

# Chemistry 5850 Summer 2004 Assignment 7

Due: Tuesday, July 6

Weight of this assignment: 43 marks

1. Prove that  $L(\mathbf{x}, \mathbf{y})$  is a constant of the motion for a Hamiltonian system if  $\{H, L\} = 0$ . [4 marks]
2. Consider the two-particle Hamiltonian in one spatial dimension

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(x_1, x_2).$$

Under what condition(s) will the net momentum  $p = p_1 + p_2$  be a constant of the motion? [8 marks]

Bonus: Provide a mechanical interpretation for your condition(s), i.e. relate your mathematical result to concepts learned in your physics classes.

3. (a) Find the equilibrium points of the dynamical system defined by the Hamiltonian

$$H = \frac{1}{2}p^2 - \frac{1}{2}x^2 + \frac{1}{4}x^4.$$

Carry out a linearized stability analysis to classify the equilibria. [10 marks]

- (b) Using a computer program, draw the orbits of this system. Your drawing should be exact, i.e. not based on the numerical integration of the differential equations. Relate the features of your drawing to the results of the stability analysis. [6 marks]
- (c) Using `xppaut`, try a few (three or four) different numerical methods to obtain trajectories of this dynamical system. Have your `xpp` program compute the energy (using an `aux` statement). Report on any interesting behavior you observe. Which methods do the best job of keeping the energy constant? What happens when the energy isn't constant?  
`xppaut` has a symplectic integrator which you should try out. To use this, you *must* put the equations in your `.ode` file in the order `x', p'`. How well does this integrator work? [15 marks]