

Homework 5A Due Mon Nov 6

Part A. More problems will be assigned throughout next week.

Levine 6.16, 6.17, 6.47, 7.27, 7.29

1) A Dirac notation equivalent of our integrals for finding Fourier coefficients is the “projection operator” $P_n = |n\rangle \langle n|$ (it may look strange but you know how to “use” it). P_n projects out the component of any arbitrary ket that lies along the basis ket $|n\rangle$. (i.e. if $\psi = a|1\rangle + b|2\rangle + c|3\rangle$) then $P_n \psi = |1\rangle (\langle 1| a|1\rangle + \langle 1| b|2\rangle + \langle 1| c|3\rangle) = a|1\rangle$. Combine the definition of completeness in Levine 7.39 with Levine 7.71 to show that

$$\sum_n |n\rangle \langle n| = 1$$

This is the more common statement of completeness for an orthonormal basis set.

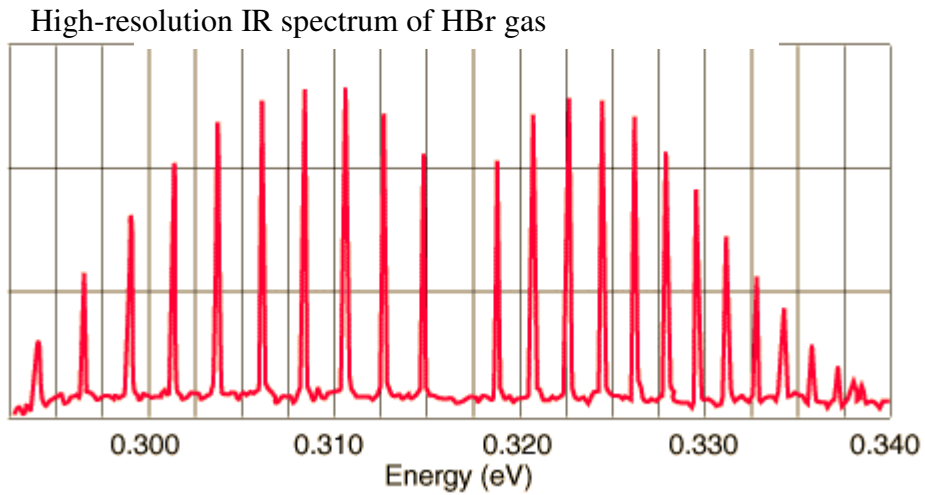
Note: this is really a notational problem—just translate Levine’s equations into Dirac notation, and using the definitions you are familiar with show that this new operator must return f when operating on any function f .

2) What is the most probable distance (in meters) of finding a 1s electron from a Uranium nucleus that has been ionized of all but 1 electron? What is the potential energy of an electron this far away from a uranium nucleus (in Joules)? The virial theorem (an important result from chapter 14 that we haven’t had time to cover) tells us that $2 * \langle KE \rangle$ of this electron will equal $-\langle U \rangle$ (or that $\langle KE \rangle = -\langle U \rangle$), the average PE of this electron. Use a classical estimate to calculate how fast such an electron is moving. *Comment.*

3) Following Levine, use a computer to make linear combinations of $Y(1,-1)$, $Y(1,1)$, $Y(1,0)$ to generate the familiar p_x , p_y and p_z orbitals. Make 3D plots of the angular components to verify that you indeed get the angular factors from p_x and p_y . *Why can we take linear combinations of these eigenfunctions and create new eigenfunctions of H , when we know that in general, linear combinations of eigenfunctions are not also eigenfunctions.*

4) See next page:

4) *Rotational-Vibrational Spectra*



4) A) Calculate the ratio of molecules in the ground and first excited rotational states at 300K for HBr.

B) Discuss why we see a whole series of lines around the fundamental vibrational transition in the above IR spectrum.

C) Label the peaks according to the quantum numbers n and l of the initial and final states responsible for each of the 6 central lines in the spectrum above.

This data contains information about which of the following:

A) Energy of the electrons in a rotating HBr

B) Bond length

C) Bond strength

D) Isotopic distribution of H and Br