5.74 Introductory Quantum Mechanics II Spring 2009

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## 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:  $D_e = 6.091 \times 10^{-19} \text{ J}$ Equilibrium bond length:  $r_0 = 9.109 \times 10^{-11} \text{ m}$   $x = r - r_0$ Force constant:  $k = 1.039 \times 10^3 \text{ J} \text{ m}^{-2}$   $\alpha = \sqrt{k/2D_e}$ 

(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

$$\dot{b}_{k} = \frac{-i}{2\hbar} b_{\ell} V_{k\ell} e^{i(\omega_{k\ell} - \omega)t}$$
$$\dot{b}_{\ell} = \frac{-i}{2\hbar} b_{k} V_{\ell k} e^{-i(\omega_{k\ell} - \omega)t}$$

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  $V_{\ell k} / hc = 100 cm^{-1}$ . Compare the behavior for detuning from resonance of  $(\omega_{k\ell} - \omega) / 2\pi c = 0 cm^{-1}$  and  $100 cm^{-1}$ .

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