

Lecture 7: February 10

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7.1 Reformulations of the laws of mechanics

After the laws of mechanics were articulated by Newton in precise mathematical terms, and calculus was available to work out their consequences, there was a growing interest in how best to carry out the mathematical analysis. Every advance in the efficiency of the analysis expanded the scope of physics to new applications. Efficient representations of mechanical systems, formulations that make their dynamics both more transparent and tractable, will also be our motivation in the next several lectures. While these considerations carry much less weight in the era of computers, the impact of these reformulations on physics is recognized today by the new kinds of mechanics — statistical and quantum — that they helped launch.

7.1.1 Degrees of freedom

One way to economize on the description of a mechanical system is to minimize the number of variables. We say a mechanical system has N *degrees of freedom* when N real-valued variables are required to uniquely specify the state of the system (*e.g.* positions of all the particles). Often there are several choices of sets of variables, and the choice we make is one of convenience. The standard notation for these variables, in a general discussion, is q_1, q_2, \dots, q_N . These might correspond to distances, angles, or even charges on capacitor plates.

Let's do a degrees-of-freedom analysis of the cyclo-heptane molecule. We model the molecule as seven mass points (carbon atoms) joined by seven rigid struts (bonds) to form a ring. Chemistry also requires that the two struts impinging on each mass have a fixed angle. The two sets of conditions, on the bond lengths and angles, are called constraints.

To count the number of degrees of freedom we start by ignoring the constraints. Seven mass points, each free to move in space, have altogether $7 \times 3 = 21$ degrees of freedom. Each constraint on the system reduces this number of degrees of freedom by one. Since cyclo-heptane has seven bond length and seven bond angle constraints, the number of remaining degrees of freedom is $21 - 7 - 7 = 7$.

Some degrees of freedom are guaranteed by symmetry. The rigid translations of the molecule (which preserve all the constraints) have three degrees of freedom, as do the rigid rotations. There are thus six degrees of freedom of a trivial kind, just because the molecule exists in three dimensional space. Not counting those, cyclo-heptane then has just $7 - 6 = 1$, or a single non-rigid degree of freedom!

The q 's are called *generalized coordinates*. By definition, the position of every particle in our N -degrees-of-freedom system is uniquely specified by N q 's:

$$\mathbf{r}_i = \mathbf{r}_i(q_1, \dots, q_N). \quad (7.1)$$

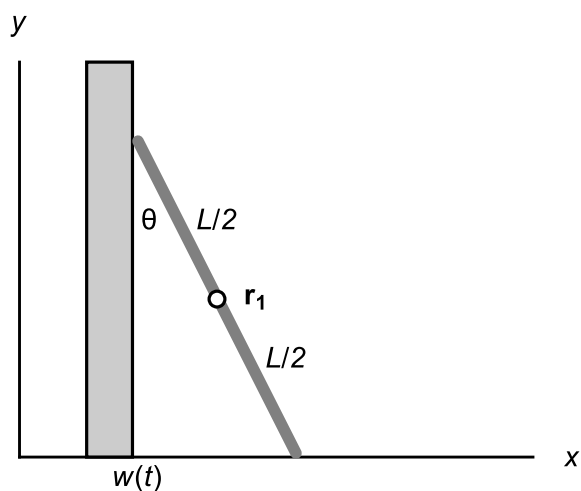
This is to be read as “the vector variable \mathbf{r}_i (position of the i^{th} particle) is a function of q_1, \dots, q_N ”. In the case of cyclo-heptane, $\mathbf{r}_1, \dots, \mathbf{r}_7$ are the positions of the carbon atoms, q_1, q_2, q_3 are center-of-mass coordinates of the molecule, q_4, q_5, q_6 are three angles that specify the molecule’s orientation, and q_7 is the single generalized coordinate that specifies the shape of the molecule.

Sometimes the environment of the system changes with time, in which case we write

$$\mathbf{r}_i = \mathbf{r}_i(q_1, \dots, q_N, t). \quad (7.2)$$

Because the environment is not considered part of the system, there are no q ’s associated with it.

As a simple example of a system with one degree of freedom we consider a ladder of length L leaning against a frictionless, moving wall.



The point $\mathbf{r}_1 = x\hat{\mathbf{x}} + y\hat{\mathbf{y}}$ is the ladder’s center of mass and where the force of gravity would be applied. To specify the state of the ladder we need a single generalized coordinate: the angle θ it makes with the wall. The time dependent position of the wall, $w(t)$, corresponds to the environment. This is not a degree of freedom but a given function of time. For example, $w(t) = vt$ corresponds to a moving frame, $w(t) = at^2/2$ an accelerating frame, and $w(t) = A \cos(\omega t)$ might be a way to model the presence of an earthquake. Here are expressions for the components of \mathbf{r}_1 in terms of our generalized coordinate and environment function:

$$x = (L/2) \sin \theta + w(t) \quad (7.3)$$

$$y = (L/2) \cos \theta. \quad (7.4)$$

7.1.2 Generalized velocities and forces

Time derivatives of the generalized coordinates are *generalized velocities*. They are related to the particle velocities by the chain rule of calculus:

$$\dot{\mathbf{r}}_i = \sum_{k=1}^N \frac{\partial \mathbf{r}_i}{\partial q_k} \dot{q}_k + \frac{\partial \mathbf{r}_i}{\partial t} \quad (7.5)$$

We will think of the \dot{q} ’s as independent of the q ’s. This is something we are already familiar with, when they are evaluated at the same instant of time and their values correspond to initial conditions. We will

apply this independence principle more generally. That was why we were very careful to spell out in (7.2) all the variables that \mathbf{r}_i is a function of. As you see, it is not dependent on any \dot{q} 's, and therefore $\partial\mathbf{r}_i/\partial q_k$ and $\partial\mathbf{r}_i/\partial t$ are also not dependent on any \dot{q} 's. However, from (7.5) we see that $\dot{\mathbf{r}}_i$ does have dependence on \dot{q} 's, a very simple one, from which we get the identity

$$\frac{\partial\dot{\mathbf{r}}_i}{\partial\dot{q}_k} = \frac{\partial\mathbf{r}_i}{\partial q_k}. \quad (7.6)$$

Taking time derivatives of (7.3),

$$\dot{x} = (L/2)\dot{\theta} \cos\theta + \dot{w} \quad (7.7)$$

$$\dot{y} = -(L/2)\dot{\theta} \sin\theta, \quad (7.8)$$

we can verify (7.6) for the ladder system:

$$\frac{\partial\dot{x}}{\partial\dot{\theta}} = (L/2) \cos\theta = \frac{\partial x}{\partial\theta} \quad (7.9)$$

$$\frac{\partial\dot{y}}{\partial\dot{\theta}} = -(L/2) \sin\theta = \frac{\partial y}{\partial\theta}. \quad (7.10)$$

Now consider the forces acting on our system. We will be primarily interested in the work performed by these forces, for all conceivable motions as the generalized coordinates are varied. Forces whose role is to impose constraints on the particles, called *constraint forces*, can be neglected. For example, we do not need to consider the forces that maintain the constant carbon-carbon bond distances in cyclo-heptane, or the normal forces keeping the ladder from penetrating the floor or wall. By definition, these forces perform no work because there is zero displacement in the direction of the force.

Let $\delta q_1, \dots, \delta q_N$ be arbitrary, infinitesimal changes in the generalized coordinates. Using the chain rule, the corresponding particle displacements are

$$\delta\mathbf{r}_i = \sum_{k=1}^N \frac{\partial\mathbf{r}_i}{\partial q_k} \delta q_k. \quad (7.11)$$

Let \mathbf{F}_i be the (non-constraint) force on particle i . The net work performed by all forces on the system is then

$$\delta W = \sum_i \mathbf{F}_i \cdot \delta\mathbf{r}_i. \quad (7.12)$$

Substituting (7.11) into this expression,

$$\delta W = \sum_i \mathbf{F}_i \cdot \left(\sum_{k=1}^N \frac{\partial\mathbf{r}_i}{\partial q_k} \delta q_k \right), \quad (7.13)$$

and rearranging, we arrive at

$$\delta W = \sum_{k=1}^N f_k \delta q_k, \quad (7.14)$$

where

$$f_k = \sum_i \mathbf{F}_i \cdot \frac{\partial\mathbf{r}_i}{\partial q_k} \quad (7.15)$$

is the *generalized force* associated with generalized coordinate k . We could have included constraint forces in this expression, because in all possible motions the vector $\partial\mathbf{r}_i/\partial q_k$ must be perpendicular to the constraint force on particle i .