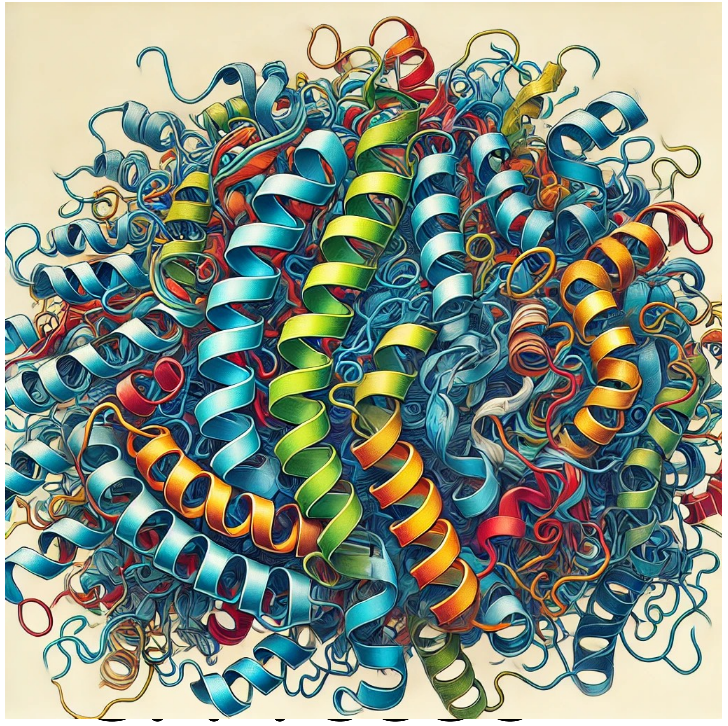
CBP Summer School
Aug 5-16
Lecture 2



Physics Dept., ASU
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What are the classical laws of motion?

Why do these laws apply to atoms?

What is “Molecular Dynamics”?

What forces matter for motions of atoms?

For today, we will just do a bit of math and see how far it takes us.

What are the classical laws of motion?

Classical laws are explained in terms of displacements, velocities, accelerations:

$$x, v, a$$

Velocities give rise to changes in displacement and acceleration gives rise to changes in velocity

$$\Delta x, \Delta v$$

How are all these related?

$$x_f = x_i + v\Delta t$$

$$v_f = v_i + a\Delta t$$

Sometimes we prefer to write these as

$$x_{\text{new}} = x_{\text{old}} + v\Delta t$$

$$v_{\text{new}} = v_{\text{old}} + a\Delta t$$

How are all these related?

Suppose I drive at 60 miles/hr and travel for 2 hrs, how far will I have gotten?

Suppose an object starts falling vertically downward and accelerates at 9.8 meters/ second^2 what will my velocity be if the object is initially at rest after 1 second?

How are all these related?

Velocity makes position change.

Acceleration makes velocity change.

What makes acceleration change?

What makes acceleration change?

$$F = ma$$

Applied forces set the acceleration!

What if you have many forces? The acceleration is the result of the net force.

$$\sum F = ma$$

$$a = \frac{v_f - v_i}{\Delta t} = \frac{F}{m}$$

$$v_f = v_i + \frac{F}{m}\Delta t$$

$$\frac{x_f - x_i}{\Delta t} = v_i + \frac{F}{m}\Delta t$$

$$x_f = x_i + v_i\Delta t + \frac{F}{m}\Delta t^2$$

When no force is applied, objects keep move with the same velocity (they do not accelerate).

The net force on a 1kg block resting on a frictionless surface is 2N to the right. Suppose the object starts at the origin (x=0) at rest.

What is the velocity after 1 sec?

What is the position after 1 sec?

We use the same formula!!

$$x_f = x_i + v_i \Delta t + \frac{F}{m} \Delta t^2$$

What if forces depend on position?

$$m\ddot{x} = F$$

$$\dot{x}(t) = v(t)$$

$$\int \ddot{x}(t)dt = \int \frac{F(x(t))}{m}dt$$

$$x_{\mathrm{new}} = x_{\mathrm{old}} + \int v_{new}(t)dt$$

$$\dot{x} - v_{\mathrm{old}} = \int \frac{F(x(t))}{m}dt$$

$$v_{\mathrm{new}} = v_{\mathrm{old}} + \int \frac{F(x(t))}{m}dt$$

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$$x_{\text{new}} = x_{\text{old}} + \int v(t) dt$$

$$v_{\text{new}} \approx v_{\text{old}} + \frac{F(x_{\text{old}})}{m} \Delta t$$

$$x_{\text{new}} \approx x_{\text{old}} + v_{\text{new}} \Delta t$$

What if forces depend on position?

$$x_{\text{new}} \approx x_{\text{old}} + v_{\text{new}}\Delta t$$

$$\boxed{v_{\text{new}} \approx v_{\text{old}} + \frac{F(x_{\text{old}})}{m}\Delta t}$$

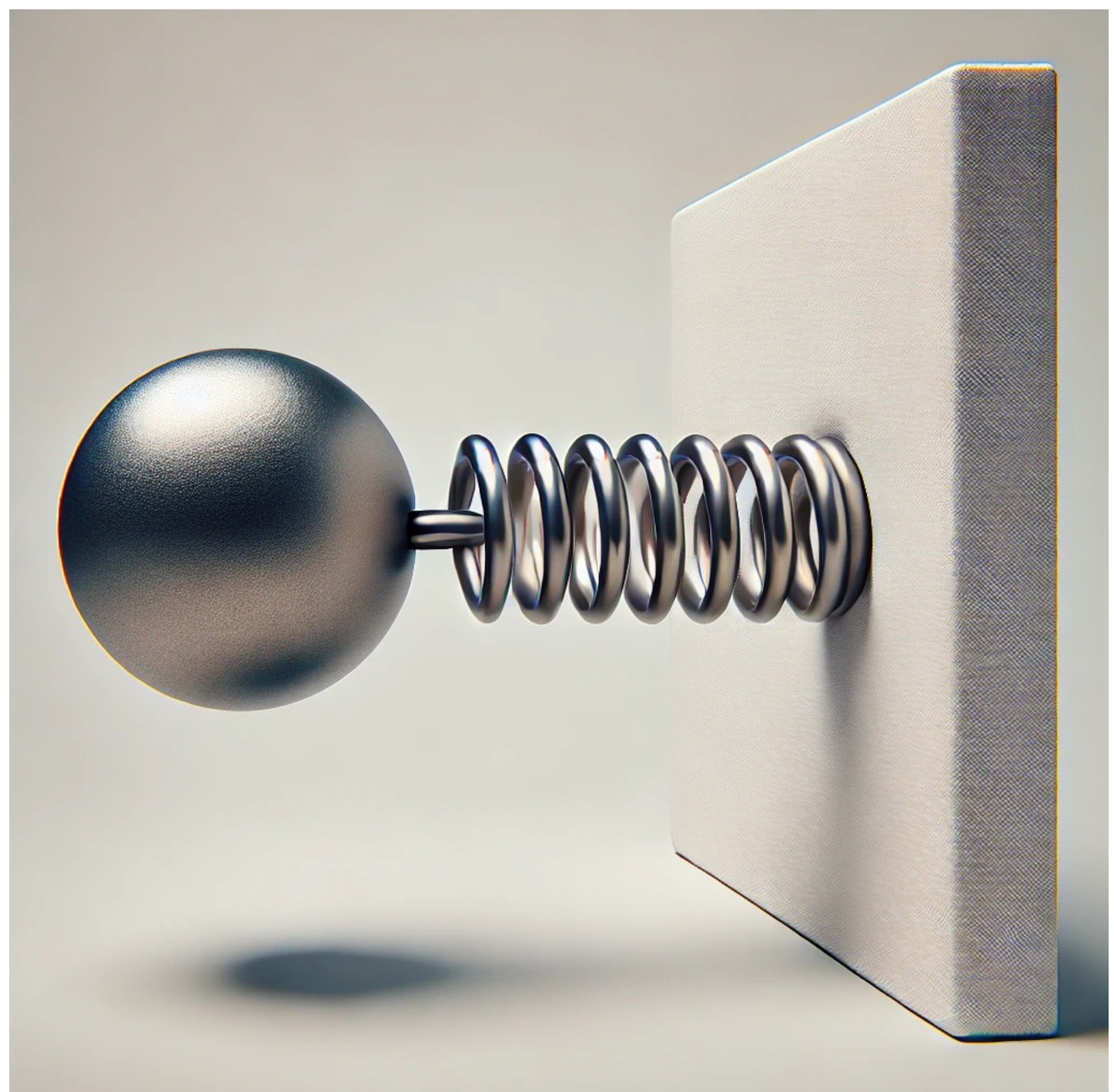
Computers don't know calculus. They know addition/subtraction. Calculus is used to derive results that we plug into computers.

$$v_{\text{new}} \approx v_{\text{old}} + \frac{F(x_{\text{old}})}{m}\Delta t \qquad x_{\text{new}} \approx x_{\text{old}} + v_{\text{new}}\Delta t$$

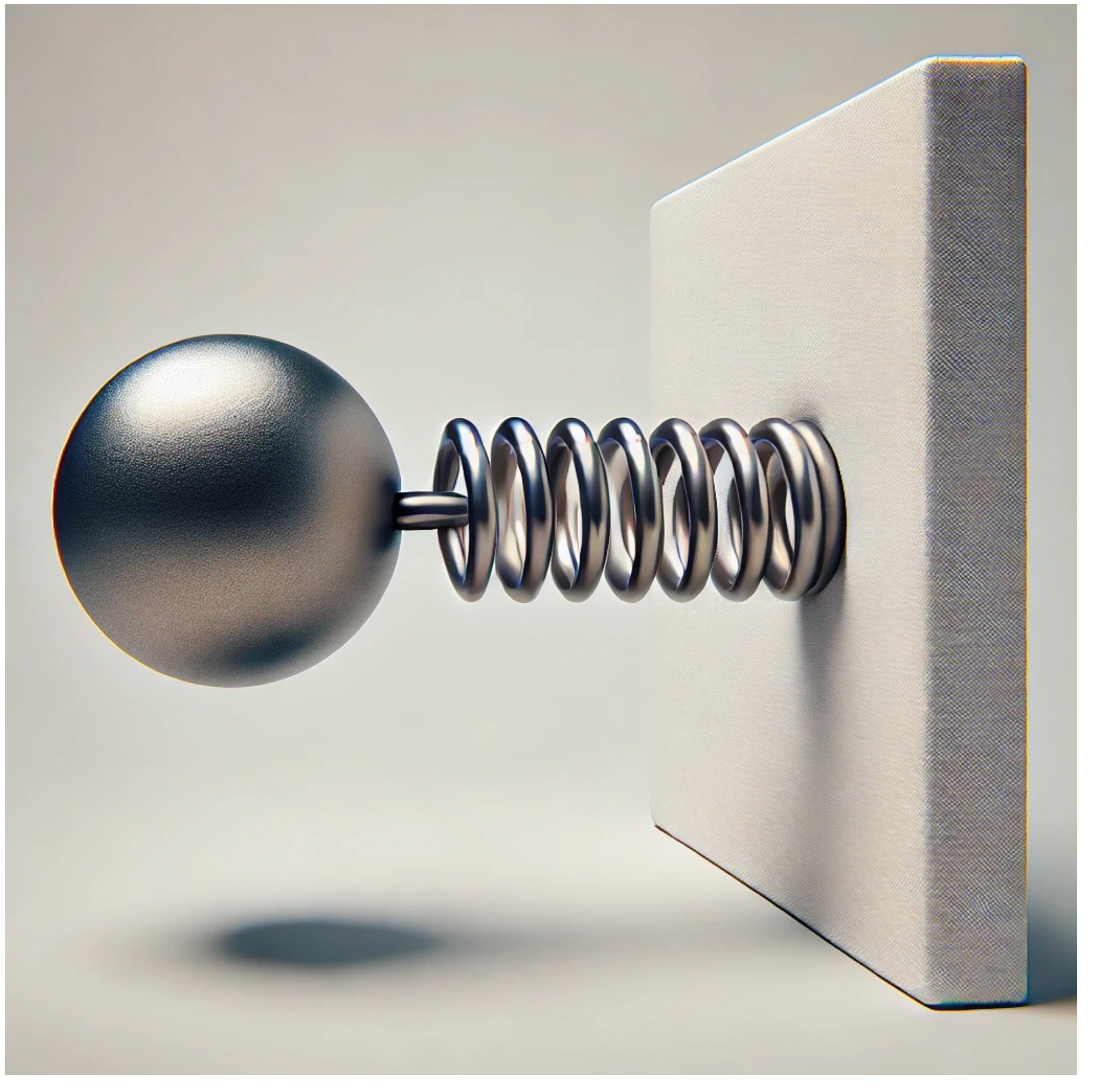
At every time step, from old x,v,F calculate new x,v

What’s a good example of a force that depends on position?

$$v_{\text{new}} \approx v_{\text{old}} + \frac{F(x_{\text{old}})}{m}\Delta t \qquad\qquad x_{\text{new}} \approx x_{\text{old}} + v_{\text{new}}\Delta t$$



If I try to keep the bead at the same (constant) acceleration, then from F=ma then this means that I need to keep applying a stronger and stronger force because my spring wants to recoil!



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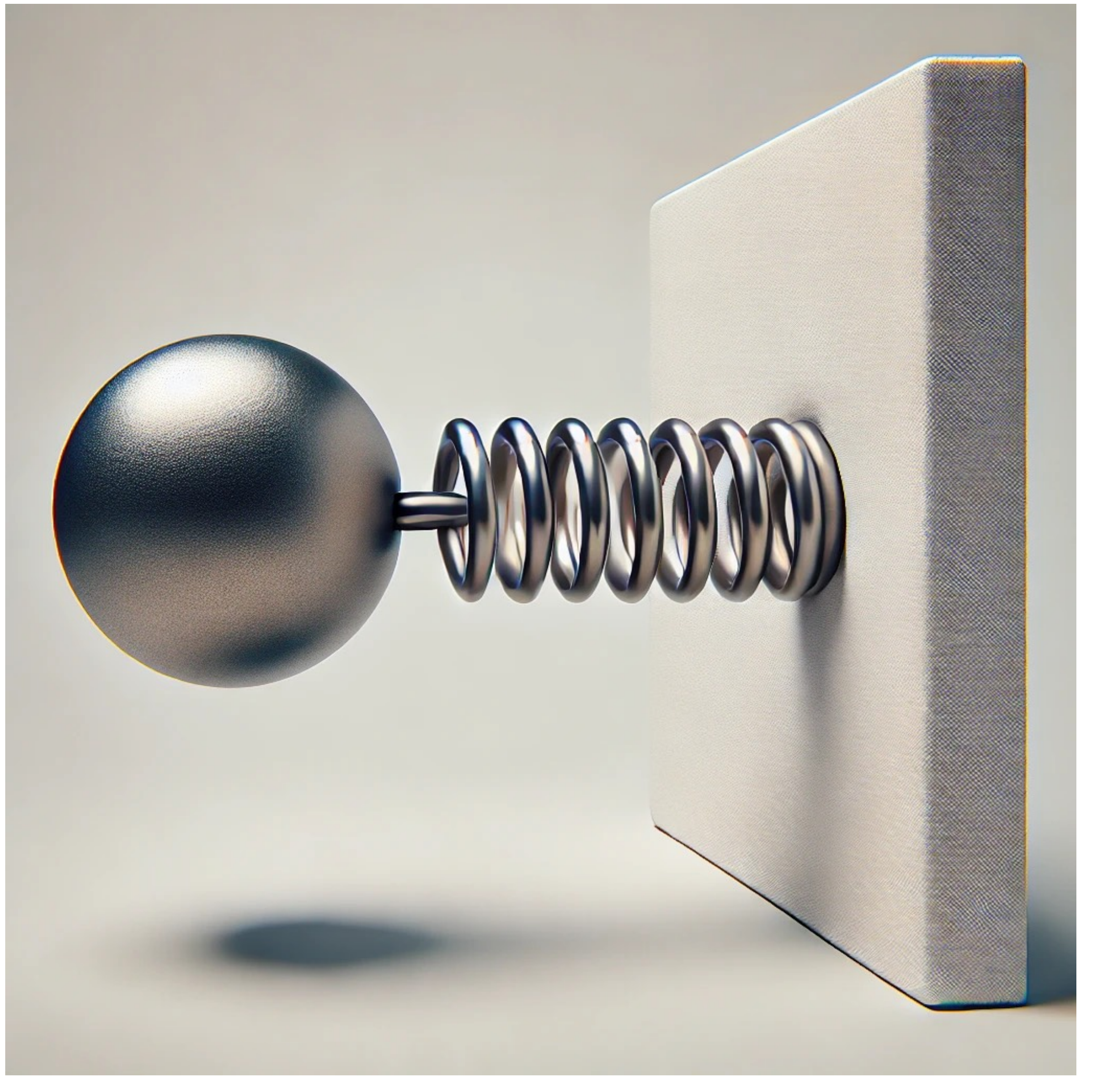
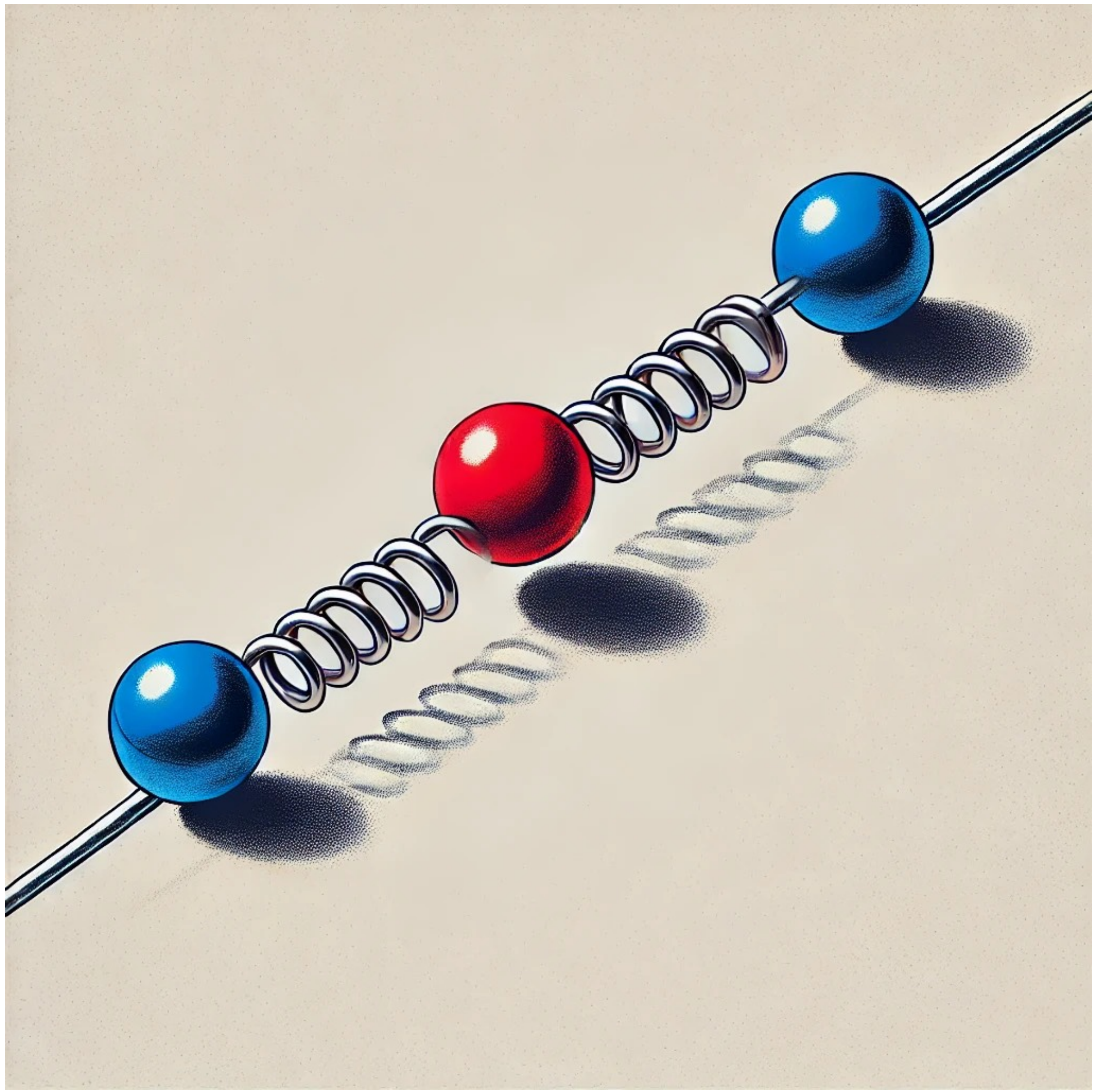


So now force depends on position!!

In fact, this is how atoms interact! If they are far away there is no force between them. But as they come closer there is a force that often depends on the distance between them.



What is energy and how is it related to force?

$$W = F \times d$$

So the sum of the force multiplied by the distance is the work.

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What if the force depends on position?

$$W = \sum F(x)\Delta x$$

We can also write this using calculus

$$W = \int F(x)dx$$

In classical mechanics, we often write

$$F = -\frac{dU}{dx}$$

with

$$U = -W$$

What is total energy of a system in classical mechanics?

Energy of motion plus energy it takes you to get to where you are (-W)

$$E = U + K$$

$$E = U + \frac{1}{2}mv^2$$

Energy is conserved. So when you go up a mountain you spend energy (and feel tired) and when you come back down you…suck back up the energy and feel energized? What is wrong with this reasoning?

Energy is conserved. So when you go up a mountain you spend energy (and feel tired) and when you come back down you…suck back up the energy and feel energized? What is wrong with this reasoning?

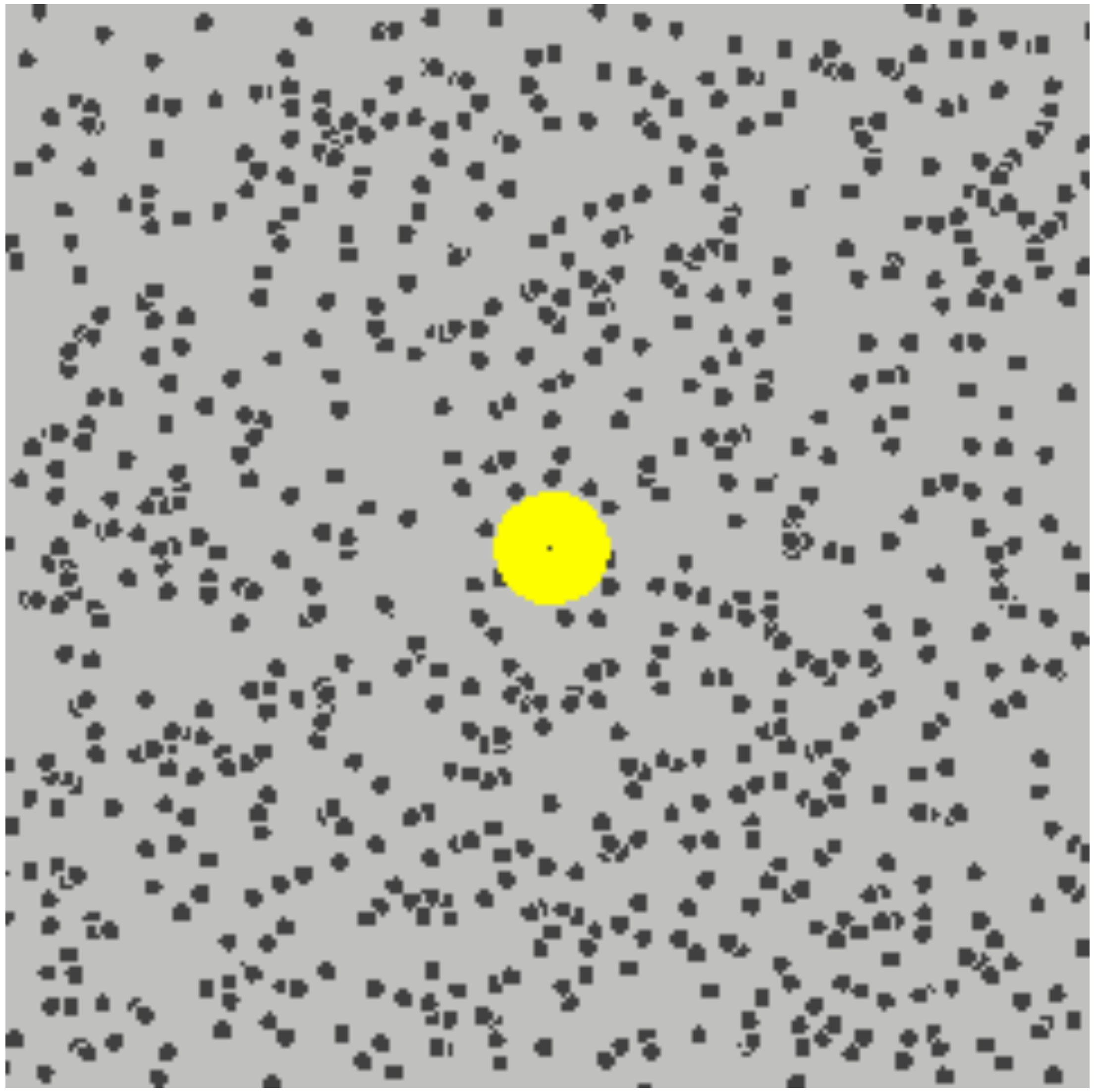
Energy is conserved in the whole universe but not in your body. You lose energy to friction the whole way up and down the mountain. That energy is “lost” to the environment. It is still there, just not accessible to you.

On small scales, the size of a atom or even a protein or pollen grain, that energy in the environment kicks things around in a way that you can see it.

Because on average the particle or “thing” getting kicked around doesn’t accumulate or lose energy then something really interesting happens.

It has to gain as much energy through kicks as it looses through friction.

Here's a "Brownian particle". No net force is being applied (on average the velocity is zero). No net energy is being pumped into the system either.



https://upload.wikimedia.org/wikipedia/commons/c/c2/Brownian_motion_large.gif

In there case of the Brownian particle, the fluid is the "environment". The size kicks it can give is basically what we call "temperature". Each fluid molecule has its own direction of motion and they collide against each other and the Brownian particle of interest.

So when we write down the force acting on an atom (or groups of atoms) of a protein, we need to worry about all the forces due to the other atoms in the protein and the fluid.

so $$\sum F = ma$$

becomes $$\sum F_{\text{atoms}} + \sum F_{\text{fluid}} = m_i a_i$$

for atom indexed i

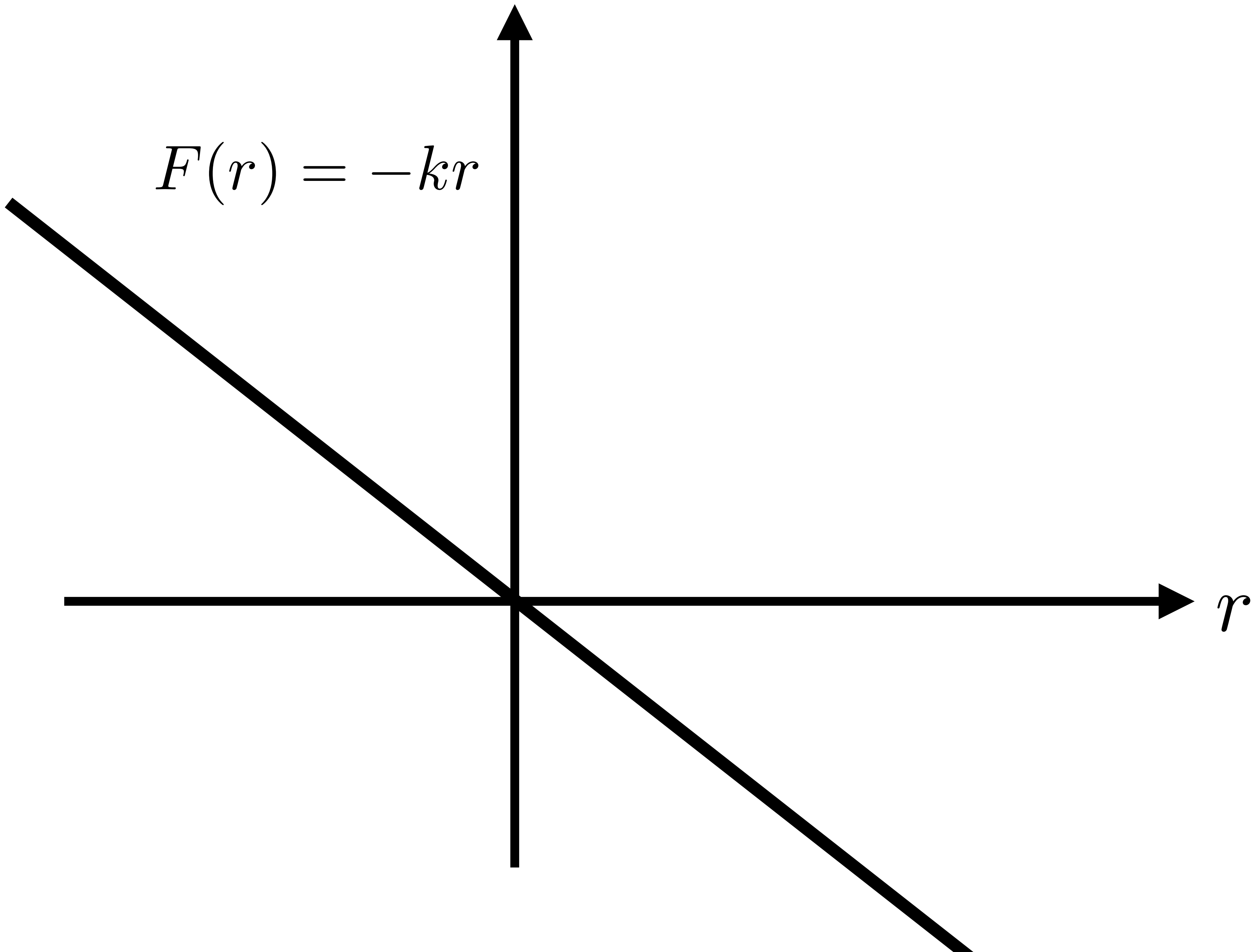
What are there forces like between atoms?

We can equivalently ask, what is the energy like as a function of distance between 2 atoms or groups of atoms?

There is normally a Coulomb term, a Lennard-Jones term, and an elastic force term between bonded atoms.

These terms will be described in later lectures.

For now let's focus on the elastic force term.



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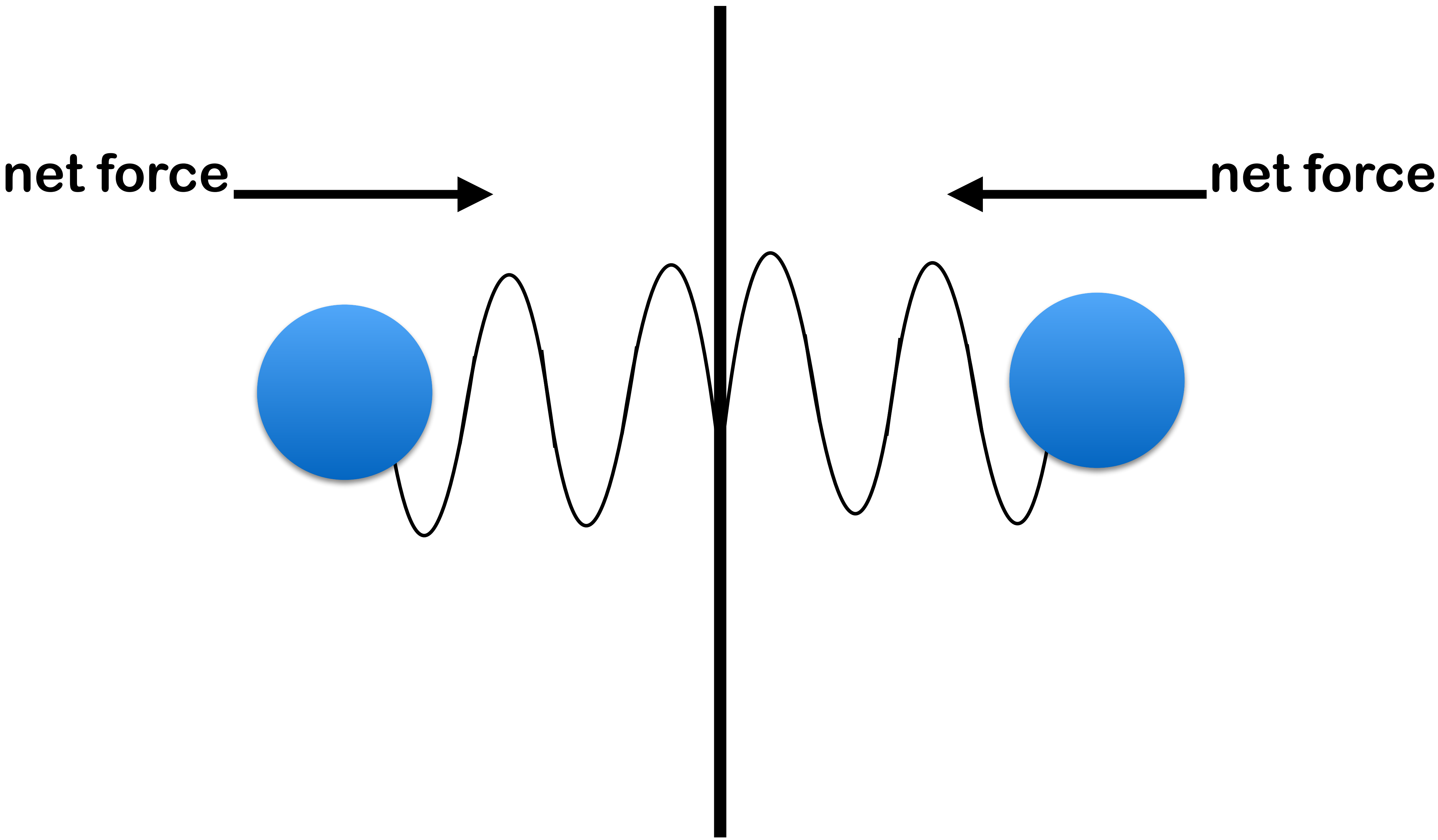

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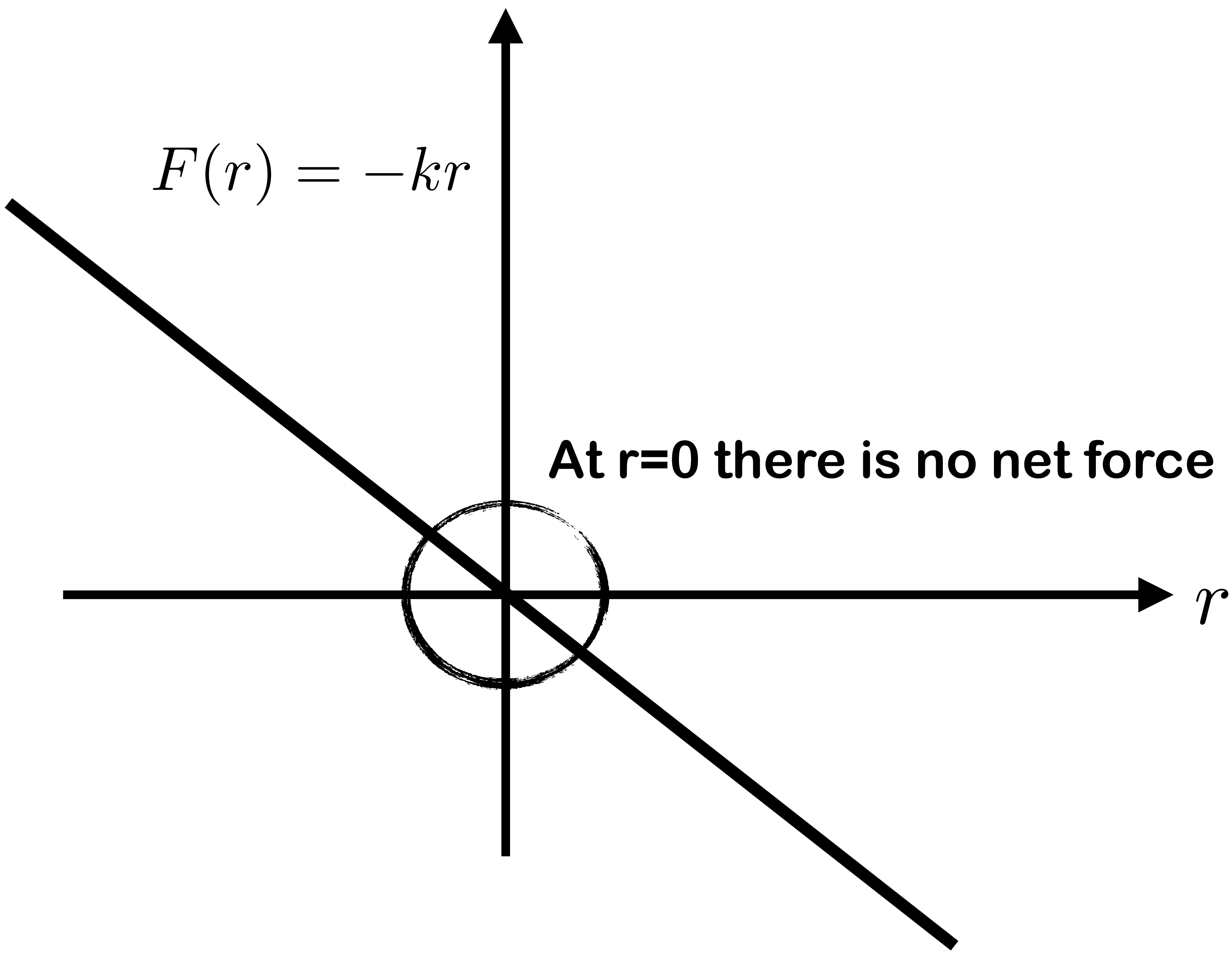
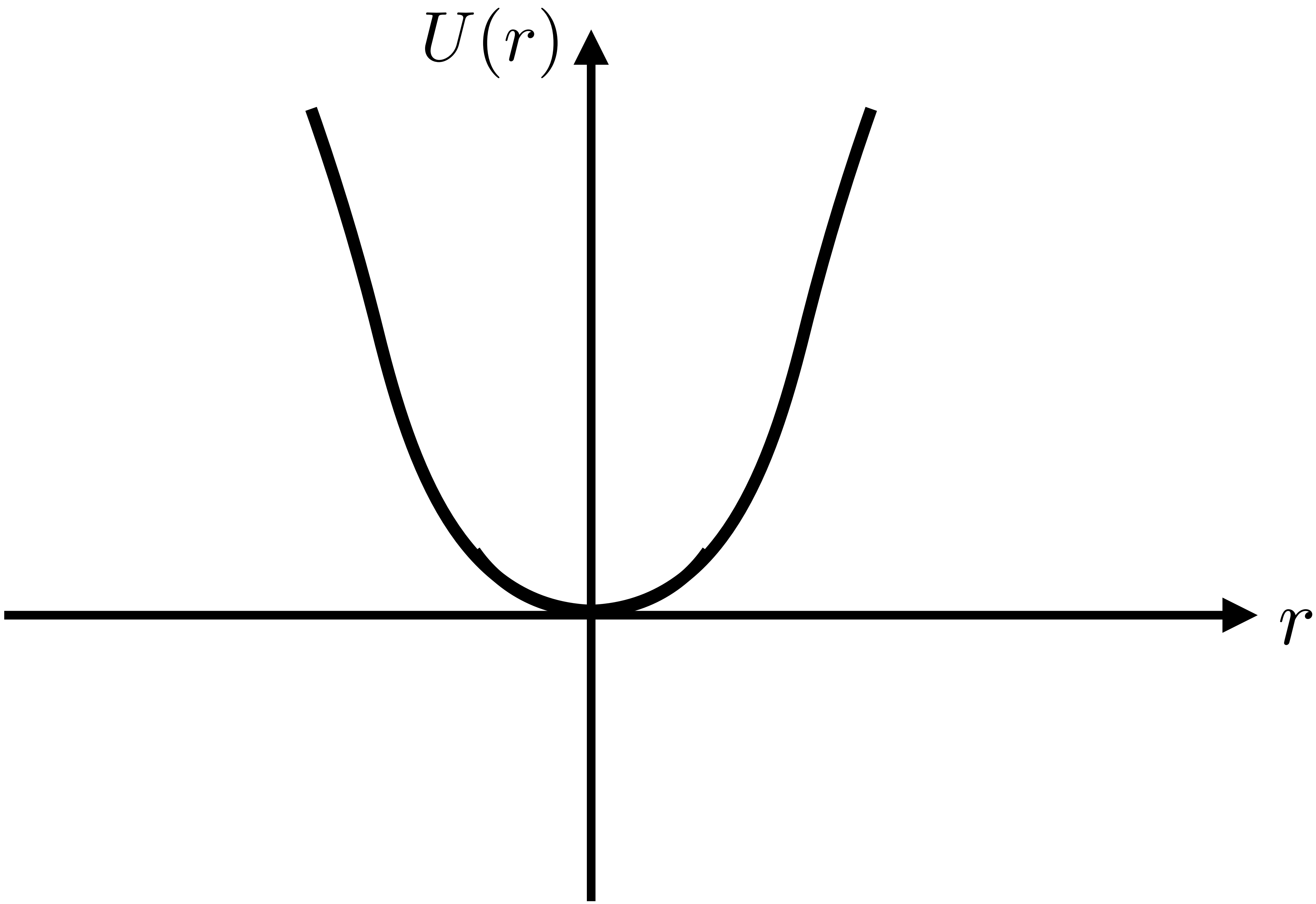


What is the corresponding potential energy, U, term?



What is the corresponding potential energy, U, term?

$$U = \frac{k}{2} r^2$$

So if r is different from zero, the energy grows in proportion to k the spring constant.

So what keeps the whole protein from collapsing into a point?

Lennard-Jones and repulsive Coulombic potential!