Homework 3

Due in class Monday, Feb. 14

From the text: 3-5, 3-30, 3-31, 3-35

1. Consider two ground state hydrogen atoms interacting via

$$V(r) = De^{-\alpha(r-r_0)}[e^{-\alpha(r-r_0)} - 2].$$

This is a Morse potential and only approximates the real H+H interaction for

$$D = 0.174$$
$$\alpha = 1.1$$
$$r_0 = 1.4.$$

All of these quantities are given in atomic units (*i.e.* $\hbar = e = m_e = 1$). Make sure all calculations below are accurate to at least 0.1%.

(a) Is this a short-range or long-range potential? Is its asymptotic behavior physical — that is, does it correctly reproduce the real asymptotic behavior expected for the H+H potential?

(b) Calculate the scattering angle $\Theta(s)$ for at least 10 different collision energies E in the range $0 \leq E \leq 1$ a.u. Make sure that you include large enough s to represent all of the scattering.

(c) For each of your $\Theta(s)$ in (b), calculate the differential scattering cross section $d\sigma/d\Omega$. Plot your results from (b) and (c) in some organized manner and discuss them.

(d) Pick values of E and s that give a/an

(i) Orbiting trajectory

(ii) Spiraling trajectory

(iii) Rainbow trajectory

(iv) Glory trajectory

(v) "Normal" repulsive trajectory (like you might see for a purely repulsive potential)

(vi) "Normal" attractive trajectory (like you might see for a purely attractive potential).

In each case, be sure to give the parameters that produce the given kind of trajectory and say how you identified/calculated these parameters. Identify each of these trajectories in your plots from (c). Plot the trajectories and discuss them. If a particular kind of trajectory doesn't exist, say so, and say why it doesn't (*i.e.* what condition cannot be satisfied).