CHAPTER 5

Mechanics: Concepts, Representation of Reality, and Models

5.1 The concept of center of mass

It is the concept of center-of-mass that allows Newtonian mechanics being able to be applied to a wide variety of scenarios, to complex objects.

5.1.1 No frictional force is allowed

A frictional force on a point mass \( x(t) \) has to be dependent of the velocity \( \frac{dx}{dt} \). The simplest model for a frictional force is \( F = -\eta \frac{dx}{dt} \). Now let us consider two point masses \( m_1 \) and \( m_2 \):

\[
\begin{align*}
    m_1 \frac{d^2 x_1(t)}{dt^2} &= -\eta_1 \frac{dx_1}{dt} + F_{21}(x_1, x_2) + F^{ext}_1, \\
    m_2 \frac{d^2 x_2(t)}{dt^2} &= -\eta_2 \frac{dx_2}{dt} + F_{12}(x_2, x_1) + F^{ext}_2,
\end{align*}
\]

in which we shall assume that \( F_{12}(x_2, x_1) = -F_{21}(x_1, x_2) \) according to Newton’s third law. Then one has

\[
M_{cm} \frac{d^2 x_{cm}}{dt^2} = - \left\{ \eta_1 \frac{dx_1}{dt} + \eta_2 \frac{dx_2}{dt} \right\} + \sum_{1,2} F^{ext}_i,
\]

in which the center of mass \( x_{cm} = \frac{m_1 x_1 + m_2 x_2}{M_{cm}} \).

One notices that the term inside \( \{ \cdots \} \) cannot be expressed in terms of \( \frac{dx_{cm}}{dt} \) in general, except \( \frac{m_1}{\eta_1} = \frac{m_2}{\eta_2} \). Therefore, in order to treat a complex mechanical system in terms of its center of mass, one needs to eliminate all frictional forces by explicitly considering a viscous medium itself as collisions with a collection of point masses.

5.2 The concept of energy

Assuming there is no frictional force, then \( F \) is a function of \( x \) only, not a function of \( \dot{x} = \frac{dx}{dt} \), then we have

\[
m \frac{d^2 x}{dt^2} = F(x).
\]
If one introduces a potential of force
\[ U(x) - U(x_0) = - \int_{x_0}^{x} F(y) dy, \] (5.5)
then one has
\[ \frac{dU(x)}{dx} = -F(x), \] (5.6)
and
\[ m \left( \frac{dx}{dt} \right)^2 + U(x) = \text{constat}, \] (5.7)
in which the term \( \frac{1}{2}mv^2 \), known to Gottfried Leibniz as \textit{vis viva}, is now called \textit{kinetic energy}. Here is an excerpt from Wikipedia on “Energy”:

The word energy derives from Greek \( \epsilonν\,\epsilonρ\,\epsilonρ\,\epsilonι\,\epsilonα\,\zeta \) (energeia), which possibly appears for the first time in the work of Aristotle in the 4th century BC.

The concept of energy emerged out of the idea of \textit{vis viva} (living force), which Leibniz defined as the product of the mass of an object and its velocity squared; he believed that total \textit{vis viva} was conserved. To account for slowing due to friction, Leibniz theorized that thermal energy consisted of the random motion of the constituent parts of matter, a view shared by Isaac Newton, although it would be more than a century until this was generally accepted. In 1807, Thomas Young was possibly the first to use the term “energy” instead of \textit{vis viva}, in its modern sense. Gustave-Gaspard Coriolis described “kinetic energy” in 1829 in its modern sense, and in 1853, William Rankine coined the term “potential energy”. It was argued for some years whether energy was a substance (the caloric) or merely a physical quantity, such as momentum.

It has to wait for Einstein’s theory that unifies \textit{energy} and \textit{substance}: \( E = mc^2 \).

### 5.2.1 Energy conservation to include heat

In Eq. 5.7, the force from \( -\frac{dU}{dx} \) is called conservative since kinetic energy and potential energy can forever convert back-and-forth. This is not the case if there is an energy dissipation due to frictional force. A frictional force is proportional to the velocity of a moving object:
\[ m \frac{d^2x}{dt^2} = - \frac{dU(x)}{dx} - \eta \frac{dx}{dt}, \] (5.8)
the last term no the right-hand-side is a frictional force. It is equal to zero if velocity \( \frac{dx}{dt} = 0 \).

Now parallel to the deviation of Eq. 5.7, we now have
\[ \frac{d}{dt} \left[ \frac{m}{2} \left( \frac{dx}{dt} \right)^2 + U(x) \right] = -\eta \left( \frac{dx}{dt} \right)^2. \] (5.9)
The right-hand-side is the instantaneous rate of \textit{heat energy} produced, which is equal
The concept of energy to the rate of energy decreasing in the mechanical system. The total mechanical energy (= kinetic + potential) is no longer conserved in this system with friction. However, counting the rate of heat $dQ/dt$:

$$\frac{d}{dt} \left[ \frac{m}{2} \left( \frac{dx}{dt} \right)^2 + U(x) \right] = - \frac{dQ}{dt} \iff \frac{d}{dt} \left[ \frac{m}{2} \left( \frac{dx}{dt} \right)^2 + U(x) + Q \right] = 0.$$  

(5.10)

The total energy conservation, including mechanical and thermal, is again regained.

5.2.2 Simple harmonic oscillator with damping

Let us now consider a Newtonian mechanical system with a point mass at $x$, which is attached to a Hookean spring with re-storing force $-kx$ and a frictional force $-\eta \frac{dx}{dt}$. Then according Newton’s second law of motion:

$$m \frac{d^2x}{dt^2} = \text{total force} = -kx - \eta \frac{dx}{dt}.$$  

(5.11)

The standard way to solve this linear, constant coefficient equation (5.11) is to assume the general solution with the form $e^{rt}$. Then we obtain the characteristic polynomial for $r$:

$$mr^2 + \eta r + k = 0,$$  

(5.12)

whose two roots are

$$r_{1,2} = \frac{-\eta \pm \sqrt{\eta^2 - 4mk}}{2m}. \quad (5.13)$$

The general solution to Eq. 5.11 is

$$x(t) = c_1 e^{r_1 t} + c_2 e^{r_2 t}.$$  

(5.14)

We see that if $\eta \neq 0$ ($\eta$ has to be positive from the physical requirement), then with increasing $t$, $x(t)$ in (5.14) tends to zero.

However, depending on whether $\eta^2 \geq 4mk$ or $\eta < 4mk$, the $x(t)$ approaches to zero either monotonically or oscillatiorily with frequency $\sqrt{4mk - \eta^2}$. The latter corresponds to Eq. 5.12 having a pair of complex roots.

5.2.3 Heavily overdamped system

When $\eta^2 \gg 4mk$, the mechanical system is called heavily overdamped. In this case, one can approximate the two roots in (5.13). We use the important formula

$$(1 + s)^{1/2} \approx 1 + \frac{s}{2} - \frac{s^2}{8} + \cdots$$  

(5.15)
for small $s$. Then

$$r_{1,2} = \frac{-\eta \pm \sqrt{\eta^2 - 4mk}}{2m} = \frac{-\eta \pm \eta\sqrt{1 - 4mk/\eta^2}}{2m}$$

$$\approx \frac{-\eta \pm \eta(1 - 2mk/\eta^2 - 2m^2k^2/\eta^4)}{2m}$$

$$= \left\{ \begin{array}{ll}
-k/\eta (1 + mk/\eta^2) & \approx -k/\eta \\
-\eta/m (1 - mk/\eta^2 - m^2k^2/\eta^4) & \approx -\eta/m
\end{array} \right.$$

Both $r_1$ and $r_2$ are negative. Since $\eta^2 \gg 4mk$, $|r_2| \gg |r_1|$. Therefore, an over-damped system has a very rapid acceleration phase in which “inertia balancing friction”, e.g., $m\ddot{x} = -\eta\dot{x}$, and a relatively slow motion in which “friction balances elasticity”, i.e., $\eta\dot{x} = -kx$.

5.2.4 Underdamped system

What happens if $\eta^2 \ll 4mk$? In this case, we have

$$r_{1,2} = \frac{-\eta \pm \sqrt{\eta^2 - 4mk}}{2m} = \frac{-\eta \pm i\sqrt{4mk}\sqrt{1 - \eta^2/(4mk)}}{2m}$$

$$\approx \frac{-\eta}{2m} \pm i\sqrt{\frac{k}{m}}.$$

We have a decaying oscillation with frequency $\omega = \sqrt{k/m}$ and a much slower decaying rate $\eta/(2m) \ll \omega$. On the fast time scale, the inertia balances the elasticity: $m\ddot{x} = -kx$, just like a Harmonic oscillation without damping.

5.3 Mechanistic modeling of biomolecular mechanics

In this section, we shall develop a mathematical model for the phenomenon of “forced biomolecular bond rupture” first observed by Florin, Moy and Gaub in 1994. Their experimental observations were published in Science.* However, their “interpretations” were quite erroneous.

The problem, even though it is on a single biological molecule (a protein) and its natural partner (called a ligand) in water, is a very ideal Newtonian mechanical system. One can develop a mechanistic model (or theory) based two laws: Newton’s law of motion and van der Waals’ formula for the force between two molecules, together with a list of further assumptions.

Figure 5.1 Upper panel: A schematic overview of protein-ligand complex separation with the AFM. Lower panel: One-dimensional model. The position of the ligand will be denoted by $x$.

We model the external force exerted by a cantilever from an atomic force microscope (AMF) as a linear, harmonic spring:

$$m \frac{d^2 x}{dt^2} = -F_{\text{int}}(x) + k(x - d) - \eta \frac{dx}{dt},$$

in which $x$ is the distance between the center-of-mass of the ligand to the center-of-mass of the protein, which is assumed to be fixed. $m$ is the mass of the ligand, $\eta$ is its frictional coefficient in water, $k(x - x_0)$ represents the force exerted by the AFM cantilever, with $d$ being the position of the base of the cantilever. $F_{\text{int}}(x)$ is the interaction force between the ligand and the protein, it has the celebrated van der Waals potential $U_{\text{vdw}}(x)$

$$F_{\text{int}}(x) = \frac{dU_{\text{vdw}}(x)}{dx}, \quad U_{\text{vdw}}(x) = -U_0 \left[ 2 \left( \frac{x_0}{x} \right)^6 - \left( \frac{x_0}{x} \right)^{12} \right].$$

Because water is a rather viscous medium, we further assume that (1) the mechanical system is overdamped, i.e., we can neglect the mass term. Therefore, Eq. (5.16) can

† This immediately gives the insight that the internal structure of the protein can change under the pulling. But if our measurement for $x$ is precisely the distance between the center-of-masses, then it does not matter. However, in real-world experiments, this is nearly impossible. So there will be consequences.
be simplified into
\[ \eta \frac{dx}{dt} = -F_{\text{int}}(x) + k(d - x). \] (5.18)

We now ask the question: When \( d \) is slowly increased, i.e., the AFM is pulling the ligand away from the protein, how does the position of the ligand change?

This is in fact a static, force balance problem: \( F_{\text{int}}(x) = k(d - x) \). That is,
\[ U_0 \left[ \frac{1}{12} \left( \frac{x_0}{x} \right)^7 - 12 \left( \frac{x_0}{x} \right)^{13/2} \right] = k(d - x). \] (5.19)

The solution \( x \) to the equation, as a function of \( d \), is the answer to our question.

There are many parameters in the equation. But they can be grouped together:
\[ z = \frac{x}{x_0}, \quad \delta = \frac{d}{x_0}, \quad \text{and} \quad \alpha = \frac{kx_0^2}{12U_0}, \]
then,
\[ z^{-7} - z^{-13} = \alpha (\delta - z). \] (5.20)

Note that all three quantities, \( z \), \( \delta \), and \( \alpha \) are dimensionless, non-dimensionalization is a very useful way to simplify mathematical models without involving any approximation. It uses the internal scales as units for physical quantities in a model.

This equation can not be solved in a closed form for \( z(\delta) \). However, one can obtain a parametric equation for the function:
\[ z = \left( \frac{1 \pm \sqrt{1 - 4\xi}}{2} \right)^{-\frac{2}{3}}, \quad \delta = z + \frac{\xi}{\alpha z}, \quad \xi \in \left[ -\infty, \frac{1}{4} \right]. \] (5.21)

Fig. 1 shows several \( z \) as functions of \( \delta \) with different \( \alpha \)’s. We see with increasing \( \alpha \), i.e., the spring becoming more stiff, the “sluggish” behavior disappears.

One can also understand the behavior in the figure in terms of the “potential energy function”:
\[ \eta \frac{dx}{dt} = -\frac{dU_{\text{tot}}}{dx}, \] (5.22)
where
\[ U_{\text{tot}}(x) = U_{\text{vdw}}(x) + \frac{1}{2}k(x - d)^2 = -U_0 \left[ 2 \left( \frac{x_0}{x} \right)^6 - \left( \frac{x_0}{x} \right)^{12} \right] + \frac{1}{2}k(x - d)^2. \] (5.23)

In non-dimensionalized form, it is
\[ \frac{U_{\text{tot}}(z)}{U_0} = -\left[ 2 \left( \frac{1}{z} \right)^6 - \left( \frac{1}{z} \right)^{12} \right] + 6\alpha(z - \delta)^2. \] (5.24)

Fig. 2 shows the total potential energy function \( U_{\text{tot}}(z) \) for three different \( \delta \).
Figure 5.2 Mechanical equilibrium position of the ligand, $z$, as a function of $\delta$, the position of the base of the cantilever, with several different $\alpha$s, the stiffness of the cantilever. $z = 1$ is the equilibrium position of the ligand in the absence of the AFM force. Red: $\alpha = 0.1$; blue: $\alpha = 0.3$, and green: $\alpha = 0.7$. 
Figure 5.3 Total mechanical energy, $U_{\text{tot}}(z)$, as a function of the ligand-protein (center of mass) distance $z$ for several different values of $\delta$. Red: $\delta = 1.3$, green: $\delta = 2.2$, and orange: $\delta = 3.3$. All with $\alpha = 0.1$, correspond to the red curve in Fig. 1.