

## Lecture 1

### **The Hamiltonian approach to classical mechanics. Analysis of a simple oscillator.**

Program:

1. Hamiltonian approach to classical mechanics.
2. Vibrations of an electron in a lattice: simple oscillator

Questions you should be able to answer by the end of today's lecture:

1. How to construct a Hamiltonian for a classical system of particles?
2. How to derive the equations of motion for a classical system?

References:

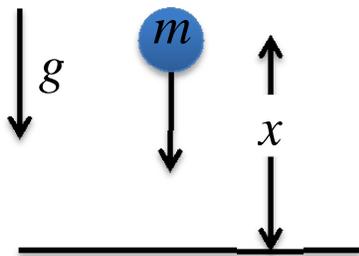
1. Kittel, Chapter 4, page 99.
2. Ashcroft and Mermin, Chapter 22, page 422.

## Introduction:

While this course is primarily focused on electronic structure and its relation to EOM properties it is useful to briefly review the Hamiltonian or *energetics* approach to classical mechanics. We will begin with an analysis of lattice vibrations, which determine the speed of sound in materials, mediate heat conduction, define the heat capacity and play a key role in limiting the electrical conductivity in metals. Later in the course we will also learn that lattice vibrations enable optical absorption and emission in indirect band semiconductors.

## The Hamiltonian approach to classical mechanics

Let's begin with an example: a particle such as an atom falling under gravity:



The energy of this falling particle can then be written as:

$$E = K + V = \frac{mv^2}{2} + V(x),$$

Where  $K$  is kinetic energy and  $V(x)$  is potential energy.

Remembering that  $p=mv$ , we can also write the total energy as:

$$E = \frac{p^2}{2m} + V(x)$$

In this representation energy looks like a function of momentum  $p$  and height  $x$ . This function is usually referred to as a **Hamiltonian**  $H(x,p)$ . For the system consisting of a particle falling under gravity Hamiltonian is:

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

Why is this function important? – Let's take a look how the Hamiltonian changes with respect to momentum and position:

$$\frac{\partial H}{\partial p} = \frac{p}{m} = v = \frac{dx}{dt}$$

$$\frac{\partial H}{\partial x} = \frac{dV(x)}{dx} = -F(x) = -m \frac{d^2 x}{dt^2} = -\frac{d}{dt} \left( m \frac{dx}{dt} \right) = -\frac{dp}{dt}$$

The resulting pair of equations is referred to as Hamilton's equations, which provide an alternative (to Newtonian) description for a mechanical system.

$$\begin{cases} \frac{\partial H}{\partial p} = \frac{dx}{dt} \\ \frac{\partial H}{\partial x} = -\frac{dp}{dt} \end{cases}$$

These equations are very powerful because they imply that knowing a Hamiltonian for any system one can derive equations of motion and learn about the time evolution of this system.

In general case our systems will consists of numerous particles with different momenta  $p_i$  and positions  $x_i$  and consequently the Hamiltonian will be in the form of:

$$H(x_1, \dots, x_N, p_1, \dots, p_N, t) = \sum_{i=1}^N \frac{p_i^2}{2m_i} + V(x_1, \dots, x_N, t)$$

And for every particle  $i$  we would be able to write a pair of Hamilton's equations:

$$\begin{cases} \frac{\partial H}{\partial p_i} = \frac{dx_i}{dt} \\ \frac{\partial H}{\partial x_i} = -\frac{dp_i}{dt} \end{cases}$$

Let's go back to our initial example.

### Example I: Particle falling under gravity:

The Hamiltonian in this case is:

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

Then the Hamilton's equations are:

$$\begin{cases} \frac{\partial H}{\partial p} = \frac{dx}{dt} = \frac{p}{m} \\ \frac{\partial H}{\partial x} = -\frac{dp}{dt} = mg \end{cases} \Rightarrow \begin{cases} \frac{dx}{dt} = \frac{p}{m} \\ \frac{dp}{dt} = -mg \end{cases} \Rightarrow \frac{d^2x}{dt^2} = \frac{1}{m} \frac{dp}{dt} = -g$$

Now we can solve resulting equation of motion and obtain:

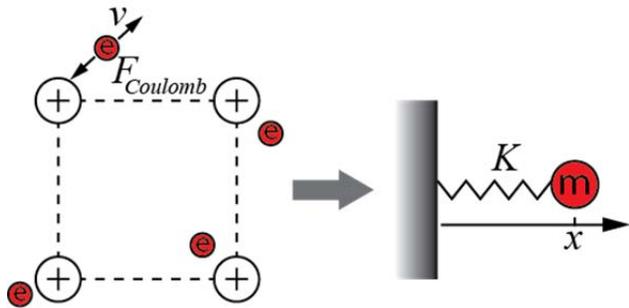
$$\frac{dx}{dt} = \int g dt = -gt - \frac{dx}{dt} \Big|_{t=0} = -gt - v(t=0)$$

$$x(t) = \int (-gt - v(t=0)) dt = x(t=0) - v(t=0) \cdot t - \frac{1}{2} gt^2$$

**Example II: Electron vibrations with respect to the lattice  $\Rightarrow$  simple harmonic oscillator**

In insulating crystalline materials electrons are fairly closely bound to the ions in the lattice. However electrons are not stationary – they have thermal velocity, which allows them to move away from the ions, while the Coulombic attraction to the ions pulls them back. In the very simplistic case we can model this system as a ball (electron) on a spring attached to a wall (massive ion).

**I. The system:**



Electron = ball of mass  $m$  is bound by a stretchable spring of length  $l$  and stiffness  $K$ .

**II. The Hamiltonian:**

The energy for this system is:

$$E = \frac{mv^2}{2} + K \frac{(x-l)^2}{2} = \frac{p^2}{2m} + \frac{K}{2}(x-l)^2$$

Then the Hamiltonian for this system is simply:

$$H(p, x) = \frac{p^2}{2m} + \frac{K}{2}(x-l)^2$$

**III. The Hamilton's equations of motion for this system are:**

$$\left\{ \begin{array}{l} \frac{\partial H}{\partial p} = \frac{dx}{dt} = \frac{p}{m} \\ \frac{\partial H}{\partial x} = -\frac{dp}{dt} = -K(x-l) \end{array} \right. \Rightarrow \left\{ \begin{array}{l} \frac{dx}{dt} = \frac{p}{m} \\ \frac{dp}{dt} = -K(x-l) \end{array} \right. \Rightarrow \frac{d^2x}{dt^2} = \frac{1}{m} \frac{dp}{dt} = -\frac{K}{m}(x-l)$$

$$\Rightarrow \frac{d^2x}{dt^2} + \frac{K}{m}(x-l) = 0 \Rightarrow \frac{d^2(x-l)}{dt^2} + \omega^2(x-l) = 0, \quad \omega = \sqrt{\frac{K}{m}}$$

The last equation is simply an equation for a simple harmonic oscillator. The solution for this equation is:

$$x-l = Ae^{i\omega t} + Be^{-i\omega t}$$

We can find coefficients A and B from the initial conditions.

Let's say at time  $t = 0$ , we have stretched the spring to the length of  $2l$  and released with initial zero velocity:

$$\left. \begin{array}{l} x(0) = 2l \Rightarrow 2l - l = l = Ae^{i\omega 0} + Be^{-i\omega 0} = A + B \\ \frac{dx}{dt}(0) = 0 \Rightarrow 0 = i\omega Ae^{i\omega 0} - i\omega Be^{-i\omega 0} \end{array} \right\} \Rightarrow A = B = \frac{l}{2}$$

Then the solution to the equations of motion is:

$$x = l + \frac{l}{2}(e^{i\omega t} + e^{-i\omega t}) = l + l \cos \omega t$$

Oscillatory behavior as expected from a ball on a spring.

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