PHYS 3142 Sping 2019
Computational Methods in Physics
Assignment 5
Due: 17th April 2019

Before you submit your assignment, do remember:

1. the due day
2. submit a report which contains your figures and results
3. make sure your code can run
4. do not upload a compressed file(e.g. rar, zip, ...)

Quantum oscillators

Consider the one-dimensional,time-independent Schrödinger equation in a harmonic (i.e., quadratic) potential $V(x) = V_0 x^2/a^2$, where V_0 and a are constants.

1. Write down the dimensionless version of the Schrödinger equation for this problem and convert it from a second-order equation to two first-order ones. Write a program using the 4th order Runge Kutta method to find the energies of the ground state and the first two excited states for these equations when m is the electron mass, $V_0 = 50\,\text{eV}$, and $a = 10^{-11}\,\text{m}$. Note that in theory the wavefunction goes all the way out to $x = \pm\infty$, but you can get good answers by using a large but finite interval. Try using $x = -10a$ to $+10a$, with the wavefunction $\psi = 0$ at both boundaries. (In effect, you are putting the harmonic oscillator in a box with impenetrable walls.) The wavefunction is real everywhere (only in one-dimensional system), so you don't need to use complex

variables, and you can use evenly spaced points for the solution. Hint: Please refer to the lecture note (Lec 14.pdf) about the secant method for solving eigen energies.

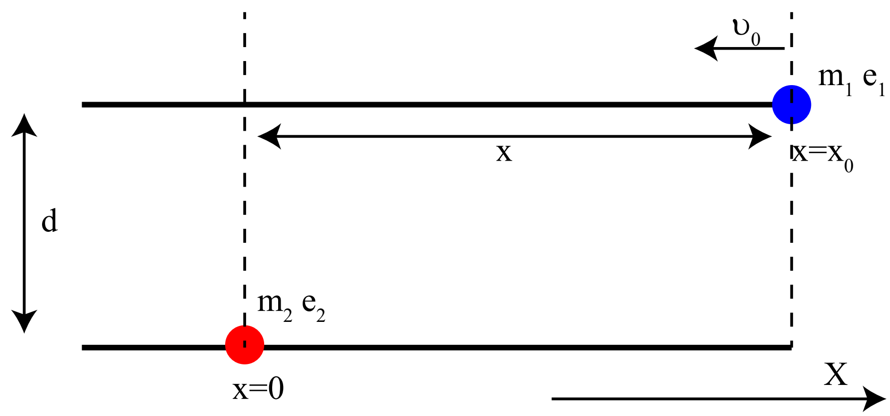
The quantum harmonic oscillator is known to have energy states that are equally spaced. Check that this is true, to the precision of your calculation, for your answers. (Hint: The ground state has energy in the range 100 to 200 eV.)

2. Now modify your program to calculate the same three energies for the anharmonic oscillator with $V(x) = V_0 x^4/a^4$, with the same parameter values.

Coulomb Drag

Consider two parallel wire with distance d. A negative charged object(m_1) is moving along the wire with initial velocity v_0. One positive charged object(m_2) is located on another wire with zero initial velocity and located at the original point($x = 0$). The initial distance between two objects(x), velocity(v_0), charges and(e_1,e_2) masses(m_1,m_2) are arbitrary. Relativity effect can be ignored.

1. Write down the equations of motion for these two objects for this problem and convert it from a second-order equation to two-first order ones. Write down a program using the time-reversal symmetric methods such as leapfrog or Verlet method to give the relations between time-velocities and time-distance of these two objects.(please use initial conditions: $m_1 = 1;\ m_2 = 1;\ e_1 = -1;\ e_2 = 1;\ d = 1;\ x = 100;\ v_0 = -5$)
2. Keep the original distance, masses and charges unchanged($m_1 = 1;\ m_2 = 1;\ e_1 = -1;\ e_2 = 1;\ d = 1;\ x = 100$), please plot the final velocity of m_2 with different v_0 ($v_0 \in (-10, 0)$). (here, you may need to enlarge the total time to find the stable final velocity of m_2, roughly should be $\delta v < 10^{-4}$). In the distance figure, we can always find that m_2 first move along positive direction and then move along negative direction. Please find the maxinum distance($D2_{max}$) of m_2 in the positive direction at different v_0 and plot this relation between v_0 and $D2_{max}$



υ0
m1 e1
x
x=x0
d
m2 e2
x=0
X