5.74, Problem Set #0  
Spring 2009  
Not graded

These are some problems to make sure that you are up to speed on the basics of solving numerical problems.

1. **Numerically solving for eigenstates and eigenvalues of an arbitrary 1D potential.**
   Obtain the energy eigenvalues \( E_n \) and wavefunctions \( \psi_n(r) \) for the anharmonic Morse potential below. (Values of the parameters correspond to HF). Tabulate \( E_n \) for \( n = 0 \) to \( 5 \), and plot the corresponding \( \psi_n(r) \).

   \[
   V = D_e \left[ 1 - e^{-\alpha x} \right]^2
   \]

   Equilibrium bond energy: \( D_e = 6.091 \times 10^{-19} \) J

   Equilibrium bond length: \( r_0 = 9.109 \times 10^{-11} \) m \( x = r - r_0 \)

   Force constant: \( k = 1.039 \times 10^3 \) J m\(^{-2}\) \( \alpha = \sqrt{k/2D_e} \)

   (If you aren’t familiar with these problems, study the notes and worksheets on the Discrete Value Representation).

2. **Resonant driving of two level system.** If two states \( k \) and \( l \) are coupled with a sinusoidal potential, the differential equations that describe their probability amplitude are

   \[
   \dot{b}_k = \frac{-i}{2\hbar} b_k V_{kl} e^{i(\omega_{kl} - \omega)t}
   \]

   \[
   \dot{b}_l = \frac{-i}{2\hbar} b_k V_{lk} e^{-i(\omega_{kl} - \omega)t}
   \]

   Numerically solve for the probability of being in state \( k \) and \( l \) for times \( t = 0 \) to \( t = 1 \) ps given that the system is in state \( k \) at \( t = 0 \). You can take the coupling to be \( V_{kl}/\hbar c = 100 \text{ cm}^{-1} \). Compare the behavior for detuning from resonance of \( (\omega_{kl} - \omega)/2\pi c = 0 \text{ cm}^{-1} \) and 100 cm\(^{-1}\).

   (If you aren’t familiar with numerically solving differential equations, study your software’s implementation of the Runga-Kutta method).