

Re: How to calculate entropy of particles?

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- *From:* Rick Giuly <rgiuly.group@xxxxxxxxxx>
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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?

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

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

Re: How to calculate entropy of particles?

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).

–Rick