CHEM352: Physical Chemistry II
Homework Set I - due 25^{th} of Feb, 5.00 pm
Each problem is worth 2 pts, 20 pts in total.

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1. (a) Derive from Rydberg formula the wavelength limits of Lyman, Balmer and Paschen series for a hydrogen atom. Identify the spectral regions of these wavelengths.
   (b) Generalize the Rydberg formula for $\bar{\nu}$ for any nuclei with atomic number Z.
2. Starting from Planck's expression for black body radiation, derive Wien's displacement law. Consult 1-5 problem for hints how to solve numerically the expression after taking the derivative. Use the resulting equation to estimate temperature of the brightest star in the night sky, Sirius.
3. Using your favorite web-search engine, social network or encyclopedia, find the work function of lithium, sodium, potasium, iron and aluminium. Next, calculate the kinetic energy of electrons emitted from a metal surface that is irradiated with radiation of wavelength of 200 nm.
4. Calculate the wavelenght for:
   (a) an electron with a K.E. of 1 keV,
   (b) a proton with a K.E. of 1 keV,
   (c) an alpha particle with a K.E. of 1 keV.
   (d) an electron in the second Bohr orbit in hydrogen atom.
5. (a) Solve the equation:
   $$\frac{d^2x}{dt^2} + \omega^2 x(t) = 0$$
   Subject to the initial conditions $x(0) = A$ and $\frac{dx}{dt} = v_0$ at $t = 0$.
   (b) The general solution to the above differential equation is:
   $$x(t) = c_1 \cos \omega t + c_2 \sin \omega t$$
   Fot convenience, the solution is often presented in the equivalent forms: $x(t) = A \sin(\omega t + \phi)$ or $x(t) = B \cos(\omega t + \psi)$. Using trigonometric identities, derive expressions for A and ϕ (and B and ψ) in terms of c_1 and c_2.
6. Calculate $< x >$,$< x^2 >$, $< p >$ and $< p^2 >$ for the n=2 state of a particle in one dimensional box. Next, calculate respective standard deviations and show that Heisenberg uncertainty principle holds.
7. (a) Use a partice in a box model to estimate the electronic excitation energies in a haxatriene. Compare predicted and experimental values.
   (b) Use a particle in a 1D-cyclic box to estimate eigenstates of cyclohexatriene (benzene). Show that periodic boundary condition causes degeneracy of eigenstates.
8. The wave function and of the particle in the 3 dimensional box with lengths of a, b and c has the following form:
   $$\Psi(x, y, z) = A_x A_y A_z \sin \frac{n_x \pi x}{a} \sin \frac{n_x \pi y}{b} \sin \frac{n_z \pi z}{c}$$
   where n_x, n_y and n_z are independent, positive integers.
   (a) Derive the normalization constant $(A_x A_y A_z)$

(b) Derive the expression for the energy of the particle in the 3D box.

(c) Show that the eigenfucntions are orthonormal to each other.

(d) Sketch the particle's energy diagram for the box of a size $a = b = 1$ and $c = 1.5a$,

9. (a) Show that:

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$$
$$[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$$
$$[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$$

(b) Show that each of the above operators commutes with $\hat{L}^2$

10. Take a look at 4-35 - quantum-mechanical tunneling and analyze the solution. The problems are mostly self-explanatory however the solution require your independent work.