# An Einstein Solid

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This project is devoted to study statistical properties of an Einstein solid both analytically and by performing numerical simulations. In particular, we derive the dependence of the temperature of an Einstein solid on the total energy $E$ and number of particles $N$; we show that numerical simulations follow our theoretical expectations. For numerical simulations we use the so-called demon algorithm.

## I. PRELIMINARIES

Einstein developed a very simple model for mechanical vibrations on a lattice. This model is called the Einstein solid and consists of a 3-d lattice which contains $N/3$ lattice sites, with one atom attached to each lattice site. Each atom can oscillate about its lattice site in three independent spatial directions, $(x, y, z)$. Thus, each lattice site contains three independent oscillators. The entire lattice contains a total of $N$ oscillators, which are assumed to be harmonic oscillators, all having the same radial frequency $\omega$. The vibrations of the solid are due these $N$ harmonic oscillators. A single harmonic oscillator has an energy $\varepsilon = 1/2\bar{h}\omega + n\bar{h}\omega$ , where $\bar{h}$ is Planck's constant, $1/2\bar{h}\omega$ is the zero-point energy of the harmonic oscillator, and $n = 0, 1, 2, \ldots, \infty$ is an integer.

## II. MULTIPLICITY OF AN EINSTEIN SOLID

First to simplify the notation lets shift the energy levels of the Einstein solid and introduce dimensionless energy scale $E$ such that $E = n$.

Let us assume that "$E$ quanta on the lattice" is a macroscopic state, and let us determine the multiplicity of this macroscopic state. We need to determine how many ways $E$ quanta can be distributed among $N$ distinct pots. This is straightforward if we draw a picture. Represent a quantum of energy by an $x$ and $N$ pots by N-1 vertical lines. For example, if $E = 9$ and $N = 6$, then one way to distribute the quanta is represented by the picture $\{xx|xxx||x|xx|x\}$. We can determine all possible ways to distribute $E = 9$ quanta among $N = 6$ pots by finding the number permutations of nine $x$s and five vertical lines. More generally, the number of ways to distribute q quanta among $N$ pots is the total number of permutations of $E$ "$x$" s with $N - 1$ vertical lines. This number is the multiplicity, $\Omega(N, E)$ of the macrostate $E$ "quanta on the lattice" and is given by

$$\Omega(N, E) = \frac{(N + E - 1)!}{E!(N - 1)!}.$$

## III. ENTROPY AND TEMPERATURE OF AN EINSTEIN SOLID

Using micro canonical ensemble it is straightforward to derive the entropy

$$S(N, E) = k_B \ln \frac{(N + E)^{N+E}}{N^N E^E}. \tag{1}$$

and the temperature (measured in $\bar{h}\omega$)

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_N = k_B \ln \left(1 + \frac{N}{E}\right) \tag{2}$$

or

$$\beta = \ln \left(1 + \frac{N}{E}\right). \tag{3}$$

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From the last equation we can also obtain

$$E(N,T) = \frac{Ne^{-\beta}}{1-e^{-\beta}}. \tag{4}$$

The demon is in thermal equilibrium with the rest of the system. The partition function of the demon is given by

$$Z_d(\beta) = \sum_{E=0}^{\infty} e^{-\beta n} = \frac{1}{1-e^{-\beta}} \tag{5}$$

The average demon energy is then

$$\langle E_d \rangle = Z_d^{-1} \sum_{E=0}^{\infty} e^{-\beta n} = -\frac{\partial}{\partial \beta} Z_d(\beta) = \frac{e^{-\beta}}{1-e^{-\beta}}. \tag{6}$$

Hence the average demon energy coincides (in thermodynamic limit) with the energy per particle $E/N$.

## IV. COMPARISON WITH NUMERICAL SIMULATIONS USING THE DEMON ALGORITHM

Applying the code to obtain the energy of a demon in each trial

```
python p1.py > Ed.dat
```

A sample of the file:

```
...
2
3
4
3
2
3
3
2
2
3
2
1
0
0
0
0
...
```

Constructing the probability distribution (Mac OS or Unix):

```
cat Ed.dat|awk '{A[$1]=A[$1]+1; N=N+1} END{ for(x in A){print x,A[x]/N}}'  |
sort -g > probab_Ed.dat
```

(one command line!) A sample of the probability file:

```
0 0.20454
1 0.16399
2 0.12944
3 0.10228
4 0.08177
5 0.06688
6 0.05336
7 0.04258
8 0.03401
9 0.02743
10 0.02163
11 0.01669
12 0.01284
13 0.00981
14 0.00771
15 0.00656
...
```

See the results of numerical simulation in Fig. 1.

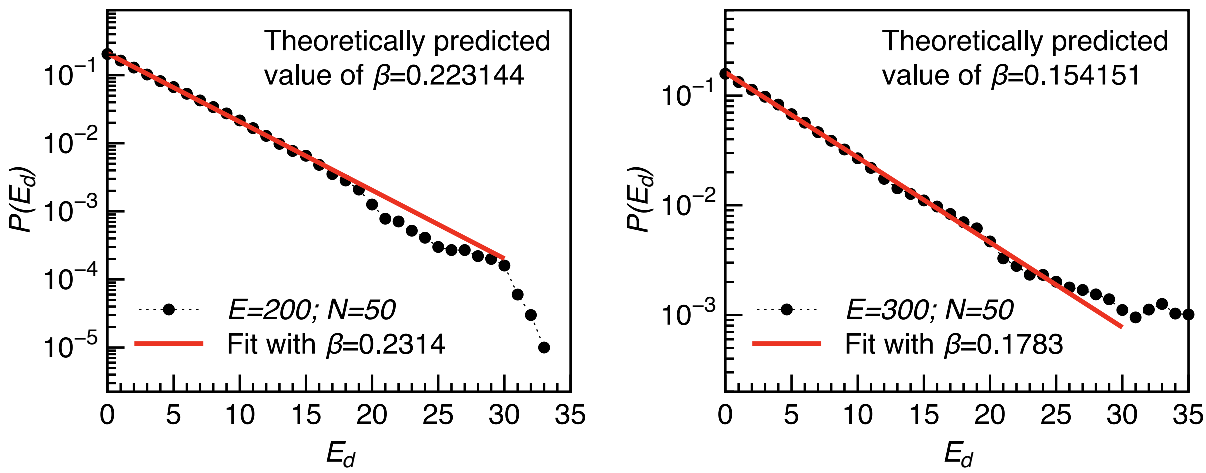


FIG. 1: The probability distribution of the demon energy for two different system energies $E = 200$ and $E = 300$. The number of particles is fixed, $N = 50$. The theoretical prediction for $\beta$ is obtained from Eq. (3). The fit is motivated by the Boltzmann distribution $P(E_d) \propto e^{-\beta E_d}$, used because the demon represents a small sub-system within an isolated system (the demon plus the particles).