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Phys 466: Atomic Scale Simulation

Homework #5 – MonteCarlo

**Problem #1**

(a)

Given:

$$P(\{r\} \rightarrow \{r\}') = T(\{r\} \rightarrow \{r\}')\, A(\{r\} \rightarrow \{r\}')$$

Where T is the sampling probability as r is changed to r' and A is the acceptance probability.

$$A(\{r\} \rightarrow \{r\}') \equiv \min\left(1, \frac{\pi\{r\}' \, T\{r\}' \rightarrow \{r\}}{\pi\{r\} \, T\{r\} \rightarrow \{r\}}\right)$$

Since the acceptance ratio takes the minimum of these values and the second value is a ratio, we utilize the ratio as the acceptance probability.

Thus, plugging this for equation 1 we get

$$P(\{r\} \rightarrow \{r\}') = T(\{r\} \rightarrow \{r\}') \frac{\pi\{r\}' \, T\{r\}' \rightarrow \{r\}}{\pi\{r\} \, T\{r\} \rightarrow \{r\}}$$

$$P(\{r\} \rightarrow \{r\}') = \frac{\pi\{r\}' \, T\{r\}' \rightarrow \{r\}}{\pi\{r\}}$$

So

$$\pi\{r\} \, P(\{r\} \rightarrow \{r\}') = \pi\{r\}' \, T\{r\}' \rightarrow \{r\}$$

On the right side, A the ratio will be greater than 1. As a result the minimum between the two will be 1. This will mean that $T\{r\}' \rightarrow \{r\}$ = $P\{r\}' \rightarrow \{r\}$

So

$$\{r\} \, P(\{r\} \rightarrow \{r\}') = \pi\{r\}' \, P\{r\}' \rightarrow \{r\}$$

(b)

Given that

$$C = k_B \beta^2 \left( (E^2) - (E)^2 \right)$$

$$E = K + V$$

$$Var\,(E) = < E^2 > - < E >^2 = < (K+V)^2 > - < K + V >^2$$

$$= < K^2 + 2KV + V^2 > - (< K > + < V >)^2$$

$$= < K^2 > + 2 < KV > + < V^2 > - < K >^2 - 2 < K >< V > - < V >^2$$

$$= (< K^2 > - < K >^2) + (< V^2 > - < V >^2) + (< KV > + < K >< V >)$$

Therefore

$$= Var(K) + Var(V) + 2 * 0 = Var(x) + Var(V)$$

(c)

$$< K^2 > - < K >^2 = 3N/2\beta \, , < K > = 3N/2\beta$$

$$< K^2 > = \frac{\int d\{p\} K^2 e^{-\beta \mathrm{K}}}{\int d\{p\} e^{-\beta \mathrm{K}}} = \int_{-inf}^{inf} d\{p\} (\frac{p^2}{2m})^2 e^{-\beta(\frac{p^2}{2m})} = \frac{90}{\beta^2}$$

$$< K^2 > - < K >^2 = \frac{90}{\beta^2} - \frac{9N^2}{4\beta^2}$$

Given that N = 6

$$< K^2 > - < K >^2 = \frac{90}{\beta^2} - \frac{9N^2}{4\beta^2} = \frac{18}{2\beta^2} = 3N/2\beta$$

**Problem #2**

(a)

$$\tau_l(25\% \; acceptance \; ratio) = 0.0002$$
$$\tau_m(50\% \; acceptance \; ratio) = 0.000084$$
$$\tau_h(75\% \; acceptance \; ratio) = 0.00002$$

(b)

$$\tau(50\% \; acceptance \; ratio) = 0.0005$$
$$\tau(80\% \; acceptance \; ratio) = 0.00004$$
$$\tau(99\% \; acceptance \; ratio) = 0.00007$$

(c)

0.0002: time = 2.85, time for simulation = 515
0.000084 = time = 14.132 time for simulation = 545 seconds
0.00002: time = 25.245, time for simulation = 502 seconds
0. 0005: time = 1.316, time for simulation = 501 seconds
0.00004 : time = 14.329, time for simulation = 512 seconds
0.00007: time =17.211, time for simulation = 511 seconds

(d)

The minimum product between the correlation time and real time pass was found for this. Of the six choices the smallest product was found to be smart montecarlo method at 50% acceptance.

**Problem #3**

The variance was found from a list of potentials and the variance between those values were calculated.

Temperature prior to transition = 1.06
Heat capacity = 121.418

Temperature at transition = 1.13
Heat capacity = 118.367

Temperature after transition = 1.31
Heat capacity = 112.642

At the transition, heat capacity decreases more with an increase in temperature indicating the increase in how much less increase in temperature needed to increase the temperature of the entire system.