Lecture #1

Today’s Program

1. Classical States - trajectories
2. Hamiltonians
3. Time evolution (ref. Goldstein 2nd edition Ch. 8 p339).

Suggested References for today’s lecture:

Classical Mechanics, Goldstein 2nd edition Ch. 8 p339

By the end of today’s lecture you should:

Know how to analyze a system of particles moving in a potential field classically in particular:

(a) Understand what the classical definition of a state is, and what are the state variables.
(b) Know how to generate a classical Hamiltonian function.
(c) Know how to predict the time evolution of a classical system by generating the equations of motion from the Hamiltonian.
(d) Remind yourself how to solve systems of coupled differential equations
(e) Learn how to use Mathematica to solve systems of coupled first order equations.
Classical States, Hamiltonians and time evolution

The system

Physical description

The state

The state of a classical system is determined by the variables $x(t)$ and $p(t)$.

The Hamiltonian

All physical quantities of the system (energy, angular momentum) can be expressed in terms of these variables. For example the total energy of the system is determined by its classical Hamiltonian which can be defined as,

$$H(x, p, t) = \frac{p^2}{2m} + V(x, t)$$

Time evolution of the state

Once the state $(x(t), p(t))$ is known at a particular time $t_0$, the state of the system at any other time $t$ is determined completely by the equations of motion.

$$\frac{\partial H(x, p, t)}{\partial p} = \frac{dx}{dt}$$

$$\frac{\partial H(x, p, t)}{\partial x} = -\frac{dp}{dt}$$

the complete set of $(x(t), p(t))$ is called the trajectory of the system.

Example: Mass in a gravitational field

The system consists of a single mass $m=1\text{kg}$ which is released at $t=0$ from a height of $1\text{m}$ above the floor the state of the system at $t=0$ is $(x(t=0) = 1, p(t=0) = 0)$ the total energy is given by the Hamiltonian,

$$H(x, p, t) = \frac{p^2}{2m} + mgx = 1[kg] \frac{m}{s^2} [1[m]] = 9.8[J] = 6.11\times10^{19}[eV]$$

The time evolution of the state is given by,
\[ \frac{\partial H(x, p, t)}{\partial p} = \frac{p}{m} = \frac{dx}{dt} \rightarrow \int gtdt = \int dx \rightarrow x_0 - g \frac{t^2}{2} = x(t) \]
\[ \frac{\partial H(x, p, t)}{\partial x} = mg = -\frac{dp}{dt} \rightarrow \int mgdt = \int dp \rightarrow \int_0^x p_0 = mg t = p(t) \]

**Example: Diatomic molecule**

[I] The system:

![Diatomic molecule diagram](image)

\[ x_1, p_1 \quad \quad x_2, p_2 \]

[II] The Hamiltonian:

\[ H(x_1, p_1; x_2, p_2) = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{k}{2} (x_2 - x_1 - l)^2 \]

k is the spring constant and l is the equilibrium position of the spring (i.e. at that distance the spring is not exerting any force on the masses)

[III] The equations of motion:

\[ \frac{\partial H(x_1, p_1, x_2, p_2; t)}{\partial p_1} = \frac{p_1}{m} = \frac{dx_1}{dt} \]
\[ \frac{\partial H(x_1, p_1, x_2, p_2; t)}{\partial x_1} = -\frac{dp_1}{dt} = -k(x_2 - x_1 - l) = -\frac{dp_1}{dt} \]
\[ \frac{\partial H(x_1, p_1, x_2, p_2; t)}{\partial p_2} = \frac{p_2}{m} = \frac{dx_2}{dt} \]
\[ \frac{\partial H(x_1, p_1, x_2, p_2; t)}{\partial x_2} = \frac{dp_2}{dt} = k(x_2 - x_1 - l) = \frac{dp_2}{dt} \]
\[ \dot{x}_1 = \frac{p_1}{m}, \quad \dot{x}_2 = \frac{p_2}{m}, \quad \dot{p}_1 = k(x_2 - x_1 - l), \quad \dot{p}_2 = -k(x_2 - x_1 - l) \]

these coupled first order equations can be solved by generating uncoupled second order equations (attached is an example of a Mathematica code which can be used to solve such a system of coupled first order equations):

```
k = 1;
m = 1;
solution = NDSolve[
  9x1\[Prime]\[Prime] = \frac{p1}{m},
  x2\[Prime]\[Prime] = \frac{p2}{m},
  p1\[Prime]\[Prime] = \frac{k}{m} x2 - x1 - 1,
  p2\[Prime]\[Prime] = -\frac{k}{m} x2 + x1 - 1,
  x1[0] == 0,
  x2[0] == 1,
  p1[0] == -0.25,
  p2[0] == 0.25
  ];

Plot[8x2 - x1, Solution, 8t, 0, 10];
```

The relative distance between the atoms as a function of time is plotted below \((x_2 - x_1)\)