PHY441 Final Project

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Intro

Using the Metropolis algorithm, an Einsten-model solid is simulated. A series of N quantum harmonic oscillators coupled with a heat bath at temperature T will cause the average energy $\langle E(T) \rangle$ to eventually reach a stable, converging value.

The probability of a given energy level being populated in a canonical ensemble is given by

$$P(E_n) = \frac{e^{-n\beta h\nu}}{Z}$$

In our system we have set $h\nu = 1$, and the thermodynamic beta $\beta = 1/T$ (we are working in units such that the Boltzmann constant is 1):

$$P(E_n) = \frac{e^{-n\beta}}{Z}$$

The partition function is

$$\begin{aligned} Z &= \sum_{n=0}^{\infty} e^{-n\beta} \\ &= \frac{1}{1-e^{-\beta}} \end{aligned}$$

And the average energy is

$$\begin{aligned} \langle E \rangle &= \sum_{n=0}^{\infty} e^{-n\beta} \\ &= \frac{e^{-\beta}}{1-e^{-\beta}} \end{aligned}$$

The Metropolis algorithm has been implemented as follows, where we have pre-selected fixed T, n, N (N = number of Monte Carlo steps/iterations to perform):

1. For n particles, create a microstate with corresponding $E_0 = n$ energy.
2. For the first step, set $E_i = E_0 = N$.
3. Set the value of $E_j = E_i \pm 1$, where the sign is randomly picked. Ensure that it can never be negative.
4. For all sequential steps, calculate the value of $\Delta E = E_j - E_i$.
   (a) If $\Delta E < 0$, accept the change, and set $E_i = E_j$ and proceed to the next iteration.
   (b) If $\Delta E > 0$, choose a random number between $r = (0, 1)$. Then, choose another number $w = e^{-\beta \Delta E}$:
      i. If $r \leq w$, accept the change.
      ii. If $r > w$, $E_i = E_j \cdot w = E_j \cdot e^{-\beta \Delta E}$. *This is the key part of the algorithm!*

Results

Note that in these plots we have done 2500 iterations in the Monte Carlo simulation. The results of higher iterations do not seem to differ much at these temperatures, so it is safe to assume that these results have allowed a sufficient progression for us to distinguish divergent and convergent behaviors.

- In the first category of the attached figures, we see the plots for both $n = 20, 100, 200$ and $0.5 < T < 9$. There are multiple Monte Carlo simulations composited in each plot.
  - We can see pretty clearly that the $\langle E \rangle$ values converge eventually.
  - For smaller temperature values, the behavior converges quickly; for larger temperature values, the behavior is still convergent but takes longer.
- In the second category of the attached figures, again we see the plots for $n = 20, 100, 200$ particles for $\langle E(T) \rangle$ values.
  - The analytical $\langle E(T) \rangle$ trend is easily distinguished, colored in turquoise.
  - We can see that for larger T, the $\langle E(T) \rangle$ values begin to diverge but still stay relatively near each other.
  - The analytical and simulated results show a similar trend in general, but there are noticeable differences between the two.