Consider a single atom, which has the potential energy *E(x)=kcx2* , where *x* is atom’s coordinate and *kc*=0.1 is a constant. Develop a Monte Carlo (MC) program, which computes the average energy *<E>* of this atom at the temperatures *T* from 0.1 to 1.0 with the increment of 0.1. For simplicity assume that *kB*=1. Set maximum position displacement during MC move to *dx*=10. Also, set at each temperature the initial coordinate value *x* to 100.

If MC code works correctly, then *<E> ≈ T/2*. The deviation of *<E>* from the theoretical result *T/2* should not exceed 10%. Present the results as a plot *<E>* vs *T* and as a table. Include in the table the number of MC steps performed to obtain *<E>* at each *T*. I also need to see your code.

*Optional assignment for extra credit*: Compute the acceptance rate at each temperature and investigate its dependence on temperature.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Temperature (T) | Expected <E> as T/2 | Calculated <E> | Iterations to <E> goal | Accepted Iterations | Acceptance Rate |
| 1.0 | 0.5 | 0.54999 | 98239 | 14247 | 0.1450 |
| 0.9 | 0.45 | 0.49499 | 97382 | 14213 | 0.1460 |
| 0.8 | 0.4 | 0.439998 | 75352 | 10922 | 0.14495 |
| 0.7 | 0.35 | 0.384997 | 91730 | 13342 | 0.1454 |
| 0.6 | 0.3 | 0.329998 | 138199 | 19824 | 0.1434 |
| 0.5 | 0.25 | 0.274998 | 128048 | 36528 | 0.2853 |
| 0.4 | 0.2 | 0.219999 | 213298 |  |  |
| 0.3 | 0.15 | 0.164999 | 210398 |  |  |
| 0.2 | 0.1 | 0.109999 | 264597 |  |  |
| 0.1 | 0.05 | 0.054999 | 451197 |  |  |

I used Excel to calculate the average energy. See Excel document attached.

A description of the code is as follows;

1. Find the potential energy at the initial X of 100.
2. Added a random step for X, I used positive and negative steps. And calculated the new energy state.
3. Evaluated the new energy state.
   1. If new energy was lower than the original energy, I accepted the new X position, if not then b
   2. I generate a uniform random number “a” and calculated a Relative Boltzmann Factor (BRF).
      1. If a <= to the BRF, I accepted the new X position, if not then ii
      2. I kept the previous X position.
   3. I average the potential energy with the current X value
4. I would repeat the iterations till the average the energy was less than 110% of the Temperature divided by 2,

I was only able to calculate the accepted iteration down to the calculation for temperature equal to 0.5 because Excel could not handle the calculations beyond 150,000 iterations. I added a modification to the calculations to add more iterations assuming that the atom would stay at potential energy state of zero for infinity and continue to add iterations with zero potential energy till the stopping condition was meet. At High Temperatures, I see no effect on the Acceptance Rate in the data. Looking at the Relative Boltzmann factor equation (e-E/kT), I can see that at higher temperatures, high energy increases are more likely to be accepted. On the other hand, at lower temperatures there is a greater probability of rejecting the state.