CHEM442-001
College of Charleston
Spring 1999
Exam I

1(15). For a nitrogen molecule moving at a speed of 333 m s^{-1}, determine the

A) deBroglie wavelength

B) frequency corresponding to the deBroglie wavelength

C) the wavenumber (in cm^{-1}) corresponding to the deBroglie wavelength

2(18). Identify the term corresponding to each of the following topics discussed in class:

(example: $\langle o \rangle = \int \psi^* \hat{o} \psi \, d\tau$	$\langle o \rangle$ is an <u>expectation value</u>)
A) $\int \psi^* \psi \, d\tau = 1$	ψ is ________________
B) $\int \psi_2^* \psi_1 \, d\tau = 0$	ψ_2 and ψ_1 are ________________
C) $\psi(x,y,z) = \psi(x)\psi(y)\psi(z)$	________________ method
D) E(trial wave function) $\geq E$(real value)	postulate of ______________ method
E) ψ for an e^- must be antisymmetric	________________ principle
F) $(\Delta x)(\Delta p_x) \geq \hbar/2$	________________ principle

3(10). Write out the complete internal Hamiltonian operator for atomic Be. (Do not use summations–write out all the terms.)

Write the (Slater) determinant expressing an antisymmetric trial wave function for atomic Be using hydrogen atom wave functions. (Do not expand the determinant.)

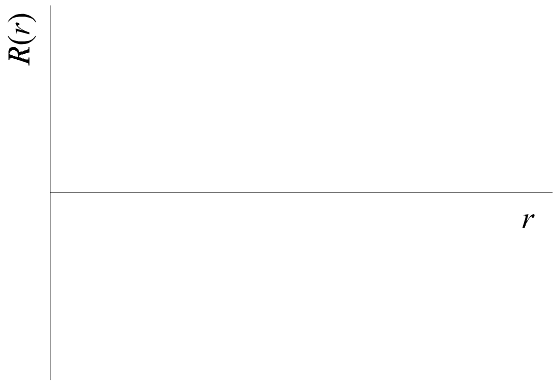
4(15). A trial wave function is obtained by the linear combination of ψ_1 and ψ_2

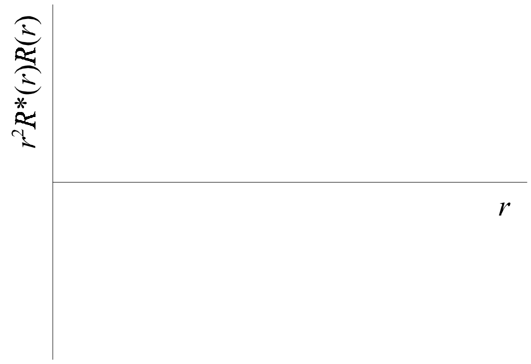
$$\phi = A(\psi_1 + \psi_2)$$

where $\int \psi_1^* \psi_1 \, d\tau = \int \psi_2^* \psi_2 \, d\tau = 1$ and $\int \psi_2^* \psi_1 \, d\tau = \int \psi_1^* \psi_2 \, d\tau = 0$. Determine the normalization constant A.

5(25). Determine the associated Laguerre polynomial for a 2s subshell and write the normalized radial wave function. (The answer may be left in terms of the variable ρ.)

Make a sketch of $R(r)$ and of $r^2 R^*(r) R(r)$.





6(10). Using the Bohr theory for atomic hydrogen, calculate $\Delta\epsilon$ for an electronic transition between $n_2 = 3$ and $n_1 = 1$.

What is the ratio of atoms in this excited level to that in the ground state at $T = 100$ K?

7(7). Name the three principles/rules that are used when writing the ground state atomic electron configurations of polyelectronic atoms.