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
\[ x_1 + c_2 + c_4 = 0 \\
 c_1 + x_2 + c_3 = 0 \\
 c_2 + x_3 + c_4 = 0 \\
 c_1 + c_3 + x_4 = 0 \]

2. Show that
\[
\begin{bmatrix}
  \cos \theta & -\sin \theta & 0 \\
  \sin \theta & \cos \theta & 0 \\
  0 & 0 & 1 
\end{bmatrix} = 1
\]

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
\[
A = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\
B = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \\
C = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}
\]
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 \( 0 \leq x \leq a \) in a potential given by
\[
V(x) = \begin{cases} 
V_0 x & 0 \leq x \leq \frac{a}{2} \\
V_0(a-x) & \frac{a}{2} \leq x \leq a 
\end{cases}
\]
As a trial function, use a linear combination of the first two particle-in-a-box wave functions:
\[
\phi(x) = c_1 \left(\frac{2}{a}\right)^{1/2} \sin \left(\frac{\pi x}{a}\right) + c_2 \left(\frac{2}{a}\right)^{1/2} \sin \left(2\frac{\pi x}{a}\right)
\]

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

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