**Physics 401 - Homework #7**

1) **Time evolution of expectation values (seven points total).** If an observable (A) has a quantum mechanical operator ($\hat{A}$) which does not depend on time, then the time-rate change of the expectation value of that observable in any arbitrary state is given by

$$\frac{d\langle A\rangle}{dt} = \left\langle \frac{i}{\hbar}\left[\hat{H},\hat{A}\right]\right\rangle$$

    a) (three points) Prove that this is true. Hint #1: Write down an expression for the expectation value of A using the position basis, where the (arbitrary) state function is the spatial wavefunction $\Psi(x,t)$. Hint #2: Your proof should make use of the Time Dependent Schroedinger Equation. Hint #3: Your proof will also make use of the complex-conjugate of the Time Dependent Schroedinger Equation.

    b) (three points) Apply the result shown above to the case where the observable (A) is the momentum. Let the Hamiltonian for the system be that of a particle moving in an arbitrary one-dimensional potential function V(x) . Hint: you will need to know the commutator between the Hamiltonian and momentum. You calculated this commutator on Exam #1, and the solution is posted on the course website.

    c) (one point) What famous law of classical physics does the result from part (b) correspond to?

2) **Orthogonality of the stationary states of the harmonic oscillator (three points).**
Since energy is an observable quantity, it is represented by a Hermitian operator ($\hat{H}$), and this guarantees that the energy eigenstates (or stationary states) are orthogonal.

We would like to demonstrate that the stationary states are, in fact, orthogonal, for a few specific cases. To do this, show that the ground state, first excited state, and second excited state of the harmonic oscillator have zero overlap, working in the position basis. In other words, prove that $\langle 0|1\rangle = \langle 1|2\rangle = \langle 0|2\rangle = 0$ using the spatial wavefunctions of these states:

$$\psi_n(x) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n\, n!}} H_n(\xi)e^{-\xi^2/2} \ , \ \ \xi \equiv \sqrt{\frac{m\omega_0}{\hbar}}x$$

$$H_0 = 1$$
$$H_1 = 2\xi$$
$$H_2 = 4\xi^2 - 2$$

Hint: By examining the even-odd properties of the integrands, you can easily show that some of these integrals are zero without any real work.

3) **Games we play with the promotion and demotion operators (eight points).**
Calculate the expectation values for position, momentum, position squared, and momentum squared, for the $n^{th}$ harmonic oscillator state. <u>Do not attempt to do these calculations by evaluating any integrals.</u> Instead, write the position and momentum operators in terms of the promotion and demotion operators, and use the following properties of these operators to evaluate the appropriate Dirac brackets:

$$\hat{a}|n\rangle = \left(\sqrt{n}\right)|n-1\rangle$$
$$\hat{a}^{\dagger}|n\rangle = \left(\sqrt{n+1}\right)|n+1\rangle$$

Please use Dirac notation!

4) **Classical motion of a quantum harmonic oscillator (three points).** A quantum mechanical harmonic oscillator is in the initial state

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

Show that as time goes forward, the expectation value of the position for this system will execute the motion that we expect of a classical harmonic oscillator:

$$\langle x\rangle = C\cos(\omega_0 t)$$

Hint: use the method suggested in question #3 to evaluate this expectation value.

5) **Carbon monoxide molecule (six points total).** Diatomic molecules have vibrational energy levels which are evenly spaced, just as expected for a harmonic oscillator. We can infer from these measurements that the potential energy of the two atoms in such a molecule depends on the distance between them in a roughly quadratic fashion, at least near the equilibrium point.

We observe the effect of the vibrational energy levels by measuring the frequency of the electromagnetic radiation emitted when the molecule makes a transition from one level to another.[1] For the carbon monoxide molecule, we find that the wavenumber of the emitted EM radiation is $\Delta k$ = 2170 cm$^{-1}$. This wavenumber corresponds to the difference in energy between adjacent levels in the molecule. (It is not the energy of any one particular energy level.)

     a) What is the fundamental frequency ($\omega_0$) of the harmonic oscillator for this molecule? Please report your answer in Hz.
     b) When interpreting a diatomic molecule as a harmonic oscillator, the relevant mass is the reduced mass, given by (mM)/(m+M), where m is the mass of the lighter atom, and M is the mass of the heavier atom. Calculate the reduced mass of the carbon monoxide molecule, and report your answer in kilograms.
     c) What is the effective spring constant (K) for this harmonic oscillator? Please report your answer in kg/s$^2$.

6) **The quantum number of a classical oscillator (three points).** A harmonic oscillator consists of a one kilogram mass on a spring. Its oscillation frequency is one Hertz, and when it passes through the equilibrium point, its velocity is one meter per second. What is the order-of-magnitude of the quantum number (n) associated with this oscillator?

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[1] By the way, during the transition from one state to another, the expectation value for the position of the atoms in the molecule oscillates exactly as shown in question #4.