Honors Stat Mech
Project 3

Physics 423 Spring 2017

Due: Thurs, Mar. 10 ***No Writeup Required, Only Plot***

Canonical Ensemble and Importance Sampling. (Gould & Tobochnik 4.33)

The canonical ensemble describes the probability distribution of microstates of any system coupled to a large heat bath of temperature T:

$$P(s) \propto e^{-E(s)/T} \tag{1}$$

in units where $k = 1$. Simulating the canonical ensemble requires care because of the exponential suppression of high-energy states. For example, in the naïve approach, one would generate a large number of microstates at random and then compute mean quantities by averaging over this sample, weighting each contribution by $P(s)$. However, this approach is extremely inefficient, because in general a large number of high-energy microstates are included that make negligible contribution to any observable.

A more efficient algorithm uses *importance sampling*, which is a technique to generate a sample in which microstates with larger $P(s)$ are more likely to appear. The sample is a Markov chain in which element t is a microstate x_t. The simplest way to implement it, known as the Metropolis algorithm, is as follows:

- Choose an initial microstate at random. Set it to x_0.
- The update step: Make a trial change in the microstate, for example by changing the state of a single degree of freedom at random. This change induces a change in the energy of the microstate ΔE.
- If $\Delta E < 0$, keep the change. (Set x_{t+1} to the new microstate. This way it is both saved and used as the starting point for the next update step.) If $\Delta E > 0$, keep the change with probability $e^{-\Delta E/T}$. For example, generate a random number between 0 and 1, and keep the change or not depending on whether the random number is less than $e^{-\Delta E/T}$. If the change is *not* kept, set $x_{t+1} = x_t$, so that the current microstate is reused at the next step.
- Repeat the previous two steps many times, generating an ensemble of microstates.

Averages can then be computed directly from this ensemble without additional weighting.

1. Implement importance sampling to generate the canonical ensemble for an 20-particle one-dimensional Einstein solid (20 one-dimensional harmonic oscillators). For the initial state, choose something where the total energy is not too far from NT. For the update step, increment or decrement a random oscillator's energy by one unit. Generate sufficiently large ensembles that the average energy of the solid stabilizes.
2. Change T and make a plot of $\bar{E}(T)$. Compare to the expectation from equipartition, $\bar{E}(T) \to NT$, which should hold in the classical limit of large temperatures.