1.1: The Lagrangian Formulation of Classical Mechanics

In order to begin to make a connection between the microscopic and macroscopic worlds, we need to better understand the microscopic world and the laws that govern it. We will begin placing Newton's laws of motion in a formal framework which will be heavily used in our study of classical statistical mechanics.

First, we begin by restricting our discussion to systems for which the forces are purely *conservative*. Such forces are derivable from a potential energy function $U(r_1, \cdots, r_N)$ by differentiation:

$$F_i = -\frac{\partial U}{\partial r_i}$$

It is clear that such forces cannot contain dissipative or friction terms. An important property of systems whose forces are conservative is that they conserve the total energy

$$E = K + U = \frac{1}{2}\sum_{i=1}^{N} m_i \dot{r}_i^2 + U(r_1, \cdots, r_N)$$

To see this, simply differentiate the energy with respect to time:

$$\begin{aligned} \frac{dE}{dt} &= \sum_{i=1}^{N} m_i \dot{r}_i \cdot \ddot{r}_i + \sum_{i=1}^{N} \frac{\partial U}{\partial r_i} \cdot \dot{r}_i \\ &= \sum_{i=1}^{N} \dot{r}_i \cdot F_i - \sum_{i=1}^{N} F_i \cdot \dot{r}_i \\ &= 0 \end{aligned}$$

where, the second line, the facts that $\ddot{r}_i = \frac{F_i}{m_i}$ (Newton's law) and $F_i = -\frac{\partial U}{\partial r_i}$ (conservative force definition) have been used. This is known as the law of *conservation of energy*.

For conservative systems, there is an elegant formulation of classical mechanics known as the *Lagrangian* formulation. The *Lagrangian* function, L, for a system is defined to be the difference between the kinetic and potential energies expressed as a function of positions and velocities. In order to make the nomenclature more compact, we shall introduce a shorthand for the complete set of positions in an N-particle system: $r \equiv r_1, \cdots, r_N$ and for the velocities: $\dot{r} \equiv \dot{r}_1, \cdots, \dot{r}_N$. Then, the Lagrangian is defined as follows:

$$L(r, \dot{r}) = K - U = \sum_{i=1}^{N} \frac{1}{2} m_i \dot{r}_i^2 - U(r_1, \cdots, r_N)$$

In terms of the Lagrangian, the classical equations of motion are given by the so called *Euler-Lagrange* equation:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}_i}\right) - \frac{\partial L}{\partial r_i} = 0$$

The equations that result from application of the Euler-Lagrange equation to a particular Lagrangian are known as the *equations of motion*. The solution of the equations of motion for a given initial condition is known as a *trajectory* of the system. The Euler-Lagrange equation results from what is known as an *action principle*. We shall defer further discussion of the action principle until we study the Feynman path integral formulation of quantum statistical mechanics in terms of which the action principle emerges very naturally. For now, we accept the Euler-Lagrange equation as a definition.

The Euler-Lagrange formulation is completely equivalent to Newton's second law. In order to see this, note that

$$\begin{aligned} \frac{\partial L}{\partial \dot{r}_i} &= m_i \dot{r}_i \\ \frac{\partial L}{\partial r_i} &= -\frac{\partial U}{\partial r_i} = F_i \end{aligned}$$

Therefore,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{r}_i}\right) - \frac{\partial L}{\partial r_i} = m_i \ddot{r}_i - F_i = 0$$

which is just Newton's equation of motion.

An important property of the Lagrangian formulation is that it can be used to obtain the equations of motion of a system in *any set of coordinates*, not just the standard Cartesian coordinates, via the Euler-Lagrange equation (see problem set #1).
