At very low T (large β), $Z \approx g_1$ and is almost equal to 1, which means that when the temperature is lower enough, almost all particles will occupy low energy level even with degeneracy. And more particles will occupy higher energy level if the temperature increase. In Figure 6, we observe a good correlation between theoretical of the high temperature partition function approximation. The calculation of partition function in higher temperature is closer to the theoretical result but for low temperature (10K), the difference is significant. So, means calculation of partition function will be more accurate in higher temperature.

4. Coupled harmonic oscillators

In a canonical ensemble with N coupled harmonic oscillators with constant total energy (U), the total energy can be distributed the energies randomly (different oscillators have different energies or all oscillators have the same energy) by looping over several cycles, and these oscillators can exchange energy with each other. The simulation scheme is shown in Figure 7 below.

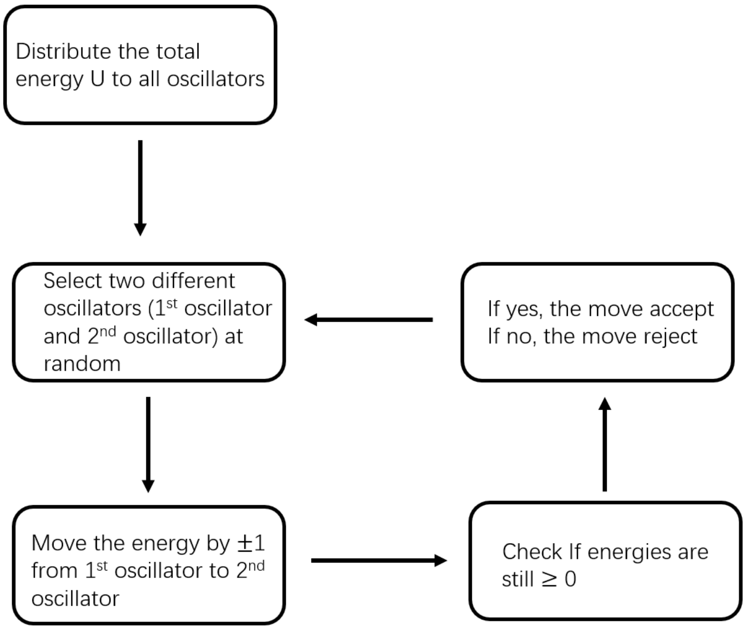

Figure 7. computational scheme for simulation of the system with coupled harmonic oscillator

As the scheme shown, first we select two different oscillators randomly with based on the RandomNumber() function shown in the code below:

```
do
{
  OscA=NumberOfOscillators*RandomNumber();
  OscB=NumberOfOscillators*RandomNumber();
} while(OscA==OscB);
```

In the next step, the program randomly decides the direction from which oscillator to which oscillators the energy moves with the code below:

```
if(RandomNumber()<0.5)
  A=UP,B=DOWN;
else
  A=DOWN,B=UP;
```

In the last step, we check if the energy of one of them is negative. If yes, the move will be rejected with the code below:

```
if(MIN(Oscillator[OscA]+A,Oscillator[OscB]+B)>=0)
{
  Oscillator[OscA]+=A;
  Oscillator[OscB]+=B;
}
```

4.1 The energy distribution of the first oscillator

In Figure 8, we consider the NVE ensemble with constant energy (U=100), we can see at constant energy, when the number of oscillators in the ensemble increase, the occupation of lower energy level will be larger. It is similar with canonical distribution at constant temperature for Boltzmann distribution especially when the number of oscillators is large enough.

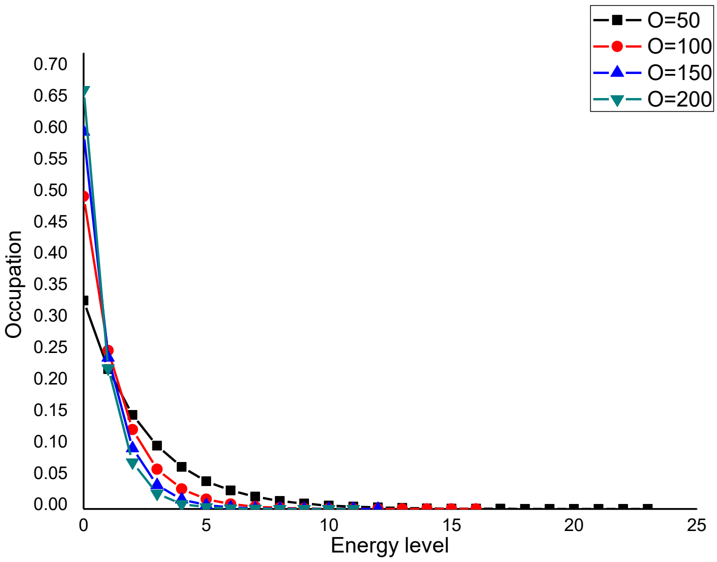

Figure 8. Energy distribution of the first oscillator for different number of oscillators

Then, we consider the NVT ensemble which only have single oscillator in the system. We run the NVT simulation with similar average energy and NVE simulation (O = 50), the comparison result is demonstrated in Figure 9. The calculation results are shown below with average energy first oscillator obtained 1.971306 for (NVE, O=50) and average energy of 1.912633 for (NVT, β=0.41).

```
Number of Oscillators? 50
Number of Cycles (x 1000)? 100
1. NVE Ensemble
2. NVT Ensemble
1
Total Energy           ?
100

Initial energy : 100

Final Energy                        : 100
Average Energy First Oscillator 1   : 1.971306
```

```
Number of Oscillators? 1
Number of Cycles (x 1000)? 100
1. NVE Ensemble
2. NVT Ensemble
2
Beta              ?
0.41

Initial energy : 0

Final Energy                        : 3
Average Energy First Oscillator 1   : 1.912633
```

In the NVT simulation, the temperature reservoir is achieved by adding several oscillators. Therefore, the single oscillator interacts with other N-1 oscillators which act as heat bath at fixed temperature and exchange energy with them. The simulation result for these two simulations is exactly similar in Figure 9 and confirm that other N-1 oscillators operate as a heat bath in NVT simulation.

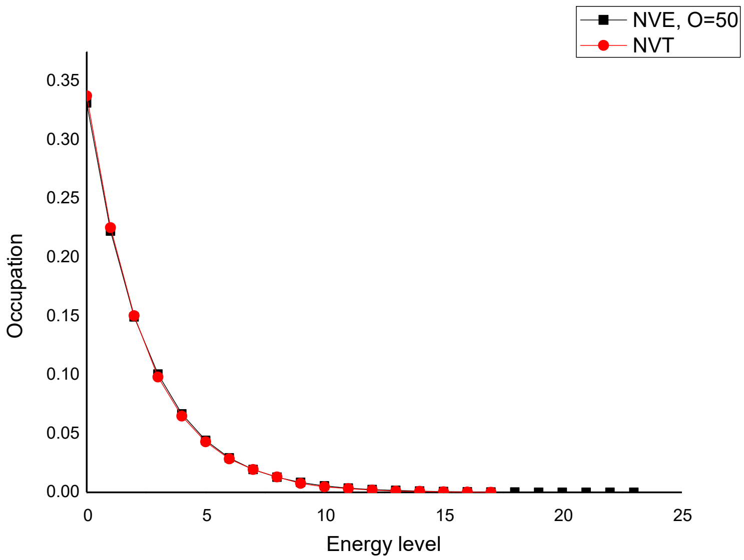

Figure 9. Comparison NVT ensemble and one oscillator of the NVE ensemble with 50 oscillators

5. Random Walk on a 1D lattice

Let us consider a system with a single particle taking random walk on a 1D lattice, this particle can jump to the right (+1) or to the left (-1). Consider p be the probability of going to the right and q the probability of going to the left, so:

$$p + q = 1 \tag{1}$$

$$p = q = \frac{1}{2} \tag{2}$$

The total number of particles jumps is N, make n_R jumps to the right and n_L to the left, and the relationship between n_R, n_L and N is: