Chemistry 651

Problem set 1

Due: 18 April 2006

1. Atomic units. Convert the Hamiltonian for the hydrogen atom to atomic units. What is the unit of length, energy and time?

2. Derive the Jacobian $J(r, \theta)$ for the transformation of a volume element from Cartesian to spherical coordinates, viz.,
$$dxdydz = J(r, \theta)d\theta d\phi dr \tag{1}$$

3. See Section 7.4 of Lowe's text and complete the calculation of the polarizability α for a H-atom in an electric field. So, calculate

$$\langle \mu_z \rangle = \int d1 \psi^*(r)(ez)\psi(r) \equiv \alpha E_z \tag{2}$$

using the variationally derived wave function in a field of arbitrary strength. Select the wavefunction that correlates with ψ_{1s} in the limit of zero electric field and use that wavefunction to compute the indicated expectation value.