Physics 131- Fundamentals of Physics for Biologists I

Professor: Wolfgang Losert wlosert@umd.edu

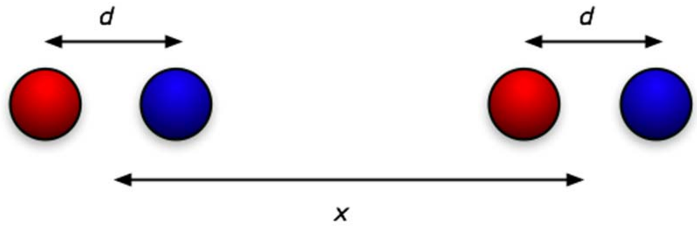
12/03/2012

Molecular Dynamics Simulations
http://www.youtube.com/watch?v=hT0c6Q4DLbk

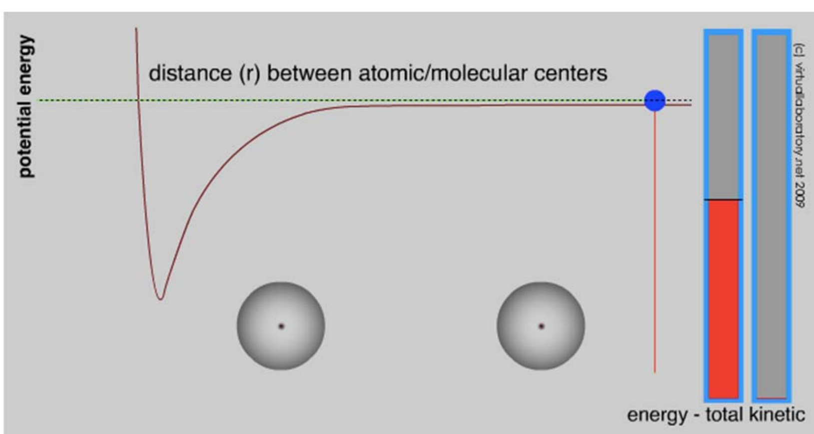
Outline

Quiz 10
Temperature
Temperature & thermal energy
Heat Capacity

What does the potential look like?

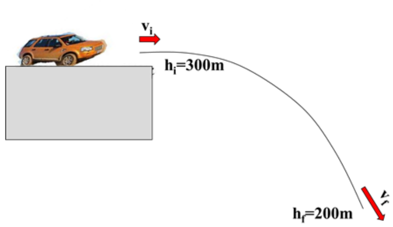


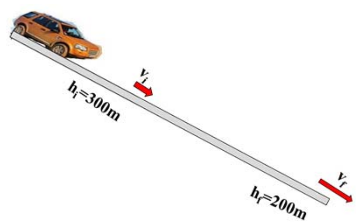
Molecular forces



http://besocratic.colorado.edu/CLUE-Chemistry/activities/LondonDispersionForce/1.2-interactions-0.html

Review: Mechanical Energy Conservation





- Total of kinetic and potential energy are conserved
- normal forces do no work

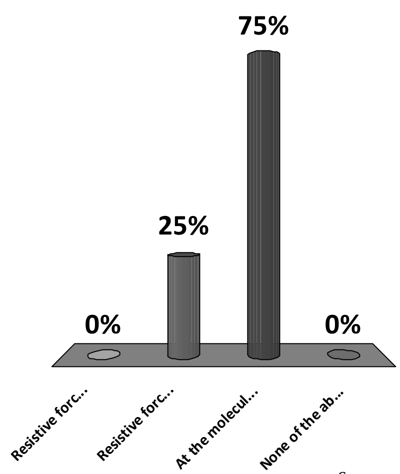
$$\Delta(\tfrac{1}{2}mv^2) = mg\Delta h$$

$$\Delta(\tfrac{1}{2}mv^2 + mgh) = 0$$

$$\tfrac{1}{2}mv_i^2 + mgh_i = \tfrac{1}{2}mv_f^2 + mgh_f$$

In the presence of resistive forces, the total energy is no longer conserved.

1. Resistive forces are dominant at the scales of molecules
2. Resistive forces are negligible at the scale of molecules
3. At the molecular scales, we can see that resistive forces are really kinetic and potential energy of molecules
4. None of the above



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"The kind of motion we call heat"

- We have a natural sense of hot and cold.
- In the 19th century it was learned that the warmth of an object was a measure of a kind of random internal motion of the object's atoms.
- It was found that there was a surprisingly large amount of "hidden" energy that objects possessed as a result of their temperature – and that under the right conditions, this energy could be put to work.

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WHERE IS THERMAL ENERGY INSIDE AN OBJECT?

Example: An objects with 9 atoms and interactions

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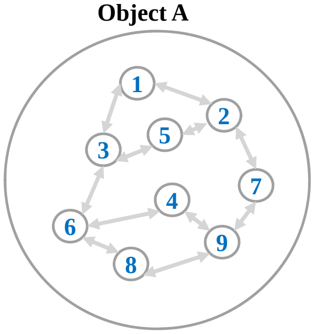
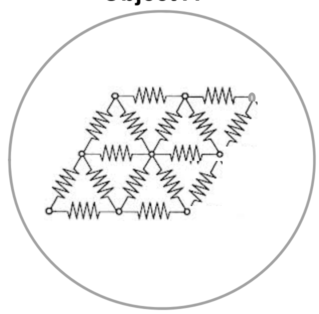
Object A



More concrete for 9 atoms

Object A

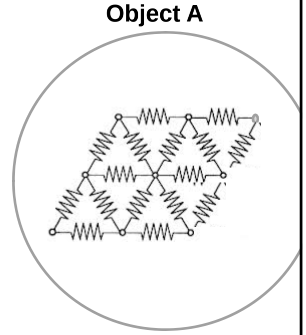


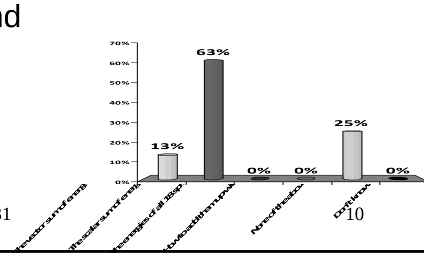
spring-like interaction potentials between atoms

The total potential energy is

1. The vector sum of energies, based on 18 springs, taking into account their orientation
2. The scalar sum of energies of all 18 springs
3. The energies of all 18 springs, counted twice since each spring interacts with two atoms
4. How to add them up will depend on the relative mass of atoms
5. None of the above
6. Don’t know

Object A





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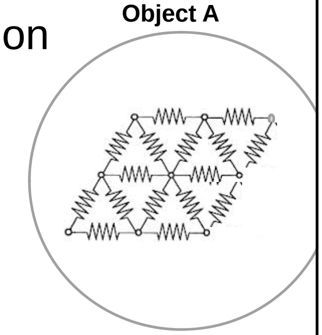
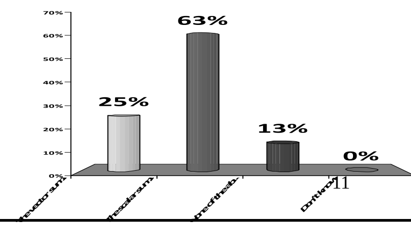
The total energy stored inside the system we call "object A" as motion of the atoms is

Object A



1. The vector sum of kinetic energies, based on the 9 atoms
2. The scalar sum of kinetic energies of all 9 atoms
3. None of the above
4. Don't know



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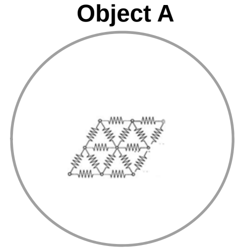
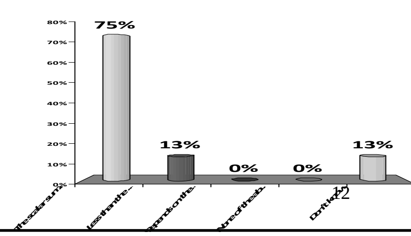
The kinetic energy **OF** "object A" is

Object A



1. The scalar sum of kinetic energies of all 9 atoms
2. Less than the scalar sum of kinetic energies of all 9 atoms
3. Depends on the direction of motion of atoms
4. None of the above
5. Don't know



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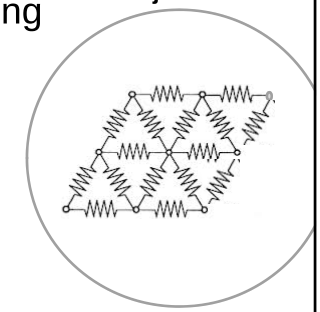
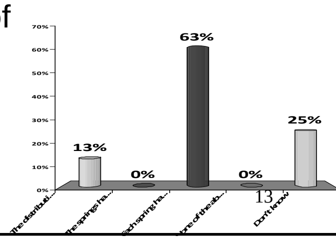
How is the total thermal energy of object A of 540 pJoules shared between spring potential energy and kinetic energy

Object A



1. The distribution of energy between springs and kinetic energy is random and cannot be predicted
2. The springs have half the share of thermal energy (270pJ), the other half of the thermal energy is in motion (270pJ)
3. Each spring has on average a share of the thermal energy of 20 pJ
4. None of the above
5. Don't know



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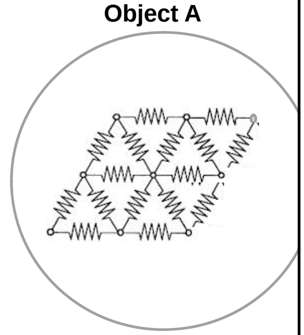
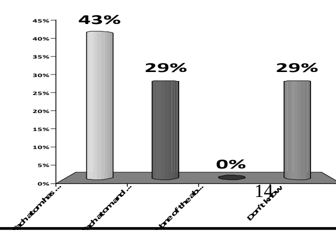
Now consider the temperature of object A at 270K

Object A



1. Each atom has on average a temperature of 270K
2. Each atom and spring interaction has on average a temperature of 10K, their temperatures add up to a temperature of 270K
3. None of the above
4. Don't know



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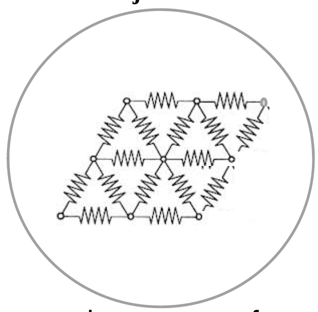
Temperature and Energy

Object A



- **Temperature:** Measures the amount of energy in each atom or interaction – the key concept is that thermal energy is on average equally distributed among all these possible locations where energy could reside.
- **Energy of object A :** Measures the TOTAL energy in the whole object. Depends on temperature and the number of locations where energy could reside.

Scales and Units

- 1 cal = the amount of thermal energy needed to change the temperature of 1gram of water by 1 degree C (from 14.5^o to 15.5^o) (by definition)
- 1 Cal = 1000 cal
- 1 Cal = 4184 J

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- Energy Sharing between objects