

## Lecture 15: March 6

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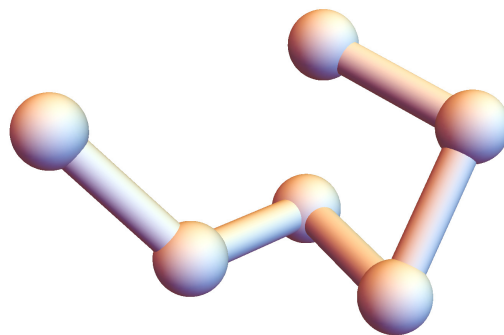
## 15.1 Constrained variations in mechanics

### 15.1.1 Holonomic constraints: the polymer model

Our first application of constraints to mechanics is for the situation where we have constraint functions on the generalized coordinates. This corresponds to the case of holonomic constraints, since a Lagrangian with the right number of generalized coordinates (equal to the number of degrees of freedom) could in principle be produced by solving the constraint equations.

We will use the method of Lagrange multipliers, as in the hanging chain problem of lecture 14. However, unlike the single constraint function we had for the hanging chain (the fixed length of the chain), in modeling a polymer we will need an infinite set of Lagrange multipliers to impose constraints at each instant of time.

Our system is comprised of  $N$  particles of mass  $m$  moving in three dimensions such that adjacent particles are always separated by distance  $d$ . This is a very simple model of a polymer, where bonds have a fixed length and bond angles are completely unconstrained.



One approach to this system is to build all the constraints into the definition of the generalized coordinates — and therefore no constraints are needed. With the position of particle 1 specified by  $\mathbf{r}_1$ , we need two angles relative to  $\mathbf{r}_1$  to specify the position of  $\mathbf{r}_2$ , another two angles (from  $\mathbf{r}_2$ ) to specify the position of  $\mathbf{r}_3$ ,

*etc.*, for a total of  $3 + 2(N - 1) = 2N + 1$  generalized coordinates (and degrees of freedom). The resulting Lagrangian will be very complicated and will poorly reflect the symmetry of the system. For example, the angle variables defined for the low-numbered particles will affect all the “downstream” particles, while angles with respect to the high-numbered particles have no affect at all on the positions of the “upstream” particles.

An alternative approach is to use the  $3N$  particle coordinates as the generalized coordinates and constraint functions for the distances between particles. To impose the distance constraint between particles  $i$  and  $i + 1$  we use the function

$$g(\mathbf{r}_i(t), \mathbf{r}_{i+1}(t)) = |\mathbf{r}_i(t) - \mathbf{r}_{i+1}(t)|^2. \quad (15.1)$$

This function takes the value  $d^2$  at every instant of time. We therefore have a Lagrange multiplier not just for each of the  $N - 1$  bonds, but also for each instant of time  $t$ . The sum over Lagrange multipliers and constraint functions we saw in lecture 13

$$f + \lambda_1 g_1 + \lambda_2 g_2 + \dots, \quad (15.2)$$

takes the form

$$S + \int_{t_1}^{t_2} dt \sum_{i=1}^{N-1} \lambda_i(t) g(\mathbf{r}_i(t), \mathbf{r}_{i+1}(t)), \quad (15.3)$$

where  $S$  is the action of the unconstrained particles. Since  $S$  is the  $t$ -integral of the Lagrangian, we define a single functional

$$S'[\mathbf{r}_1, \dots, \mathbf{r}_N] = \int_{t_1}^{t_2} dt \mathcal{L}'(\mathbf{r}_1, \dots; \dot{\mathbf{r}}_1, \dots), \quad (15.4)$$

where the new Lagrangian  $\mathcal{L}'$  includes a sum over constraint functions:

$$\mathcal{L}' = \frac{1}{2}m \sum_{i=1}^N |\dot{\mathbf{r}}_i(t)|^2 + \sum_{i=1}^{N-1} \lambda_i(t) |\mathbf{r}_i(t) - \mathbf{r}_{i+1}(t)|^2. \quad (15.5)$$

This is much more symmetrical than the minimal-generalized-coordinate approach would have produced! There is a small cost, in that the  $\lambda$ 's must be determined at each instant of time. But as the following analysis (and follow-up homework) will show, determining the  $\lambda$ 's is a simple exercise in linear algebra.

Let's work out the case  $N = 2$ . The Lagrange multiplier principle is that the gradient of (15.2) vanishes, and for our polymer functional this applies to all the variational derivatives of (15.4):

$$0 = \frac{\delta S'}{\delta \mathbf{r}_1(t)} = -\frac{d}{dt}(m\dot{\mathbf{r}}_1) + 2\lambda_1(t)(\mathbf{r}_1 - \mathbf{r}_2) \quad (15.6)$$

$$0 = \frac{\delta S'}{\delta \mathbf{r}_2(t)} = -\frac{d}{dt}(m\dot{\mathbf{r}}_2) + 2\lambda_1(t)(\mathbf{r}_2 - \mathbf{r}_1). \quad (15.7)$$

Defining a rescaled Lagrange multiplier (to simplify formulas),

$$\lambda(t) = 2\lambda_1(t)/m, \quad (15.8)$$

these equations simplify to

$$\ddot{\mathbf{r}}_1 = -\ddot{\mathbf{r}}_2 = \lambda(t)(\mathbf{r}_1 - \mathbf{r}_2). \quad (15.9)$$

The Lagrange multiplier appears as a time-dependent Hooke's law “constant” — able to adjust (in time) to keep the bond distance fixed at  $d$ .

A method for determining  $\lambda(t)$ , that generalizes to arbitrary  $N$ , begins by taking time derivatives of the constraint equations:

$$0 = \frac{d^2}{dt^2}(\mathbf{r}_1 - \mathbf{r}_2) \cdot (\mathbf{r}_1 - \mathbf{r}_2) = 2(\ddot{\mathbf{r}}_1 - \ddot{\mathbf{r}}_2) \cdot (\mathbf{r}_1 - \mathbf{r}_2) + 2|\dot{\mathbf{r}}_1 - \dot{\mathbf{r}}_2|^2. \quad (15.10)$$

Substituting the accelerations from the equations of motion (15.9),

$$0 = 4\lambda(t)|\mathbf{r}_1 - \mathbf{r}_2|^2 + 2|\dot{\mathbf{r}}_1 - \dot{\mathbf{r}}_2|^2, \quad (15.11)$$

we obtain a formula for the Lagrange multiplier:

$$\lambda(t) = -\frac{|\dot{\mathbf{r}}_1 - \dot{\mathbf{r}}_2|^2}{2d^2}. \quad (15.12)$$

The equations of motion (15.9) may now be solved with this  $\lambda$ :

$$\ddot{\mathbf{r}}_1 = -\ddot{\mathbf{r}}_2 = -\frac{|\dot{\mathbf{r}}_1 - \dot{\mathbf{r}}_2|^2}{2d^2}(\mathbf{r}_1 - \mathbf{r}_2). \quad (15.13)$$

You should check that these equations give the correct central acceleration for two equal mass particles in circular orbits about a common center — the center of the bond that joins them. Because the magnitude of the relative velocity of the two particles is constant,  $\lambda(t)$  given by (15.12) is actually constant. For  $N > 2$  the Lagrange multipliers become time-dependent. This does not further complicate the solution of the equations of motion for general  $N$ , provided it remains easy to solve for the time-dependent  $\lambda$ 's. The  $N = 3$  case in your homework assignment should convince you that the Lagrange multipliers at any time are found by solving a system of linear equations.

**Exercise:** Using freshman physics formulas for circular motion, verify that (15.13) is correct.