

## Chemistry 651

### Problem set 2

Due: 2 May 2006

1. Matrix methods. Consider the  $3 \times 3$  tridiagonal Hamiltonian matrix  $H_{ij}$

$$H_{ij} = \alpha\delta_{ij} + \beta\delta_{i,j\pm 1} \quad (1)$$

Diagonalize H and derive its eigenvalues. Using the eigenvalues, derive the three eigenvectors. Demonstrate that the eigenvectors are orthonormal and arrange them in a matrix S. Use the S matrix to prove

$$S^{-1}HS = E \quad (2)$$

where E is the diagonal matrix with eigenvalues along the diagonal.

2. Perturbed particle in a box. The particle in a box of length L has wavefunctions

$$\psi_n(x) = \sqrt{2/L} \sin(n\pi x/L) \quad (3)$$

Suppose we apply a field linear in displacement,

$$H^{(1)} = u(x/L) \quad (4)$$

Calculate the energy to first and second order in  $u$  and the wavefunction to first order in  $u$ .

3. Using the quantum mechanical angular momentum operator L,

$$L = -i\hbar r \times \nabla_r \quad (5)$$

prove that

$$[L_x, L_y] = i\hbar L_z \quad (6)$$

4. more to come ...