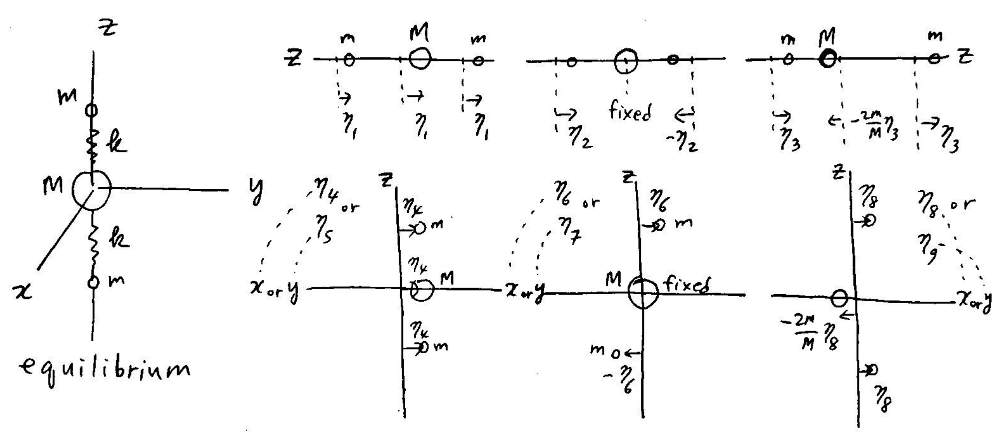
Notes for Lecture 16

Molecules, Many Body, Rigid Body

16.1 Normal modes of molecules

In the last lecture, we studied a classical mechanics model[1] for CO_2. By choice, we only considered one dimensional motions in which any atom moves only along the line of the molecule. We obtained one translational mode (zero eigen-frequency) and two vibrational modes (finite eigen-frequencies). Of course, we should expect other modes, as each atom can move in all directions, not just along the line of the molecule. Here is a sketch of all modes.



[1] The correct quantum mechanical treatment of these molecules can be made by "simply" (what I mean is that it is simple once your learn quantum mechanics) quantizing each normal coordinate η_i after, as we discussed in the last lecture, conveniently splitting the Lagrangian, and thus the Hamiltonian, into a sum of contributions from normal modes. So, the exercise of classical coupled oscillator model for molecules is a very rewarding one, as it lays a solid foundation for the correct quantum mechanical treatment.

In the above diagram, some modes ($\eta_1, \ldots, \eta_3$) are those we already considered. As with the η_1 mode, some modes turn out to be zero frequency oscillation – which means that it is not really an oscillation – but that is fine. Let us analyze the whole situation here, by asking and answering some questions.

1. Why do we have nine modes in total? Ans: because the total degrees of freedom $= 3 \times 3 = 9$.
2. What modes correspond to no restoring force, i.e. zero eigen-frequency? Ans: $\eta_1, \eta_4, \eta_5, \eta_6, \eta_7$.
3. What is the nature of each zero frequency mode? Ans: translation (η_1, η_4, η_5) and rotation (η_6, η_7).
4. Which modes are degenerate (i.e. of the same eigen-frequency)? Ans: All zero frequency modes are degenerate. The pair η_6, η_7 are degenerate, as are the pair η_8, η_9.
5. Which modes have a finite total momentum? Ans: all translational modes (η_1, η_4, η_5) only.
6. Which modes have a finite total angular momentum? Ans: All rotational modes (η_6, η_7) and all translational modes (η_1, η_4, η_5). The latter, only if the angular momentum is measured around a point that is not the center of mass.
7. Why is it that η_6, η_7 modes have no restoring force but η_8, η_9 modes have restoring force (and thus a finite frequency)? Ans: This is an excellent question. Notice that in terms of the spring force argument all these modes ($\eta_6, \ldots, \eta_9$) should have zero restoring force, since the length change of the spring is 2nd order, not 1st order, in η. So, there is more physics than just Hooke's law here. If a student answers this question well (from a general physics point of view; a simple classical mechanics point of view is obviously not enough), I will consider some bonus credit (something like a full make-up of a quiz?).

Having done this exercise, it may not be too difficult to understand the following table, which is valid for a molecule consisting of any number of atoms (tot-DOF = total degrees of freedom).

shape of molecule	Number of masses (atoms)	tot-DOF	translational modes	rotational modes	vibrational modes
line	n	$3n$	3	2	$3n - 3 - 2$
non-line	n	$3n$	3	3	$3n - 3 - 3$

The only difference for the two types (line or non-line) of molecules is the number of vibrational modes. It is meaningless to talk of a rotation of a linear molecule around its own axis – this is why a linear molecule has only two distinct rotations (η_6, η_7 of the above example), while a non-linear molecule has rotation modes in all three directions.

Knowing normal modes before solving matrices

If all normal modes are obvious from the get-go, then in principle the following is all one needs to find all normal modes. Write down all normal modes (namely all $\vec{T}_i$ vectors, as pictorially given in the above diagram), and then prove, for each normal mode, that *each* non-stationary mass vibrates at the same frequency. For the six diagrams shown above, it is rather easy to do this! [Please try this. If you submit a good report on this, then it can also fully make up a quiz.] For instance, for the 3rd digram, one can show easily that *each* of all three masses should vibrate at the angular frequency $\frac{(1+2m/M)k}{m}$, proving that this is indeed a normal mode with that angular frequency.
So, here is a question of great physical and practical importance. How can one know as much as possible about all these normal modes even before beginning to write down $\overleftrightarrow{A}$ and $\overleftrightarrow{M}$? A few guides are useful.

1. Distinguish between modes that have a finite total momentum (i.e. the center of mass is moving) and those that don't (i.e. the center of mass is fixed). The modes that do are translational modes.

2. Then, among the modes that have zero momentum, distinguish between modes that have a finite angular momentum and those that don't. Those that do are rotational modes.

3. Use "symmetry." If two masses are identical, then they can be swapped without changing physics. Then, the displacements of those two masses (say, x_1 and x_2) will appear as either the same ($x_1 = x_2$) or the opposite ($x_1 = -x_2$) in normal modes. Also, the "symmetry" is the reason why the longitudinal modes and the transverse modes can be considered separately from the get-go.

Also, note that for a linear molecule (e.g.CO_2, H_2), one can distinguish between longitudinal modes (for which atoms move along the line of the molecule) and transverse modes (for which atoms move perpendicular to the line of the molecule). For a linear molecule with n atoms, there are $n-1$ longitudinal modes (the total of n degrees of freedom within that one dimensional space minus 1 for translation). Thus, the total number of transverse vibrational modes is $3n-3-2-(n-1)=2n-4$. It is no coincidence that this is an even number. It is for the following reason. Suppose there is a transverse mode where the displacements of all atoms are in the x direction, while the linear molecule is aligned along the z axis. Then this transverse mode has a twin mode where the displacements of all atoms, while identical in value, are in the y direction. These two modes must both exist, and they have the same eigen-frequency, i.e. they are degenerate. For either direction (x or y) of displacement, then, there will be $n-2$ normal modes. Indeed, in the above example of CO_2, there was only one transverse mode per direction.

16.2 Normal modes, general remarks

In the last two lectures and in the previous section, we considered a coupled oscillator problem assuming small oscillations. This elementary treatment generally goes by the name of "**harmonic approximation**." The "stars" of this treatment were definitely those things called **normal modes**. In the harmonic approximation of coupled oscillators, all potential energies and all kinetic energies are taken only up to the quadratic terms of generalized coordinates, and the result is that the system can be described in terms of completely independent normal modes, each of which does a simple harmonic oscillation.

It should seem both satisfying and unrealistic to have such a nice picture. It is very satisfying in the sense that there is a certain beauty to this separation of the whole complex problem into completely independent and easy bits. At the same time, you might mutter to yourself that this is a bit artificial in that any small perturbation (cubic or higher terms ignored in the Lagrangian that will introduce the non-linearity – see LN 5) would spoil this ideal picture of completely independent normal modes. Indeed. Like any physics models, the harmonic approximation of coupled oscillators is a bit simplistic but immensely useful *starting point* for describing real world phenomena. For any given stable object, a small deformation will give rise to a restoring force that, in the first approximation, follows Hooke's law, and so the harmonic approximation is of relevance to *any* object.

We saw that some normal modes were "trivial." Like that of translation in which all masses move by the same amount. Or, rotation. We can call these **shape-and-size-preserving normal modes**. They are translations and rotations. You take a snap shot of the system for which only translational or rotational normal modes are excited, and you will find that the system looks just the same in every detail at any time, except for the overall position and the overall orientation. These translational and rotational modes involve no restoring force, and thus are characterized by zero eigen-frequencies. Then, there are **shape-or-size-changing normal modes**. These are all the rest – vibrations, we call them. Of course, vibrations do not change the average shape of the system, within the harmonic approximation.[2] At any given time, though, a snapshot of the system will show a distorted shape of the system.

Let us consider the following two completely different questions. First, would there be such a case when vibrational normal modes can be completely ignored? Second, would there be such a case when vibrational normal modes must be treated definitely beyond the harmonic approximation? The answers are yes and yes.

The first case is the case of a "**rigid body**." In this case, the vibrational modes are deemed unimportant and are ignored, in comparison to the translational and rotational modes. This is an important topic that we will discuss in later sections of this lecture.

The second case, while being more difficult to discuss, is also quite interesting and important nonetheless. To appreciate this second case, consider the following statement. **Within the harmonic approximation, a coupled oscillator system will always look "brand-new"**. As any object can be thought of as a coupled oscillator system to the first approximation, then this statement means the following. **No object will ever wear out, if it can be completely modeled as a harmonic coupled oscillator system**. Why so? In this nice picture of independent simple harmonic normal modes, all that can happen to the object in a collision, or any physical process, is the increase or decrease of energy of each normal mode. So, the object can, for example, vibrate more or less but on the average its shape or size can never change. In other words, it will never lose its average form – it never wears out! Our experience is quite the opposite – things wear out especially if they are subject to violent collision processes (baseball hit by a baseball bat, tennis ball hit by a racket, a tire rubbed against the road surface, etc). So, it must be the case that non-linear terms play an essential role in normal *wear and tear* processes. Indeed, without non-linear terms in the Lagrangian, it would be impossible to explain how things can (slightly) deform after a collision or why some materials can be lost during a collision.

[2] If non-linear terms are included, then the average shape or size *will* change. This is because, as we have seen in LN 5, one of the things that we saw happening due to the non-linearity was the shift of the effective equilibrium position. Remember the physical argument for the thermal expansion of materials? If the equilibrium position changes uniformly in all directions, then the size will change. More likely, the equilibrium position will change differently in different directions depending on what particular normal modes are excited – in this case the shape will change.

16.3 General properties of a many body system

Here, we summarize **a few fundamental properties of a general system of particles**. They are valid completely regardless of what type of interactions – harmonic, central, or else – particles exchange. **They are valid whenever, for whatever particles that we consider.**

For any system of particles (m_i's at $\vec{r}_i$'s),

$$\vec{P} \stackrel{def}{=} \sum_i m_i \vec{v}_i \;=\; M\dot{\vec{R}}$$

where $\vec{P}$ is the total momentum, $M \equiv \sum_i m_i$ is the total mass, and

$$\vec{R} \stackrel{def}{=} \frac{\sum_i m_i \vec{r}_i}{M}$$

is the position vector of the center of mass.

That $\vec{P} = M\dot{\vec{R}}$ is an immediate consequence of the given definition of $\vec{R}$ (exercise: just take the time derivative of this definition).

How about the angular momentum? Let us see

$$\begin{aligned}
\vec{L} &\stackrel{def}{=} \sum_i m_i \vec{r}_i \times \vec{v}_i \\
&= \sum_i m_i (\vec{R} + \vec{s}_i) \times (\dot{\vec{R}} + \dot{\vec{s}}_i) && \vec{r}_i \equiv \vec{R} + \vec{s}_i \\
&= \sum_i m_i (\vec{R} \times \dot{\vec{R}} + \vec{s}_i \times \dot{\vec{s}}_i) && \because \sum_i m_i \vec{s}_i = 0 \text{ and } \sum_i m_i \dot{\vec{s}}_i = 0 \\
&= \vec{R} \times \vec{P} + \sum_i m_i \vec{s}_i \times \dot{\vec{s}}_i
\end{aligned}$$

This result can be summarized as follows.

For any system of particles (m_i's at $\vec{r}_i$'s),

$$\vec{L} \;=\; \vec{L}_M + \vec{L}_{int,cm}$$

where $\vec{L}$ is the total angular momentum,

$$\vec{L}_M \equiv \vec{R} \times M\dot{\vec{R}}$$

is the angular momentum of the total mass $M \equiv \sum_i m_i$ located at the center of mass position $\vec{R}$, and

$$\vec{L}_{int,cm} \equiv \sum_i m_i \vec{s}_i \times \dot{\vec{s}}_i$$

where $\vec{s}_i \equiv \vec{r}_i - \vec{R}$, is the internal angular momentum of the system measured in the center of mass reference frame.

Finally, let us examine the kinetic energy.

$$\begin{aligned} T &\stackrel{def}{=} \frac{1}{2}\sum_i m_i \dot{\vec{r}}_i \cdot \dot{\vec{r}}_i \\ &= \frac{1}{2}\sum_i m_i(\dot{\vec{R}} + \dot{\vec{s}}_i) \cdot (\dot{\vec{R}} + \dot{\vec{s}}_i) \\ &= \frac{1}{2}\sum_i m_i(\dot{\vec{R}} \cdot \dot{\vec{R}} + \dot{\vec{s}}_i \cdot \dot{\vec{s}}_i) \qquad \because \sum_i m_i \dot{\vec{s}}_i = 0 \end{aligned}$$

To summarize,

For any system of particles (m_i's at $\vec{r}_i$'s),

$$T = T_M + T_{int,cm}$$

where T is the total kinetic energy,

$$T_M \equiv \frac{1}{2} M |\dot{\vec{R}}|^2$$

is the kinetic energy of the total mass M at the center of mass position $\vec{R}$, and

$$T_{int,cm} \equiv \frac{1}{2}\sum_i m_i |\dot{\vec{s}}_i^2|$$

where $\vec{s}_i \equiv \vec{r}_i - \vec{R}$, is the internal kinetic energy of the system measured in the center of mass reference frame.

16.4 Rigid body – definition

A rigid body was defined already in Section 16.2. Here it is. **A rigid body is a system of particles where all vibrational modes can be ignored compared to translational and rotational modes.** This means that there are only six degrees of freedom to consider for a rigid body, greatly simplifying the mathematics required.

The standard definition of a rigid body can be stated as followed. **A rigid body is a collection of particles, for which the distance of between any pair of particles is fixed.**

This definition simply means that a rigid body is an object whose shape and size are considered fixed. Then, the only possible excitation of such a body is the shape-and-size-conserving normal modes, i.e. translations and rotations. This makes the standard definition equivalent to the first definition.

[Subtle advanced discussion here; can skip if you like] Strictly speaking, in truth, all normal modes of every object *always* have finite amplitudes.[3] However, if one is considering cases in which an object is given a total momentum or a total angular momentum that is very large so that the translational or the rotational modes of that object have much greater amplitude than all vibrational modes, then it is of little importance to consider to those vibrational modes as far as the macroscopic dynamics of the body is concerned. Thus, a notion of a rigid body.

When to apply the rigid body concept and when not. One must keep in mind that, the concept of rigid body fails in general during the short collision process. Before or after a collision, the concept of rigid body is useful. One may be well-advised, though, that even when the body "looks the same" before and after the collision, the internal state may have changed during the collision process. If it did, then we have an inelastic collision. If it did not, then, assuming that the energy was not lost to heat or sound during the collision, we have an elastic collision. In a similar vein, it is important to note that the concept of rigid body is useful even when the body is really not rigid in general. For instance, consider a figure skater spinning on ice, with arms tugged in initially and, then, arms stretched. In a typical problem to figure out how the angular velocity changes, we learn to deal with the body of the figure skater as though it was a rigid body in the initial state and another rigid body in the final state. This, despite the fact that a human body is generally not "rigid"

[3] This is because at a finite temperature the thermal energy excite them. At $T = 0$, however, all amplitudes will cease to exist, if classical mechanics were to hold at such a low temperature. However, at $T = 0$, classical mechanics is not valid, and all normal modes have finite amplitudes. This is due to the Heisenberg uncertainty principle. We also use the expression "quantum fluctuations" to describe this $T = 0$ physics. In other words, things are agitated due to "thermal fluctuations" at a finite T and "quantum fluctuations" at zero T.

as it is flexible to change. It is nevertheless correct and useful to consider a human body a rigid body in a small time window when the shape and size of the body does not change. Of course, during the stretching of her arms, the concept of rigid body is quite unsuitable to the whole body.[4]

16.5 Rigid body – general properties

In Section 16.3, we have laid out some important properties of $\vec{P}, \vec{L}, T$ – the total momentum, the total angular momentum, and the total kinetic energy – of a general system of particles.

[**Important notation matter**] As in Section 16.3, we use the index i to mean the index of point masses constituting the system. Below, we will use indices $j, k, l, \ldots$ to mean the three Cartesian coordinates. Also, note that in this section and the next, we work in the center of mass frame only.

Let us discuss these quantities for a rigid body. To specify the motion of a rigid body, one only needs to note the following.

Translation	Described by the change of $\vec{R}$. This carried the total momentum, $\vec{P} = M\dot{\vec{R}}$, as shown in Section 16.3.
Rotation	Each coordinate $\vec{s}_i \equiv \vec{r}_i - \vec{R}$ rotates around $\vec{R}$ at the same rate at any given time.

For a rotation by $d\vec{\phi}$, we have

$$d\vec{s}_i \; = \; d\vec{\phi} \times \vec{s}_i$$

For the derivation of this relation, see LN 10, page 9. Note that there we used the δ notation, $\delta\vec{\phi}$ and $\delta\vec{r}$, as we were considering a virtual rotation (fixed time). Here, we are using the notation $d\vec{\phi}$, suitable for a real dynamical rotation of a rigid body. In any case, dividing the above equation by dt, we get

$$\dot{\vec{s}}_i \; = \; \vec{\omega} \times \vec{s}_i$$

[4] Even then, (approximately) shape-and-size conserving *parts* of bodies can be considered rigid bodies.

where $\vec{\omega} \equiv d\vec{\phi}/dt$ is the angular velocity around the center of mass. This is a key relation for describing the motion of a rigid body.

Let us examine the kinetic energy of a rigid body. Let us examine the internal part, $T_{int,cm}$, only, as the part T_M remains the same as in Section 16.3.

$$\begin{aligned}
T_{int,cm} &= \frac{1}{2}\sum_i m_i \dot{\vec{s}}_i \cdot \dot{\vec{s}}_i \\
&= \frac{1}{2}\sum_i m_i (\vec{\omega} \times \vec{s}_i) \cdot (\vec{\omega} \times \vec{s}_i) \\
&= \frac{1}{2}\sum_i m_i \left(\omega^2 s_i^2 - \sum_{j,k=1}^{3} \omega_j s_{i,j} \omega_k s_{i,k} \right) \\
&= \frac{1}{2}\sum_{j,k=1}^{3} \sum_i m_i \left(\omega_j \omega_k \delta_{jk} s_i^2 - \omega_j s_{i,j} \omega_k s_{i,k} \right) \\
&= \frac{1}{2}\sum_{j,k=1}^{3} \omega_j I_{jk} \omega_k
\end{aligned}$$

where the **inertia tensor** I_{jk} is defined as

$$I_{jk} = \sum_i m_i \left(\delta_{jk} s_i^2 - s_{i,j} s_{i,k} \right)$$

Here, again, in the expression of the kinetic energy, we see a quadratic form, as in the normal mode problem,

$$T_{int,cm} = \frac{1}{2} \vec{\omega}^t \overleftrightarrow{I} \vec{\omega}$$

Now, let us consider the angular momentum vector. Again, our concern is $\vec{L}_{int,cm}$ only, as $\vec{L}_M$ remains unchanged from Section 16.3.

$$
\begin{aligned}
\vec{L}_{int,cm} &= \sum_i m_i \vec{s}_i \times \dot{\vec{s}}_i \\
&= \sum_i m_i \vec{s}_i \times (\vec{\omega} \times \vec{s}_i) \\
&= \sum_i m_i \left(\vec{\omega} s_i^2 - \vec{s}_i (\vec{\omega} \cdot \vec{s}_i)\right) \\
&= \overleftrightarrow{I}\,\vec{\omega}
\end{aligned}
$$

with the same inertia tensor as defined above. To summarize,

$$
\boxed{\vec{L}_{int,cm} = \overleftrightarrow{I}\,\vec{\omega}}
$$