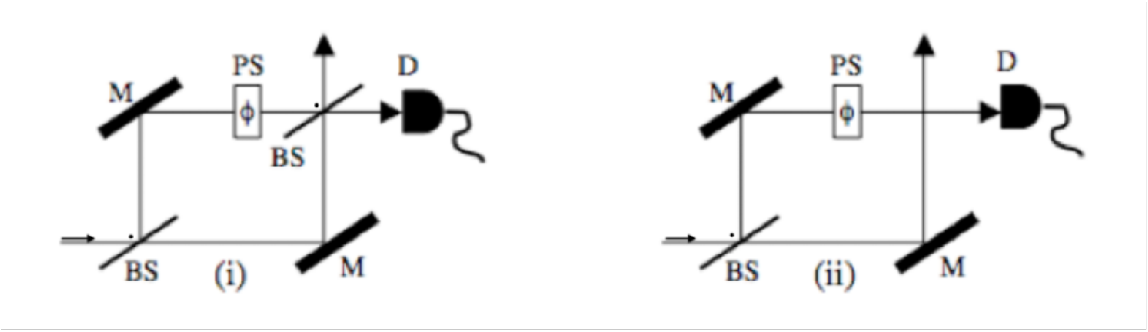
(c) Write down the spectrum of the Hamiltonian as before. Is there any degeneracy?

(d) Assume that for N-carbons there are N many π-electrons. What is the gap between the "highest occupied molecular orbital" and "lowest unoccuped molecular orbital"?

(e) The absorption peak for cryptocynanine is λ=648nm. How does this compare to the model with N=9 carbons? The hopping parameter is β=3.1eV.

Section V(Nov. 1)

1. Interferometry



We can consider the path taken of a photon as (approximately) a two-state quantum system spanned by $|\mathsf{u}\rangle, |\mathsf{d}\rangle$ for whether it went up or down respectively. Consider the two interferometers shown above.

The left one is a balanced Mach-Zender interferometer, and the right is the same but with the final beam splitter removed. The elements BS are mean splitters which implement the Hadamard gate on the incoming beam: $H = \frac{1}{\sqrt{2}}[(|u\rangle + |d\rangle)\langle u| + (|u\rangle - |d\rangle)\langle d|]$

The elements M are mirrors which transform $|\text{In}\rangle \to |\text{Out}\rangle = -|\text{In}\rangle$

The element PS is a phase shifter which transform $|\text{In}\rangle \to |\text{Out}\rangle = e^{i\phi}|\text{In}\rangle$

The element D is a detector which measures photons going in.

For each device, determine the probability for detecting a photon as a function of ϕ.

2. Time-energy uncertainty

Consider an observable A which has no explicit dependence on time. Define the variance of A in a state ϕ to be

$$\Delta\text{A} \equiv \sqrt{\left\langle \left(A - \langle A\rangle_\phi\right)^2 \right\rangle_\phi} \tag{13}$$

Let

$$\Delta\text{T} \equiv \frac{\Delta\text{A}}{\left|\partial_t \langle A\rangle_\phi\right|} \tag{14}$$

This is a measure of the time required for $\langle\text{A}\rangle$ to change significantly, i.e. by an amount comparable to its variance ΔA. Show that

$$\Delta\text{E}\,\Delta\text{T} \geq \frac{\hbar}{2}, \tag{15}$$

where ΔE is the variance of H.

3. Entropy and thermodynamics

Consider a quantum system with hamiltonian H and Hilber space $\mathcal{H} = \text{span}\{|n\rangle,\ n = 0, 1, 2 \ldots\}$. Its behavior at finite temperature can be described using thermal density matrix

$$\rho_\beta = \frac{e^{-\beta \text{H}}}{Z} \tag{16}$$

where $\beta = \frac{1}{T}$ specifies the temperature and Z is normalization factor.

(a) Find a formal expression for Z by demanding that $\rho_\beta$is normalized appropriately.

(b) Show that the von Neumman entropy of $\rho_\beta$can be written as

$$S_\beta = E / T + \log Z \tag{17}$$

where $E \equiv \langle H \rangle_\rho$ is the expectation value for the energy. The expression above for $S_\beta$is the thermal entropy.

(c) Evaluate Z and E for the case where the system is a simple harmonic oscillator

$$H = \hbar\omega\left(n + \frac{1}{2}\right) \tag{18}$$

with $\hat{n}\,|n\rangle = n\,|n\rangle$.

Section VI(Nov. 15)

1. Schmidt Decomposition

In the problems below, consider a bipartite system $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, with the factors not necessarily of the same dimension. Consider a state of the system

$$|a\rangle = \sum_{i=1}^{N} \sum_{r=1}^{N} a_{i\,r}\,|i\rangle_A \otimes |r\rangle_B \tag{19}$$

(a) We defined the Schmidt number of the state $|\,\mathsf{a}\,\rangle$ to be the rank of the matrix $a_{i\,r}$. Show that this is the same as the number of nonzero eigenvalues of

$$\rho_A = \mathrm{Tr}_B\,|a\rangle\,\langle a|. \tag{20}$$

Show that it is also the same as the number of nonzero eigenvalues of

$$\rho_B = \mathrm{Tr}_A\,|a\rangle\,\langle a|. \tag{21}$$

[Hint: To solve this problem, it is useful to take advantage of changing basis. In particular, the problem does not depend on what basis we choose for $\mathcal{H}_A$ and $\mathcal{H}_B$. If w were a Hermitian matrix, we could find a basis where it was diagonal, by using its eigenvectors as the basis elements. If w is not Hermitian, or maybe not even square, such a matrix has right eigenvectors and left eigenvectors. In particular, any matrix has a singular value decomposition(SVD) of the form

$$w = U^T\,\Lambda\,V \tag{22}$$

where U and V are unitary (basis transformations) and Λ is a diagonal matrix. For non-square matrix, Λ might look like

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},\ \text{if } N > M \quad \text{or} \quad \Lambda = \begin{pmatrix} \lambda_1 & 0 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 & 0 \end{pmatrix},\ \text{if } M > N \tag{23}$$

and U is $N \times N$, and V is $M \times M$. So we can choose a new basis for $\mathcal{H}_a$ which is $|i'\rangle = U\,|i\rangle$, and $|r'\rangle = V\,|r\rangle$. In the new basis, we have

$$|w\rangle = \sum_{i'\,r'} \Lambda_{i'\,r'}\,|i'\rangle \otimes |r'\rangle \tag{24}$$

and Λ is diagonal.

2. Entanglement cannot be created locally

Define a local unitary to be an operator of the form $U_A \otimes U_B$. These are the operators that can be done by actors with access only to A or B. Show that by acting on a state of $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ with local unitary we cannot change the Schmidt number or the entanglement entropy. Consider both the case of a pure state of $\mathcal{H}$ and a mixed state of $\mathcal{H}$. Notice the action of a unitary U on a density matrix ρ is

$$\rho \to U\,\rho\,U^{\dagger} \tag{25}$$

3. Building Bloch's Theorem

Consider a 1D Hamiltonian with a periodic potential $V(x) = V(x + n\,a)$ for $n \in \mathbb{Z}$ and a is the lattice spacing.

(a) Define the operator T^n by $T^n\,|x\rangle = |x + n\,a\rangle$. Show this is a symmetry.

(b) Show that any eigenfunctions of this system can be chosen to obey

$$\phi_k(x - a) = e^{-i\,k\,a}\,\phi_k(x) \tag{26}$$

Recall that $T\,|k\rangle = e^{-i\,k\,a}\,|k\rangle$, and $\langle x \mid k\rangle = \phi_k(x)$.

(c) Infer from (26) that one can then write $\phi_k(x) = e^{i\,k\,x}\,u_k(x)$ where $u_k(x) = u_k(x + a)$

Notice that k is not the usual momentum, It is a crystal momentum!

(d) Show that for $P = -i\,\partial_x$that $P\,\phi_k(x) \neq k\,\phi_k(x)$.

(e) Show that $\frac{-\pi}{a} \leq k \leq \frac{\pi}{a}$.What is $k + \frac{2\,\pi}{a}$?