Fall 2011   CHEM 760: Introductory Quantum Chemistry

Homework 6   Due: Nov 3 in class

1. Determine the values of x for which the following equation will have a nontrivial solution

   $xc_1 + c_2 + c_4 = 0$

   $c_1 + xc_2 + c_3 = 0$

   $c_2 + xc_3 + c_4 = 0$

   $c_1 + c_3 + xc_4 = 0$

2. Show that

   $$\begin{vmatrix} cos\theta & -sin\theta & 0 \\ sin\theta & cos\theta & 0 \\ 0 & 0 & 1 \end{vmatrix} = 1$$

3. Solve the following set of equations using Cramer's rule (textbook p220)

   $x + 2y + 3z = -5$

   $-x - 3y + z = -14$

   $2x + y + z = 1$

4. Given the matrices

   $$A = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad B = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad C = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

   Show that $AB - BA = iC\ and\ A^2 + B^2 + C^2 = 2I$, where I is a unit matrix.

5. Determine the eigenvalues and eigenvectors of $A = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}$

6. Use the variational method to calculate the ground-state energy of a particle constrained to move within the region $0 \le x \le a$ in a potential given by

   $$V(x) = \{ \begin{matrix} V_0 x & 0 \le x \le \frac{a}{2} \\ V_0(a - x) & \frac{a}{2} \le x \le a \end{matrix}$$

   As a trial function, use a linear combination of the first two particle-in-a-box wave functions:

   $$\phi(x) = c_1(\frac{2}{a})^{1/2} \sin\frac{\pi x}{a} + c_2(\frac{2}{a})^{1/2} sin\frac{2\pi x}{a}$$

7. Calculate the ground state of a hydrogen atom using a trial function of the form $e^{-\alpha r}$. Why does the result turn out to be so good?

8. Suppose we were to use a trial function of the form $\phi = c_1 e^{-\alpha r} + c_2 e^{-\beta r^2}$ to carry out a variational calculation for the ground-state energy of a hydrogen atom. Can you guess without doing any calculation what c_1, c_2, α, and $E_{\min}$ will be? What about a trial function of the form $\phi = \sum_{k=1}^{5} c_k\, e^{-\alpha_k r - \beta_k r^2}$?