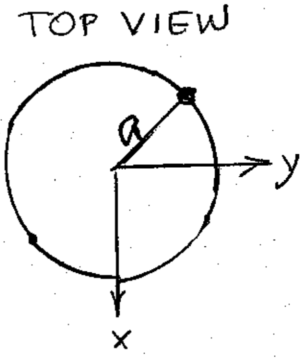
Chemistry 344

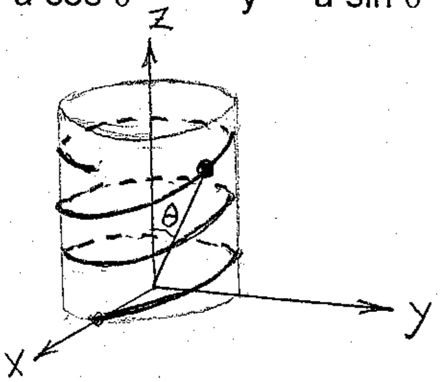
Final Exam
Dec. 10, 2002
Look at the entire exam first, then decide which problems are easiest for you to start with

1. The helix is a very important structure for biochemistry. At least some parts of important biological macromolecules have helical structure. In Problem Set 5 you could interpret the variation of the wavelength of the three bands in the ultraviolet spectrum of series of compounds containing aromatic rings by using the simple model of a particle on a circle. It turns out that many qualitative aspects of the optical rotation spectra of helical systems can be interpreted entirely by using only the electron on a helix model system. Let us see how to start. We have solved several Schrödinger equations in only one variable, for a particle on a circle, as well as a particle on a line along the x axis. Now let us consider the case which is sort of a combination of the two, that is, we take the line and wrap it on the outside of a right circular cylinder to form a helix.

A particle of mass M is constrained to move along a right-handed helix consisting of t turns (shown below). The radius of the helix is a and the pitch of the helix (the distance between successive turns) is $b2\pi$. The position of the electron anywhere on the helix is given by:

$$x = a\cos\theta \qquad y = a\sin\theta \qquad z = b\theta$$





Since there are t turns, at the bottom end of the helix $\theta = 0°$
and at the top end of the helix $\theta = t(2\pi)$.

For a free particle constrained to move on this helix of t turns, we specify that
$V(x,y,z)$ = constant = 0 on the helix and $V = \infty$ everywhere else. Obviously a complicated V!
The kinetic energy of this single particle is of course, still given by

$$\text{K.E.} = p_x^2/2M + p_y^2/2M + p_z^2/2M$$

We replace the individual components of linear momentum by the corresponding quantum mechanical operators,

$(p_x)_{op}$ =	$(p_y)_{op}$ =	$(p_z)_{op}$ =

Therefore, in terms of x,y and z, the Hamiltonian operator for this particle is

$\mathcal{H}$ =

As we have already found in other simple systems such as the particle on a circle, it is possible to make use of a change in coordinate system to simplify the form of the Schrödinger equation that needs to be solved. For the particle on a circle, we changed coordinates from the set (x,y) into the set (R,ϕ). Since the radius R of the circle is a constant we solved a Schrödinger equation in ϕ only.

For the *particle on the helix*, instead of having the operators and the eigenfunctions in terms of three variables (x,y,z), we can use a transformation to the new coordinates (a,b,θ) defined above: $x = a \cos \theta$ $y = a \sin \theta$ $z = b\,\theta$

By varying a, b, and θ one could sweep all of 3-D space, but for the helix, a and b are constants. Thus, our operators and eigenfunctions can be written in terms of only one variable, θ. In other words, to locate the particle on the helix, we only need to know the value of θ. We express the derivatives with respect to x,y,z in terms of the derivatives with respect to a, b, and θ, and since a and b are constants for the helix, we afterwards leave out all derivatives $\partial^n/\partial a^n$, $\partial^n/\partial b^n$ from the Hamiltonian, that is, we can do the following:

$$\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2 \Rightarrow (a^2+b^2)^{-1}\,\partial^2/\partial\theta^2 \text{ for } a \text{ and } b \text{ are constants}$$

Thus, in terms of θ, the Schrödinger equation to be solved is
(write the equation explicitly in terms of a, b, and θ):

Examine the above Schrödinger equation for this system, and figure out what kind of function will satisfy this equation. Remember that this system is similar in some way to the particle on a line along the x axis from 0 to L, except that here the line is wound around the outside surface of a right circular cylinder.

Try $\Psi(\theta)$ of the form: $A\sin(k\theta) + B\cos(k\theta)$

Substitute it into the Schrödinger equation and establish whether it can satisfy the equation.

What are the conditions that a function describing the state of this physical system (the single particle of mass M on the helix) has to meet in order to be an acceptable description? Hint: The particle is not allowed to exist beyond either end of the helix.

In general	Explicitly, for this system*

*That is, apply each of the requirements of acceptable state functions in mathematical terms specific to this system (in terms of the constants a, b, t, and the variable θ).

Calculate the energy eigenvalues of this system in terms of the constants a, b, t

Specify the conditions that must be satisfied by the quantities appearing in your expression for the energy eigenvalue.

Normalize the function that satisfies the above conditions:

Summarize: Explicitly write the 3 lowest energy eigenvalues and corresponding normalized eigenfunctions below:

quantum number	Energy eigenvalue	Eigenfunction

In this coordinate system, the z component of linear momentum is

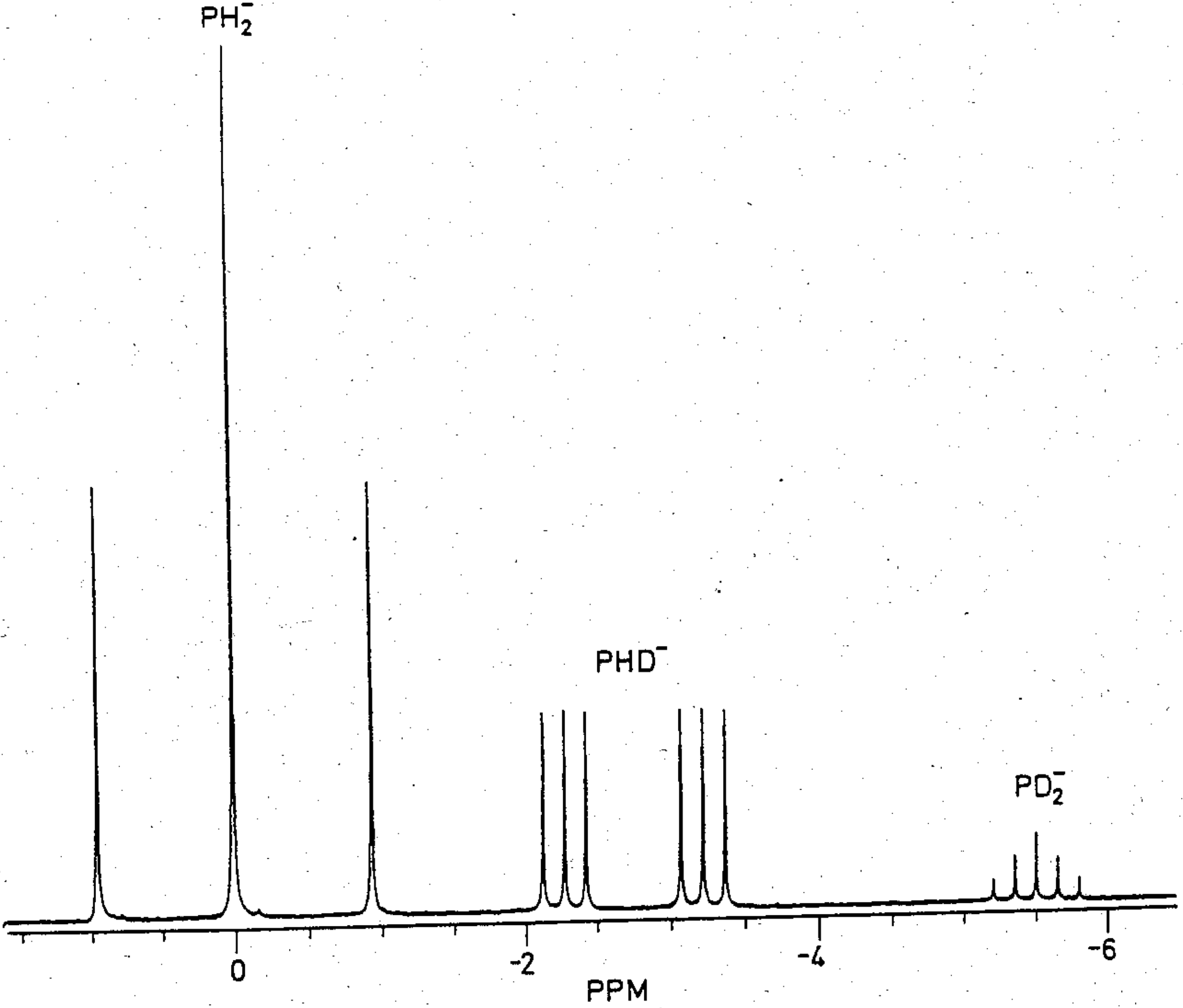
$$(p_z)_{op} = (\hbar/i)\, b\, (a^2+b^2)^{-1}\, \partial/\partial\theta$$

For the system of a particle on a helix, determine whether $(p_z)_{op}$ commutes with $\mathcal{H}$

What are the constraints, if any, on simultaneously measuring the energy and the z component of linear momentum for this system? Explain.

Calculate the expected average value of the outcomes of measurements of p_z on this system in its lowest energy state.

2. In field-free space the states having different z components of spin angular momentum are degenerate in energy. When placed in a magnetic field along the z direction, the formerly degenerate states become separated in energy on the order of several hundred MHz.
The ^{13}C NMR spectrum of $CDCl_3$ shows 3 equally spaced peaks of equal intensity. On the other hand, the NMR spectrum of the ^{31}P nucleus in a solution containing PH_2^-, PHD^-, and PD_2^- ions is shown below:
Nuclear spins are I = ½ for H, 1 for D, ½ for ^{31}P, ½ for ^{13}C



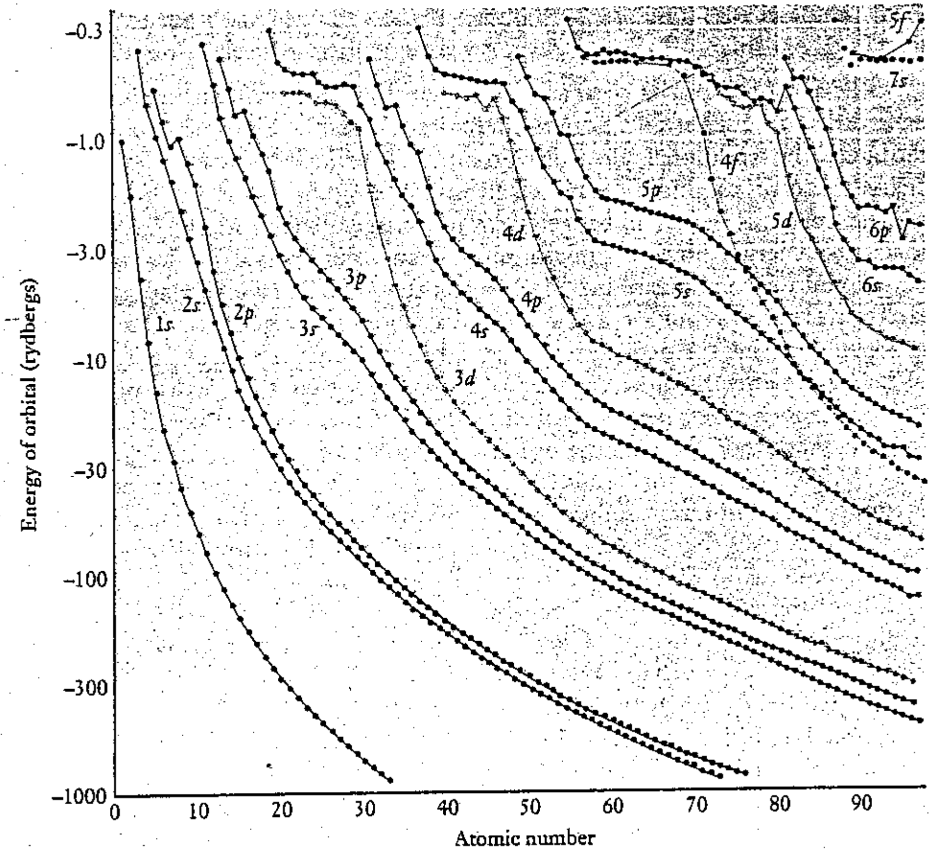
Using angular momentum properties and separation of variables, devise a concrete explanation of the observed intensities in the transitions of ^{31}P in the solution.

The PH_2^- intensities are 1:2:1

The PHD^- intensities are 1:1:1 and 1:1:1

The PD_2^- intensities are 1:2:3:2:1

3. The orbital energies of the first 97 elements, based on photoelectron spectroscopy experiments, are shown below from a Freshman chemistry textbook (Oxtoby, Gillis and Nachtrieb): Note the logarithmic energy scale. One rydberg is 13.6057 eV.



You have seen the photoelectron spectrum of Ar in Problem Set 11 and calculated the expected peaks. Pick element 10 (Ne) from this figure. Write down the electronic configuration of the ion that is produced for each of the **3** peaks that are observed for Ne:

label	Electronic configuration

Using Slater's approximation, calculate the energy of the most energetic peak in the photoelectron spectrum of Ne. Compare your answer with the value in the figure.

4. Write down the electronic configurations for the Li, N, and F atoms.

	# e	electronic configuration
Li		
N		
F		

Assuming that the ordering of the orbital energies for these molecules are the same, write down the electronic configurations expected for the Li_2, N_2 and F_2 diatomic molecules.

	# e	electronic configuration
Li_2		
N_2		
F_2		

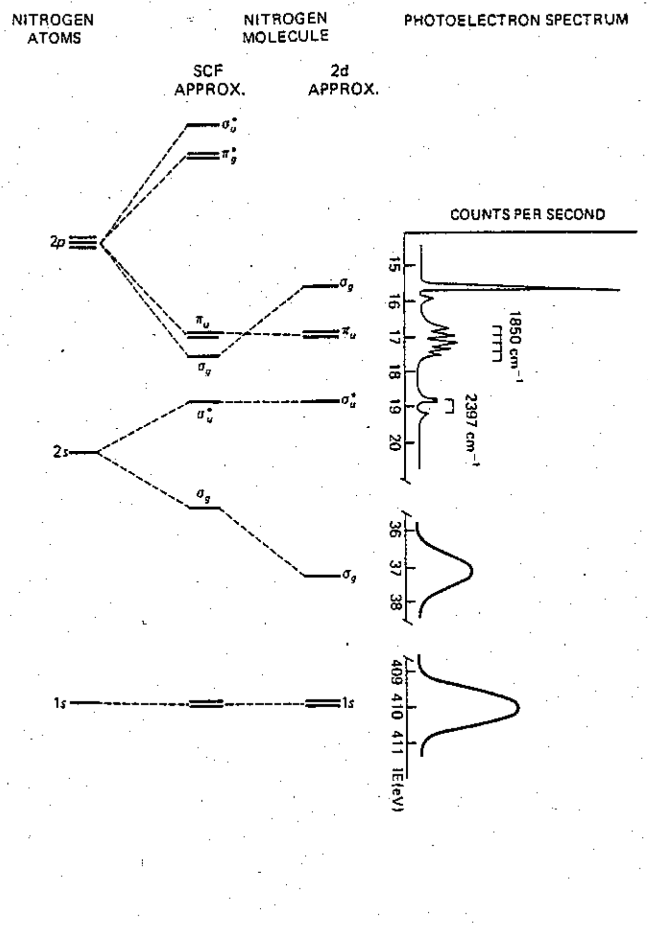
The Pauli exclusion principle states that the total wavefunction of an atom or molecule has to be antisymmetric with respect to interchange of any two indistinguishable fermions (particles having half-integer spin) and symmetric with respect to interchange of any two indistinguishable bosons (particles with integer spins). The spins of the most abundant isotopes in the above molecules are: I=1/2 for ^{19}F, I = 1 for ^{14}N, and I=3/2 for ^{7}Li nuclei. Supposing someone took the spectra of the above molecules and did not identify which molecular species the Raman spectra belonged to, is it possible to determine whether or not the molecules are homonuclear diatomics rather than heteronuclear diatomics, if you were shown the Raman spectra ($v' \leftarrow v''$: $1 \leftarrow 0$, for example) of the molecules without identification? Explain.

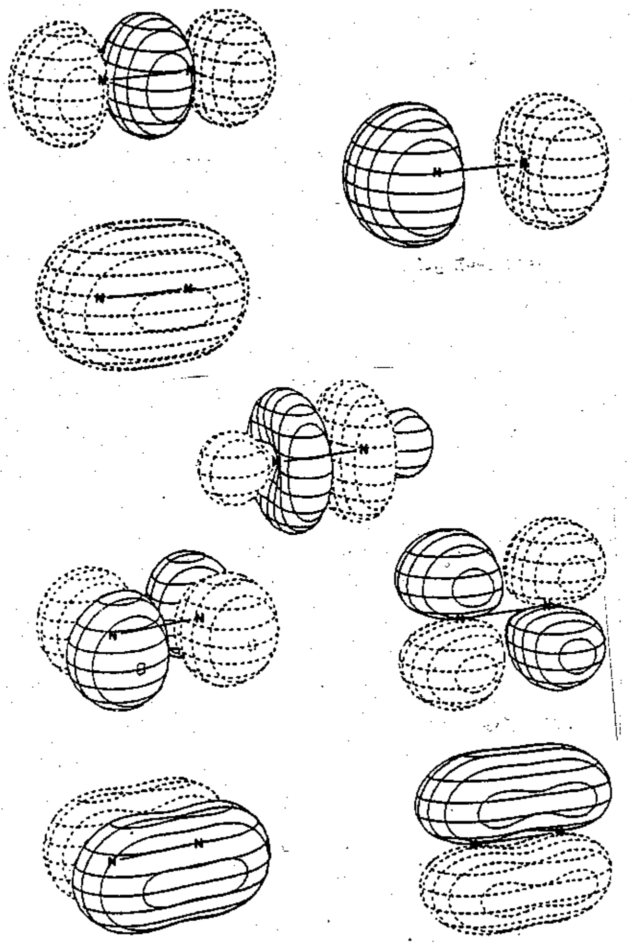
5. With what you have learned in Chemistry 344, it is now possible for you to derive or explain from first principles some facts you had learned in earlier chemistry classes. For each of the following which you would have learned in Chemistry 112, provide a quantitative explanation that is based on quantum mechanics, using mathematical equations as needed, starting from first principles.

Within a group in the Periodic Table, bond lengths in diatomic molecules usually increase with increasing atomic number Z. Thus, bond lengths increase in the series F_2 to Cl_2 to Br_2 to I_2.	
The tendency of an atom to donate or accept electrons in a chemical bond is indicated by the value of the electronegativity, which in the Mulliken definition is proportional to $(IE_1+EA)/2$. The electronegativity of F is greater than that of O.	
As orbitals are filled in order of increasing energies, in going from Ar to K the 4s orbital is filled first, before the 3d. On the other hand, Sc upon ionization to produce Sc^+ ion, loses the electron from the 4s rather than the 3d.	
Excited lithium atoms emit light strongly at a wavelength of 671 nm. This emission predominates when Li atoms are excited in a flame.	

7. Spectroscopy provides a means by which we identify the compounds that we have made by organic or inorganic synthesis, provides a means by which we determine the composition of mixtures in quantitative analytical chemistry, provides a means by which we identify interstellar matter. That each molecule has a distinct fingerprint absorption/emission spectrum in each region of the electromagnetic spectrum comes about because of the following fundamental reason: Each molecule has a unique Hamiltonian which leads to a unique set of energy eigenfunctions and eigenvalues, between which set of energy states, transitions can be induced by light. The transitions that are "allowed" by the symmetry of the molecule and the symmetry of its eigenfunctions are the only ones that can be observed under absorption and emission. Demonstrate your understanding of the energy eigenfunctions and eigenvalues of a molecule by answering the following spectroscopy questions:

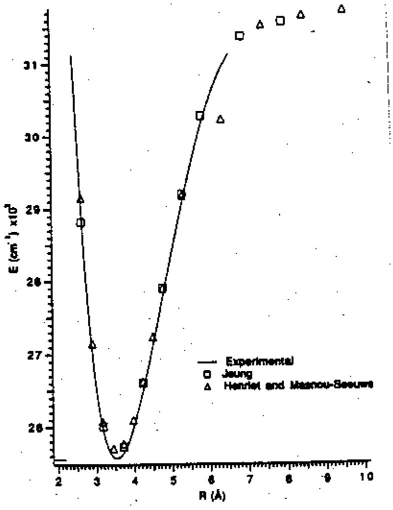
(a) Below we see the molecular orbital energies of N_2 molecule can be related to its photoelectron spectrum [in which one electron is kicked off by a photon, leaving an ion; various ionization energies are found, just as in atoms (problem 3 of this exam)]. The one-electron functions (molecular orbitals) for N_2 molecule are shown on the right, in randomized order! Draw a line connecting the orbitals on the right to the peaks in the spectrum on the left:



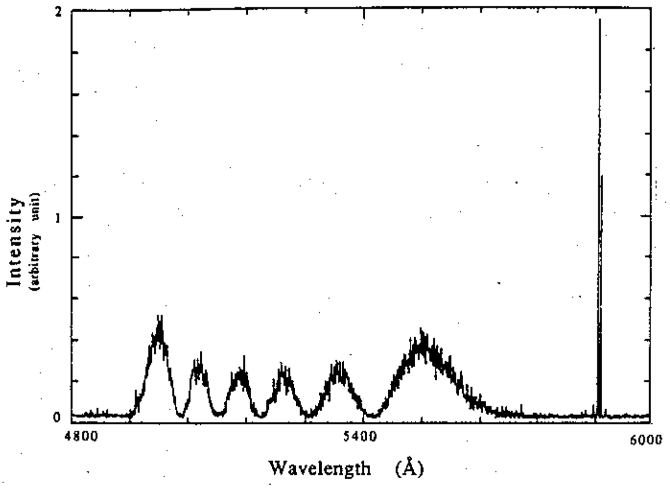


(b) The ground electronic configuration of Na_2 molecule is $(1\sigma_g)^2(1\sigma_u^*)^2(2\sigma_g)^2(2\sigma_u^*)^2(1\pi_g)^4(1\pi_u^*)^4(3\sigma_g)^2\,(4\sigma_g(3s))^2$. The excited electronic configuration $(1\sigma_g)^2(1\sigma_u^*)^2(2\sigma_g)^2(2\sigma_u^*)^2(1\pi_g)^4(1\pi_u^*)^4(3\sigma_g)^2\,(4\sigma_g(3s))^1(5\sigma_g(4s))^1$ gives a bound state $2\,^3\Sigma_g^+$, as can be seen from the plot of the U(R). The electronic transitions from the bound state of Na_2 molecule $2\,^3\Sigma_g^+$ to the free (that means, the molecule dissociates into free Na atoms after it gets there) a $^3\Sigma_u^+$ state of Na_2 is shown below. A particular vibrational state V′ of the excited $2\,^3\Sigma_g^+$ state was prepared by a pump laser and the emitted light from that prepared state to the lower free $a^3\Sigma_u^+$ (″) state was collected. Identify the V′ and draw the vibrational level and vibrational eigenfunction on the U(R) plot below.

U(R) of the excited $2\,^3\Sigma_g^+$ state



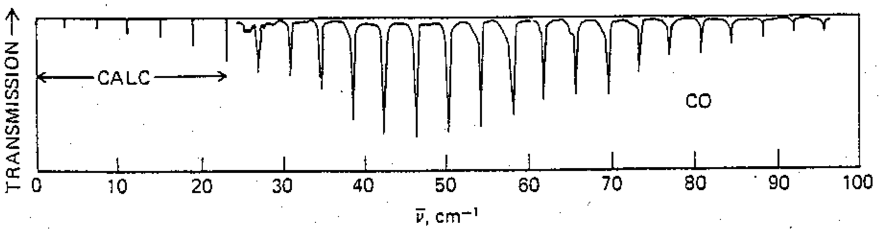
Spectrum bound $2\,^3\Sigma_g^+ \rightarrow$ free a $^3\Sigma_u^+$

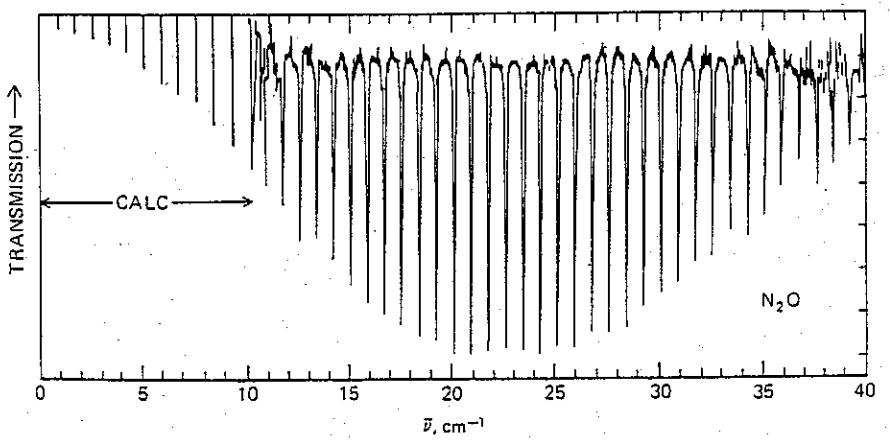


Identify electronic configurations of the two Na atoms that the above U(R) plot would approach if extrapolated well beyond 10 Å. Hint: Look at the molecular electronic configuration.

The dissociative $a^3\Sigma_u^+$ state of Na_2 gives rise to one excited and one ground state Na atom. When the excited Na atom gives up its excitation, it produces the characteristic double yellow D lines that one sees in a flame test for Na in elemental analysis. These two yellow lines are seen in the spectrum at the right hand side at wavelength 5890 and 5896 Å with one peak more intense than the other. Explain why the longer wavelength peak of the yellow doublet is less intense than the shorter wavelength peak in the atomic emission spectrum of excited Na atom. Hint: Consider the electronic configurations of the excited Na atom and the ground electronic state Na atom and remember that angular momentum vectors add.

(c) The microwave spectra of CO molecule and NNO molecules are shown below:





Which specific spectroscopic constants can be obtained from each of these spectra ()? Determine the equation that provides the frequency of each peak (the calculated peaks are shown in those regions where the spectrometer was not operational). You may neglect D_e which is obviously very small in these cases.

What is the frequency spacing (between adjacent peaks) equal to?

Why is the frequency spacing so much larger in CO than in NNO?

8. Assume that you have solved the hydrogen-like atom problem and know all the eigenfunctions and eigenvalues in terms of the number of positive charges in the nucleus.

(a) What is the hamiltonian for the motion of nuclei and electrons in the He atom?

(b) After the motion of the center of mass of the atom has been separated out, what is the hamiltonian for the electronic motion in the He atom?

(c) If we simply neglect the electron-electron repulsion in the above hamiltonian, what would the Schrödinger equation for the electronic motion in the He atom be?

(d) What are the eigenvalues and eigenfunctions of the above Schrödinger equation?

(e) If instead of total neglect of electron-electron repulsion, we use Slater's approximation, what would be the effective Hamiltonian for the He atom?

(f) If we use Slater's approximation for the He atom, what would be the electronic configuration of the ground state? Calculate the ground state energy of the He atom under this approximation.

(g) If we use Slater's approximation for the He atom, what would be the electronic configuration of the first excited state?

(h) If we use Slater's approximation for the He atom, what would be the energy difference between the first excited state and the ground state? Calculate your answer in terms of ($e^2/2a_0$) which is 13.6 eV.

9. In each of the following cases, state the particular principle (don't just name it), or the definition that has been applied in order to arrive at your answer.

The set of functions $\{\Psi_1(\phi), \Psi_2(\phi), \Psi_3(\phi), \Psi_4(\phi), \ldots\}$ are eigenfunctions of the operator $(\hbar/i)\partial/\partial\phi$ where ϕ is an angle that ranges from 0 to 2π and the particle is restricted to the circle $x^2 + y^2 = R^2$ in the xy plane and $x = R\cos\phi$ and $y = R\sin\phi$.

(a) What is the general form of the functions $\{\Psi_1, \Psi_2, \Psi_3, \Psi_4, \ldots\}$? Note: these subscripts are merely running labels to distinguish one function from another in the complete list, not necessarily parameters or quantum numbers. You will choose the identity of the functions and order the functions in your own way, according to your own choices below.

Answer	Statement of Principle

(b) Normalize each function

Answer	Statement of Principle

(c) What are the restrictions on the parameters that are involved in each of the eigenfunctions?

Answer	Statement of Principle

(d) Now that you have identified the functions and the parameters involved in them, what are the eigenvalues of the operator $(\hbar/i)\partial/\partial\phi$ corresponding to the first four eigenfunctions Ψ_1, Ψ_2, Ψ_3, Ψ_4 in the list? Write the function down and then the eigenvalue for it.

Answer	Statement of Principle
Ψ_1 : Ψ_2 : Ψ_3 : Ψ_4 :	

(e) If the physical system is found in the state described by the function Ψ_2 (whose identity is as you have specified it above) what would be the outcomes of four measurements of the property whose operator is $(\hbar/i)\partial/\partial\phi$?

Answer	Statement of Principle
Ψ_2 : (1) (2) (3) (4)	

(f) If the physical system is found in the state described by function Ψ_2, as you have specified it above, what would be the outcomes of any four measurements of the property whose operator is $-(\hbar^2/2\mu R^2)\partial^2/\partial\phi^2$?

Answer	Statement of Principle
Ψ_2 : (1) (2) (3) (4)	

(g) If the physical system is found in the state described by function $\Psi = (1/\sqrt{5})(2\Psi_2 + \Psi_4)$, as you have specified these functions above, determine the average value of the measurements of the observable whose operator is $(\hbar/i)\partial/\partial\phi$? Write down a typical set of measurement outcomes, as they would appear in your lab notbook.

Answer	Statement of Principle
Ψ:	

(g) Determine whether or not it is theoretically possible to find for this physical system that both the observables described in (e) and (f) are measured with zero standard deviation for both observables at the same time.

Answer	Statement of Principle

List of possibly useful integrals that will be provided with each exam

$\int \sin(ax)dx = -(1/a)\cos(ax)$
$\int \cos(ax)dx = (1/a)\sin(ax)$
$\int \sin^2(ax)dx = (½)x - (1/4a)\sin(2ax)$
$\int \sin^4(ax)dx = 3x/8 - (1/4a)\sin(2ax) + (1/32a)\sin(4ax)$
$\int \cos^2(ax)dx = (½)x + (1/4a)\sin(2ax)$
$\int \cos^4(ax)dx = 3x/8 + (1/4a)\sin(2ax) + (1/32a)\sin(4ax)$
$\int \sin(ax)\sin(bx)dx = [1/2(a-b)]\sin[(a-b)x)] - [1/2(a+b)]\sin[(a+b)x)]$, $a^2 \neq b^2$
$\int \cos(ax)\cos(bx)dx = [1/2(a-b)]\sin[(a-b)x)] + [1/2(a+b)]\sin[(a+b)x)]$, $a^2 \neq b^2$
$\int x \sin(ax)dx = (1/a^2)\sin(ax) - (x/a)\cos(ax)$
$\int x \cos(ax)dx = (1/a^2)\cos(ax) + (x/a)\sin(ax)$
$\int x^2 \cos(ax)dx = [(a^2x^2 - 2)/a^3]\sin(ax) + 2x\cos(ax)/a^2$
$\int x^2 \sin(ax)dx = -[(a^2x^2 - 2)/a^3]\cos(ax) + 2x\sin(ax)/a^2$
$\int x \sin^2(ax)dx = x^2/4 - x\sin(2ax)/4a - \cos(2ax)/8a^2$
$\int x^2 \sin^2(ax)dx = x^3/6 - [x^2/4a - 1/8a^3]\sin(2ax) - x\cos(2ax)/4a^2$
$\int x \cos^2(ax)dx = x^2/4 + x\sin(2ax)/4a + \cos(2ax)/8a^2$
$\int x^2 \cos^2(ax)dx = x^3/6 + [x^2/4a - 1/8a^3]\sin(2ax) + x\cos(2ax)/4a^2$
$\int x \exp(ax)dx = \exp(ax)\ (ax-1)/a^2$
$\int x \exp(-ax)dx = \exp(-ax)\ (-ax-1)/a^2$
$\int x^2 \exp(ax)dx = \exp(ax)\ [x^2/a - 2x/a^2 + 2/a^3]$
$\int x^m \exp(ax)dx = \exp(ax) \sum_{r=0 \text{ to } m} (-1)^r\ m!x^{m-r}/(m-r)!a^{r+1}$
$\int dx/x(a+bx) = -(1/a) \ln[(a+bx)/x]$

$\int_0^\infty x^n \exp(-ax)dx = n!/a^{n+1}$ $a > 0$, n positive integer
$\int_0^\infty x^2 \exp(-ax^2)dx = (1/4a)(\pi/a)^{½}$ $a > 0$
$\int_0^\infty x^{2n} \exp(-ax^2)dx = (1\cdot3\cdot5\cdot\ldots\cdot(2n-1)/(2^{n+1}a^n)(\pi/a)^{½}$ $a > 0$
$\int_0^\infty x^{2n+1} \exp(-ax^2)dx = n!/2a^{n+1}$ $a > 0$, n positive integer
$\int_0^\infty \exp(-a^2x^2)dx = (1/2a)\ (\pi)^{½}$ $a > 0$
$\int_0^\infty \exp(-ax)\cos(bx)dx = a/(a^2+b^2)$ $a > 0$
$\int_0^\infty \exp(-ax)\sin(bx)dx = b/(a^2+b^2)$ $a > 0$
$\int_0^\infty x \exp(-ax)\sin(bx)dx = 2ab/(a^2+b^2)^2$ $a > 0$
$\int_0^\infty x \exp(-ax)\cos(bx)dx = (a^2-b^2)/(a^2+b^2)^2$ $a > 0$
$\int_0^\infty \exp(-a^2x^2)\cos(bx)dx = [(\pi)^{½}/2a]\cdot\exp[-b^2/4a^2]$ $ab \neq 0$

Some useful identities:
$\sin(2x) = 2\sin x \cos x$ $\cos(2x) = \cos^2 x - \sin^2 x = 2\cos^2 x - 1$
$e^{ix} = \cos x + i \sin x$; $e^{-ix} = \cos x - i \sin x$; from which, $\cos x = ½ \{e^{ix} + e^{-ix}\}$

Slater's rules:

The effective charge seen by the $i\underline{th}$ electron whose quantum numbers are $n\ \ell$ in an atom whose atomic number is Z is given by

$$(Z_{\text{eff}})_i = Z - s_{n\ell}$$

Slater provides $s_{n\ell}$ as follows:

1. For i having $n\ \ell = 1s$

    $s_{1s} = 0.30k_{\text{same}}$

    where

    $k_{\text{same}} =$ number of other electrons in the same 1s shell

2. For i having $n > 1$ and $\ell = 0$ or 1

    $s_{n\ell} = 0.35k_{\text{same}} + 0.85k_{\text{in}} + 1.00k_{\text{inner}}$

    where

    $k_{\text{same}} =$ number of other electrons in the same shell as the screened electron of interest

    $k_{\text{in}} =$ number of electrons in the shell with principal quantum number n-1

    $k_{\text{inner}} =$ number of electrons in the shell with principal quantum number n-2

3. For the $i\underline{th}$ electron having quantum numbers $n\ \ell = 3d$

    $s_{3d} = 0.35k_{3d} + 1.00k_{\text{in}}$

    where

    $k_{3d} =$ number of other electrons in the same 3d shell

    $k_{\text{in}} =$ number of electrons with $n \leq 3$ and $\ell < 2$

For the purposes of Slater's rules, the "subshells" are taken to be in the order

innermost 1s (2s,2p) (3s,3p) 3d (4s,4p) outermost

ADDITIONAL INFORMATION

$a_0 = (\hbar^2/m_e e^2)$ the "Bohr radius", 0.529177×10^{-10} m

$(e^2/2a_0) = 13.6057$ eV one rydberg, a unit of energy = (1/2) hartree

c = frequency•wavelength = 2.997924×10^{10} cm sec^{-1} the speed of light

1 eV = 8065.6 cm^{-1}

$$\mathcal{L}^2 = -\hbar^2\{ (1/\sin\theta)(\partial/\partial\theta)\sin\theta\ \partial/\partial\theta \quad + (1/\sin^2\theta)\partial^2/\partial\phi^2\}$$

$$\mathcal{H} = -(\hbar^2/2M)\{(1/r)\partial^2/\partial r^2\ r\} \\ -(\hbar^2/2Mr^2)\{ (1/\sin\theta)(\partial/\partial\theta)\sin\theta\ \partial/\partial\theta \quad + (1/\sin^2\theta)\partial^2/\partial\phi^2\} + V(r)$$

$$E = U_\alpha(R_e) + (v+\tfrac{1}{2})\nu_e - x_e\nu_e\,(v+\tfrac{1}{2})^2 + y_e\nu_e\,(v+\tfrac{1}{2})^3 + B_eJ(J+1) - D_e[J(J+1)]^2 - \alpha_e(v+\tfrac{1}{2})J(J+1) + Y_{00}$$

where all spectroscopic quantities are expressed in energy units (or the corresponding frequency or wavenumbers). In energy units, the following are positive quantities:

$B_e \equiv \hbar^2 / 2\mu\, R_e^2$ $\qquad$ B_e rotational constant

$$h x_e\nu_e \equiv \tfrac{1}{4}\, B_e^2/(h\nu_e)^2 \cdot \{ (^{10}/_3)B_e[U'''(R_e)R_e^3]^2/(h\nu_e)^2 - U^{iv}(R_e)R_e^4 \}$$

$x_e\nu_e$ anharmonicity constant

$D_e \equiv 4\, B_e^3/(h\nu_e)^2$

D_e centrifugal distortion constant

$$\alpha_e \equiv -\,2\, B_e^2/h\nu_e \cdot \{3 + 2\, B_e[U'''(R_e)R_e^3]^2/(h\nu_e)^2\}$$

α_e vibrational rotational coupling constant

$$Y_{00} \equiv B_e^2/16(h\nu_e)^2 \cdot \{ U^{iv}(R_e)R_e^4 - (^{14}/_9)B_e[U'''(R_e)R_e^3]^2/(h\nu_e)^2 \}$$

$h\nu_e \equiv (h/2\pi)[\,U''(R_e)/\mu\,]^{1/2}$ $\qquad$ ν_e harmonic frequency

μ reduced mass $\quad 1/\mu = 1/m_A + 1/m_B$

R_e equilibrium bond length

Rotational constant for the v<u>th</u> vibrational state is B_v

$B_v = B_e - \alpha_e\,(v+\tfrac{1}{2})$

Y_{00} same anharmonic correction to <u>every</u> vibrational level

Since Y_{00} is a constant for the electronic state, it is usually put together with $U(R_e)$.

PERIODIC TABLE OF THE ELEMENTS

☐ Metals

☐ Semimetals

☐ Nonmetals

Transition elements

I	II											III	IV	V	VI	VII	VIII
1 **H** 1.0079																	2 **He** 4.0026
3 **Li** 6.941	4 **Be** 9.0122											5 **B** 10.811	6 **C** 12.011	7 **N** 14.007	8 **O** 15.999	9 **F** 18.998	10 **Ne** 20.180
11 **Na** 22.990	12 **Mg** 24.305											13 **Al** 26.982	14 **Si** 28.086	15 **P** 30.974	16 **S** 32.066	17 **Cl** 35.453	18 **Ar** 39.948
19 **K** 39.098	20 **Ca** 40.078	21 **Sc** 44.956	22 **Ti** 47.87	23 **V** 50.942	24 **Cr** 51.996	25 **Mn** 54.938	26 **Fe** 55.845	27 **Co** 58.933	28 **Ni** 58.693	29 **Cu** 63.546	30 **Zn** 65.39	31 **Ga** 69.723	32 **Ge** 72.61	33 **As** 74.922	34 **Se** 78.96	35 **Br** 79.904	36 **Kr** 83.80
37 **Rb** 85.468	38 **Sr** 87.62	39 **Y** 88.906	40 **Zr** 91.224	41 **Nb** 92.906	42 **Mo** 95.94	43 **Tc** (98)	44 **Ru** 101.07	45 **Rh** 102.91	46 **Pd** 106.42	47 **Ag** 107.87	48 **Cd** 112.41	49 **In** 114.82	50 **Sn** 118.71	51 **Sb** 121.76	52 **Te** 127.60	53 **I** 126.90	54 **Xe** 131.29
55 **Cs** 132.91	56 **Ba** 137.33	71 **Lu** 174.97	72 **Hf** 178.49	73 **Ta** 180.95	74 **W** 183.84	75 **Re** 186.21	76 **Os** 190.23	77 **Ir** 192.22	78 **Pt** 195.08	79 **Au** 196.97	80 **Hg** 200.59	81 **Tl** 204.38	82 **Pb** 207.2	83 **Bi** 208.98	84 **Po** (209)	85 **At** (210)	86 **Rn** (222)
87 **Fr** (223)	88 **Ra** (226)	103 **Lr** (262)	104 **Rf** (261)	105 **Db** (262)	106 **Sg** (263)	107 **Bh** (262)	108 **Hs** (265)	109 **Mt** (268)	110 **Uun** (269)	111 **Uuu** (272)	112 **Uub** (277)						

Lanthanide series

57 **La** 138.91	58 **Ce** 140.12	59 **Pr** 140.91	60 **Nd** 144.24	61 **Pm** (145)	62 **Sm** 150.36	63 **Eu** 151.96	64 **Gd** 157.25	65 **Tb** 158.93	66 **Dy** 162.50	67 **Ho** 164.93	68 **Er** 167.26	69 **Tm** 168.93	70 **Yb** 173.04

Actinide series

89 **Ac** (227)	90 **Th** 232.04	91 **Pa** 231.04	92 **U** 238.03	93 **Np** (237)	94 **Pu** (244)	95 **Am** (241)	96 **Cm** (247)	97 **Bk** (247)	98 **Cf** (251)	99 **Es** (252)	100 **Fm** (257)	101 **Md** (258)	102 **No** (259)