

Macroscopic vs. Microscopic Energy Systems

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Here I will discuss the relationship between the *microscopic* energy systems that have been introduced in this course, KE_{tot} and PE_{tot} , and the *macroscopic* energy systems, E_b (bond energy) and E_{th} (thermal energy).

Let's start with a system of bound molecules. The system has two general forms of microscopic energy – KE_{tot} and PE_{tot} . The total energy of our system is given by adding the constituent energies,

$$E_{tot} = KE_{tot} + PE_{tot} \quad (1)$$

Let our system be similar to the one from the computer simulation in DL 11: a small cluster of bonded particles. Let's open our system for a moment, add 2 Joules of energy to KE_{tot} , then close the system again. We saw in DL 11 (the computer simulation) that *over time, that added energy wants to equally distribute between PE_{tot} and KE_{tot}* (see Fig. 1).

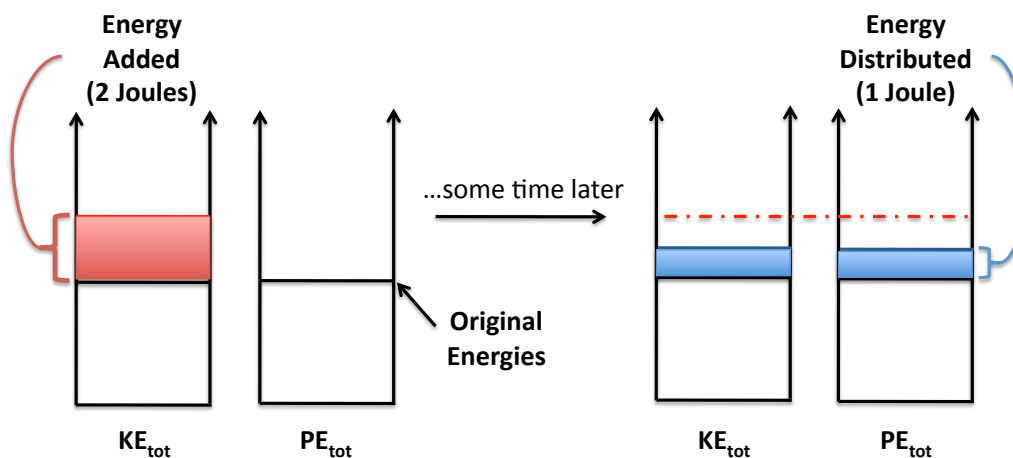


Figure 1: An initial amount of energy is added to one of the microscopic energy systems (KE_{tot}), and this energy over time becomes evenly distributed between the energy systems. Each energy system is depicted as a “reservoir” which holds some amount of the total energy.

A helpful analogy is to think of the energy systems (KE_{tot} and PE_{tot}) as containers of water (see Fig. 1). Pretend we put the two containers right next to each other, separated *only* by a mesh wall (a semi-permeable membrane). If we add 2 Liters of water to one container, we know from experience that the water will slowly flow through the “mesh” wall until the water levels are the same. The result is that each reservoir in the end will appear to have 1 Liter more than they had before we added water.

Claim 1: Like a mass-spring system, KE_{tot} and PE_{tot} in a cluster of interacting particles are equal when averaged over time. This means that if we add energy, and wait long enough, that added energy will be split evenly between KE_{tot} and PE_{tot} .

Let's turn back to our scenario. We've added some energy and let the system stabilize. We can try to relate the macroscopic picture to the microscopic one that we've been discussing, by considering the equation

$$E_{tot} = E_b + E_{th} \quad (2)$$

Does this contradict Eq. 1? *No*. In the microscopic picture, we wrote E_{tot} as the sum of all our *microscopic* energy systems, and in the macroscopic picture, we write E_{tot} as the sum of the *macroscopic* energy systems. This is perfectly fine.

Let's say our atoms are still all bonded together after we added the 2 Joules to E_{tot} . Did the bond energy of our system change? *No*. How do we know this? *We did not break any bonds!* So, if there is no change in bond energy, we see by the above equation that E_{th} must have changed by the same amount as E_{tot} .

However, if the added energy is split evenly between KE_{tot} and PE_{tot} , adding 2 Joules of energy to the system raises KE_{tot} by 1 Joule. E_{th} , on the other hand, must go up by 2 Joules. This implies that

$$KE_{tot} = \frac{1}{2}E_{th} \quad (3)$$

which indeed fits the pattern of our DL data table.

By doing some algebra, we can also find how PE_{tot} relates to E_{th} and E_b :

$$\begin{aligned} E_{tot} &= KE_{tot} + PE_{tot} \\ &= \frac{1}{2}E_{th} + PE_{tot} \\ \implies E_b + E_{th} &= \frac{1}{2}E_{th} + PE_{tot} \\ PE_{tot} &= E_b + \frac{1}{2}E_{th} \end{aligned} \quad (4)$$

What were our assumptions for getting Equations 3 and 4?

- The bond energy remains constant (because no bonds were broken).
- The time average of KE_{tot} is equal to the time average of PE_{tot} .

It turns out these equations work for liquids and solids, where the molecules are bonded even as we add energy to the system.

Claim 2: Both E_b and E_{th} contribute to PE_{tot} in a **solid or liquid**. E_{th} is from random vibrations of particles about equilibrium (so $E_{th} = 0$ at $T = 0$ Kelvin), whereas the E_b term comes from the pair-wise potential energy interactions. E_{th} is split evenly between PE_{tot} and KE_{tot} .

On the other hand, what if we do break apart all the bonds, so that we have a gas? How do these equations change when we have a bond energy of **zero**?

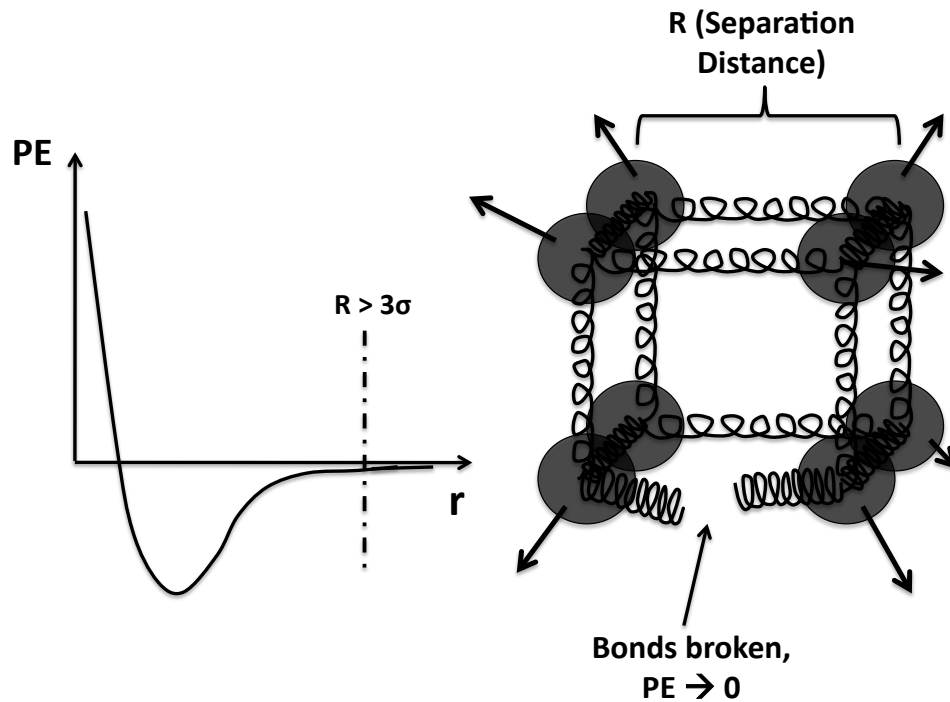


Figure 2: A Lenard-Jones potential is shown for a configuration of particles, with average separation distance R . When the molecules are bonded, or when they are separated by $< 3\sigma$, they behave like a mass-spring system. For gases, $PE_{pairs} \approx 0$ for the configuration of particles (the springs are “cut” so to speak).

If we have a gas, $E_b = 0$ by definition (solids and liquids have *negative* E_b). One can also see this in the Lenard-Jones potential (Fig. 2), noting that $PE_{pairs} \approx 0$ for gases. However, the gas particles are not interacting at all if their “springs” are broken, and therefore do not oscillate around an equilibrium position. Now we know the following:

- $E_b = 0$ in a gas.
- E_{th} does not contribute at all to PE_{tot} in a gas, because the particles have no random movement about an equilibrium position.

We must conclude that $PE_{tot} = 0$. So, we cannot use Equations 3 and 4, because *all* the energy in a gas is in KE_{tot} . We see from Equations 1 and 2 that

$$E_{tot} = KE_{tot} = E_{th} \quad (5)$$

Claim 3: For a gas, which has no PE_{tot} , all energy is in E_{th} (in the macroscopic picture) or KE_{tot} (in the microscopic picture).

It is good to introduce here the idea of a **mode**. A mode is basically an energy term of E_{tot} , i.e. PE_{tot} and KE_{tot} are modes. If E_{th} has to be split between more energy modes, then KE_{tot} will not be as great for that substance.

Take for example a gas placed next to a solid. The gas has less modes, because it does not have a PE_{tot} term, only a KE_{tot} term; the solid has both PE_{tot} and KE_{tot} . We see from the above equations that more of E_{th} goes into KE_{tot} for the gas, meaning that the gas molecules move faster so the gas is hotter. Heat flows from higher temperature to lower temperature, so we know that the heat flows from the gas to the solid.