5.73 Problem Set 2

Due Friday, Sept. 30

1. Let $|\psi_n\rangle$ be the eigenstates of some Hermitian operator, $\hat{O}$.
    a. Consider the operator $\hat{P} = \frac{1}{2}\left(|\psi_m\rangle\langle\psi_m| + |\psi_n\rangle\langle\psi_n|\right)$. Compute $\hat{P}^2$. Is $\hat{P}$ idempotent?
    b. Consider $\hat{R} = |\psi_m\rangle\langle\psi_n|$. Under what conditions is this operator Hermitian?
    c. Consider a second Hermitian operator, $\hat{O}'$. Under what conditions is $\hat{O}'\hat{O}$ Hermitian? Are there any special properties of the commutator $[\hat{O}',\hat{O}]$?
    d. Consider two Hermitian operators, $\hat{A}_1$ and $\hat{A}_2$ that *do not* commute with each other, but *do* commute with $\hat{O}$ (i.e. $[\hat{A}_1,\hat{O}] = [\hat{A}_2,\hat{O}] = 0 \neq [\hat{A}_1,\hat{A}_2]$.) Show that $\hat{O}$ must have a degenerate eigenvalue. That is, show that two of the eigenvalues, o_n and o_m, corresponding to different states are the same.

2. Consider a operator, $\hat{O}$, that depends on a parameter, λ. For example, the operator might be a Hamiltonian that depends on an electric field strength, λ.
    a. Consider the λ-dependent eigenvalue equation:
    $$\hat{O}(\lambda)|\psi(\lambda)\rangle = o(\lambda)|\psi(\lambda)\rangle$$
    Show that one can compute $\frac{do(\lambda)}{d\lambda}$ **without** knowing $\frac{d|\psi(\lambda)\rangle}{d\lambda}$. Thus, one can determine the change in the eigenvalue without knowing the change in the eigenstate. Under what conditions would $\hat{O}(\lambda)$ commute with $\hat{O}(\lambda')$?
    b. Now, consider the exponential of $\hat{O}(\lambda)$, which is defined through its power series:
    $$e^{\tau\hat{O}(\lambda)} \equiv 1 + \tau\hat{O}(\lambda) + \tfrac{1}{2}\tau^2\hat{O}^2(\lambda) + \ldots.$$
    We will later see that the exponential is closely related to *time evolution* in QM and here τ plays the role of time.

Show that $\hat{O}(\lambda)$ commutes with its exponential. That is, show that $\left[\hat{O}(\lambda), e^{\tau\hat{O}(\lambda)}\right] = 0$.

c. One often wants to compute the derivative of the exponential with respect to the external parameter λ. Show that

$$\frac{d}{d\lambda} e^{\tau\hat{O}(\lambda)} = \int_0^\tau e^{\alpha\hat{O}(\lambda)} \frac{d\hat{O}(\lambda)}{d\lambda} e^{(\tau-\alpha)\hat{O}(\lambda)} d\alpha .$$

Do not assume that $\hat{O}(\lambda)$ commutes with $d\hat{O}(\lambda)/d\lambda$. [Hint: Show that both sides ($\hat{X}$) satisfy the first order differential equation (in τ):

$$\frac{d\hat{\mathrm{X}}}{d\tau} - \hat{X}\,\hat{O}(\lambda) = e^{\tau\hat{O}(\lambda)} \frac{d\hat{O}(\lambda)}{d\lambda}$$

Then, if the two sides are equal at $\tau = 0$, they must be equal for all τ.]

3. The following concern a diatomic molecule with a simple harmonic potential between the atoms $V(\hat{x}) = \frac{1}{2}k\hat{x}^2$. Assume $\hbar = m = 1$ and denote the eigenstates of the Hamiltonian by $|n\rangle$.
   a. Find the linear combination of $|0\rangle$ and $|1\rangle$ ($|\varphi\rangle = a|0\rangle + b|1\rangle$) for which the average value of $\hat{x}$ is maximum. Repeat this process for a linear combination of $|0\rangle$ and $|2\rangle$. What are the maximum values possible in each case? Which works better?
   b. Same as b., but this time maximize the average value of $\hat{x}^2$. What conclusion do you draw from these two calculations?
   c. Now, assume that the molecule (starting in the vibrational and electronic ground state) is *instantaneously* promoted to an excited electronic state (say by a laser). In this state the potential felt by the atoms is $V(\hat{x}) = \frac{1}{3}k\hat{x}^2$. What is the average energy of the atoms in the new state? Here, we are making use of the Franck-Condon approximation by assuming the electronic state adjusts much more quickly than the nuclei.

4. For any one dimensional (1D) system, if we turn on a magnetic field of strength B perpendicular to the 1D axis, the resulting 1D Hamiltonian is:

$$\hat{H}_B = \hat{H} + B\hat{p}\ .$$

Assume that we have a harmonic oscillator of frequency ω and we subject it to a perpendicular magnetic field, B.

a. What are the observable energies for the system now that the field is on? You should determine these energies analytically (i.e. without assuming a numerical value for B).

b. We make a measurement of the energy and find a particular value E_n. Next, we measure the momentum. If we perform this sequence of measurements many, many times (i.e. we measure the energy and find E_n and then measure the momentum) what will be the average outcome? Your expression should be correct for any choice of B, n.[Hint: you should not need any explicit wavefunctions to do this.]