

Re: How to calculate entropy of particles?

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- *From:* Edward Green <spamspamspam3@xxxxxxxxxxx>
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On Feb 15, 10:12 am, Rick Giuly <rgiuly.gr...@xxxxxxxxxx> wrote:

On Feb 14, 11:40 pm, Eric Gisse <jowr...@xxxxxxxxxx> wrote:

On Feb 14, 9:22 pm, Rick Giuly <rgiuly.gr...@xxxxxxxxxx> wrote:

Hello all,

I'm working on a molecular dynamics simulation based on Lennard-Jones potential. Each particle has a position, a mass, and a velocity.

I know that temperature is the average kinetic energy of all the particles, so temperature is no problem to calculate.

But, how would you calculate the entropy of the particles?

$$S = k \ln(\text{number of states})$$
$$dS = dQ / T$$

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Any help is appreciated.

–Rick Giuly

If replying by email please use: rgiuly at ucsd dot edu

reference:http://en.wikipedia.org/wiki/Lennard-Jones_potential

The problem I have with $S = k \ln(\text{number of states})$ is that it seems like the number of states is nearly infinite, since there are multiple particles and each can be at any location in space.

$$dS = dQ / T$$

This formula tells me something about how the entropy would change when heat is added but I want to calculate the entropy as a function of the position and velocity of all the particles at an instant in time.

So I'm still not sure how to calculate the entropy (as a function of the position and velocity of all the particles at an instant in time).

Annoying people like to say that entropy is a measure of our ignorance. Specifically, it's a measure of how many microstates are compatible with a given macrostate: the "macrostate" is a description of our knowledge about the system (temperature, pressure, volume... etc.).

Given a particular microstate, I don't see any necessary meaning to its "entropy", although for extreme fluctuations, we might mean "the entropy of the resulting restricted set of microstates if we partitioned the system at that instant".

Example: by random fluctuation, more molecules will in general be in one half of a box than the other half. If we lowered a shutter at that instant, this fluctuation would be preserved in macrostate as a density and pressure differential between the sides. If we calculated the entropy of this resulting pair of systems, it would be lower than the original undivided system: i.e., the measure of the volume of microstates it could occupy would be smaller. In this sense we might say "the microstate showed an entropy fluctuation". However, the value of this fluctuation would depend on how we partitioned the system when we took the snapshot, lest you think the idea is unambiguous.

Another problem seems to be the application of $S = k \ln(\omega)$ to cases where the possible states are "nearly infinite" — i.e.,

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continuous. Presumably ω is replaced by a volume in phase space.
The first problem is more fundamental.

Entropy is not like "mass" or "energy", which have a well defined value for a microstate: it's a property of macrostates.