Two level system

Consider N impurities trapped in a solid Matrix. The microstates of this two level system are specified by the set of occupation numbers n_i, such that $n_i = \underline{0}$ or $\underline{1}$ corresponding to whether the i^{th} atom is in the ground state or the excited state.

The overall energy is thus:

$$H(\{n_i\}) = E = \epsilon \sum_{i=1}^{N} n_i = N_1 \epsilon$$ {Considering N_1 atoms are in the excited state }.

The micro-canonical probability is thus,

$$p(\{n_i\}) = \frac{1}{\Omega(E,N)} \delta_{H,E}$$

Since there are N_1 excited impurities out of a total N, the normalization Ω is the simple multiplicity

$$\Omega(E,N) = \frac{N!}{N_1!\,(N-N_1)!}$$

The entropy $S = k_B \ln \Omega = k_B \left(\ln N! - \ln N_1! - \ln (N-N_1)!\right)$

Using Stirling approximation for large N and N_1:

$$S(E,N) \approx k_B\left[N\ln N - N - N_1\ln N_1 + N_1 - (N-N_1)\ln(N-N_1) + (N-N_1)\right]$$

$$\approx k_B\left[N\ln N - N_1\ln N_1 - (N-N_1)\ln(N-N_1)\right]$$

$$\approx k_B\left[N\ln N - \frac{E}{\epsilon}\ln\frac{E}{\epsilon} - \left(N-\frac{E}{\epsilon}\right)\ln\left(N-\frac{E}{\epsilon}\right)\right] \quad \because E=\epsilon N_1$$

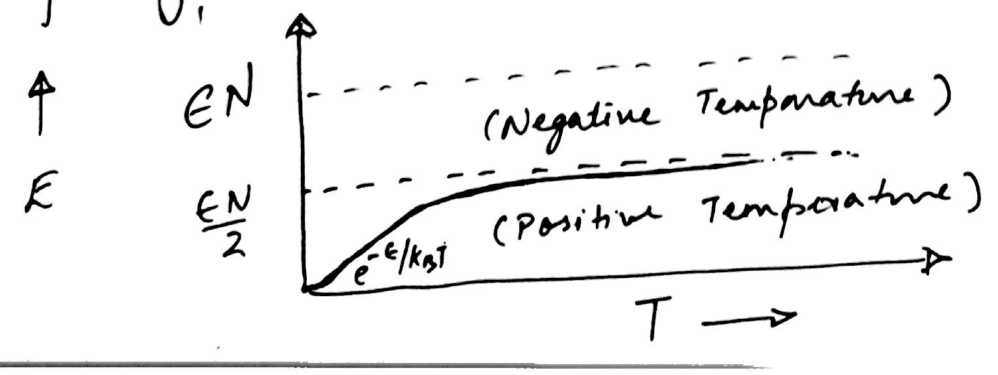
$\therefore$ The equilibrium temperature is

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_N = \frac{k_B}{\epsilon}\left[\ln\left\{\frac{(\epsilon N - E)}{E}\right\}\right] \qquad (1)$$

Solving for $E(T)$ we get:

$$E(T) = \frac{\epsilon N}{1+e^{\epsilon/k_BT}} \qquad (2)$$

plotting this behaviour, we get:



Observations.

(a) The internal energy $E(T)$ is a monotonic function of T rising from 0 at $T=0$ to becoming $N\epsilon/2$ as $T \to \infty$.

(b) From eq^n (2) it is clear that as E goes beyond $N\epsilon/2$, T becomes negative.

"The origin of negative temperature states lies in the decrease in the number of microstates with increasing energy as $E(T)$ crosses $N\epsilon/2$."

Conclusion: Two-level systems have an upper bound on their energy, and very few microstates close to this energy $E(T) = N\epsilon/2$.

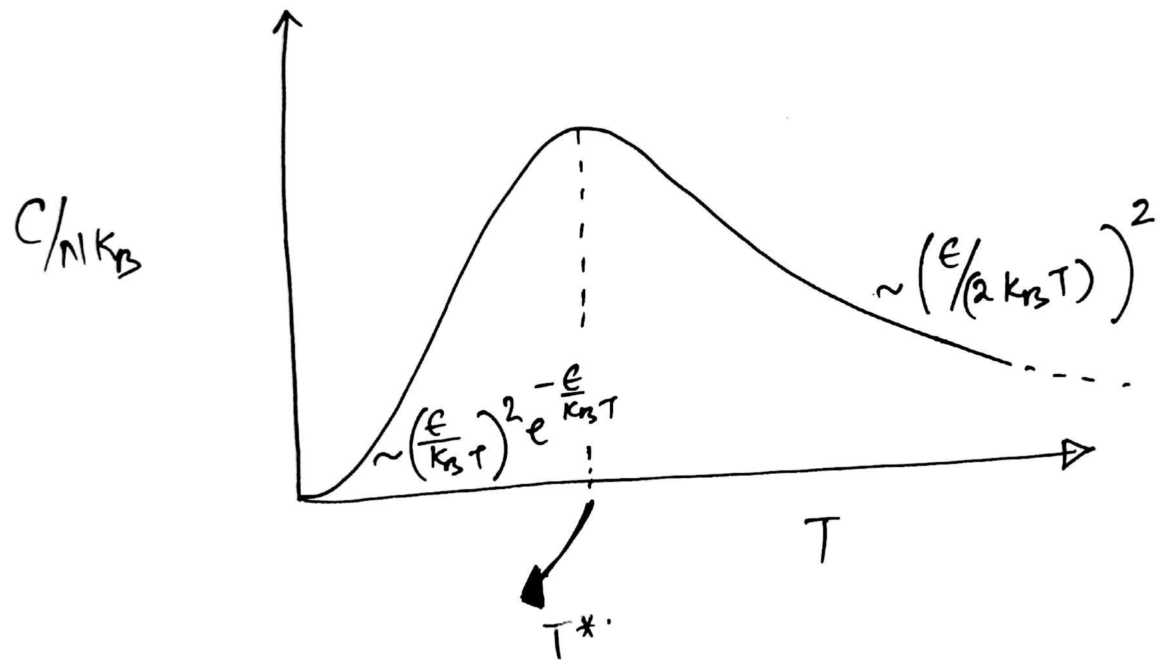
Remarks: (1) Once a system at negative temparature is brought in contact with universe, it loses E and settles at a positive temperature.

(2) A negative T system becomes hotter by giving up E & becomes cooler by taking up E.

Physical examples of such systems include lasers, magnetic spins etc.

the heat capacity of the system, given by

$$C = \frac{dE}{dt} = N k_B \left(\frac{\epsilon}{k_B T}\right)^2 \exp\left(\frac{\epsilon}{k_B T}\right)\left[\exp\left(\frac{\epsilon}{k_B T}\right)+1\right]^{-2}$$



The joint probability distribution which gives complete information on the microstates is given by

$$p(n_1, n_2, \ldots n_N) = \frac{1}{\Omega(E,N)}$$

Q. What is the unconditional probability that the j^{th} impurity has occupation number n_j ?

Ans. We know that the unconditional probability is given as:

$$p(n_j) = \sum_{\{n_1, n_2, \ldots n_{j-1}, n_{j+1}, \ldots n_N\}} p(n_1, n_2, \ldots n_N)$$

The conditional probability that the remaining $N-1$ impurities have taken up energy $E - n_j\epsilon$ is given as:

$$p(n_1, n_2, \ldots n_{j-1}, n_{j+1}, \ldots n_N \,|\, n_j) = \frac{1}{\Omega(E - n_j\epsilon, N-1)}$$

By virtue of Baye's theorem, we have:

$$p(n_j) = \frac{p(n_1, n_2, \ldots n_N)}{p(n_1, n_2, n_3, \ldots n_{j-1}, n_{j+1}, \ldots n_N \,|\, n_j)} = \frac{\Omega(E - n_j\epsilon, N-1)}{\Omega(E, N)}$$

If we take $n_j = 0$ (ground state for j^{th} impurity)

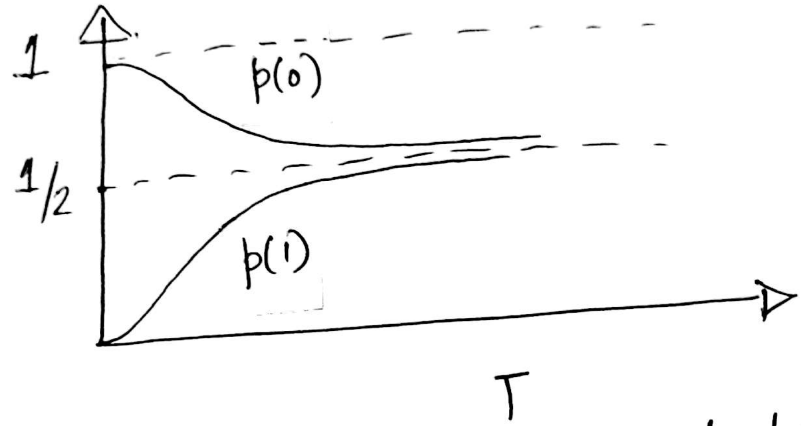
$$p(0) = \frac{\Omega(E, N-1)}{\Omega(E,N)} = \frac{(N-1)!}{N_1!\,(N-N_1-1)!} \cdot \frac{N_1!\,(N-N_1)!}{N!} = 1 - \frac{N_1}{N}$$

taking $n_j = 1$ (Excited state for j^{th} impurity)

$$p(1) = 1 - p(0) = N_1/N$$

Using the fact that $N_1 = E/\epsilon$ and the formula for $E = E(T)$, we have:

$$p(0) = \frac{1}{1 + \exp\left(\frac{-\epsilon}{k_B T}\right)} \quad \& \quad p(1) = \frac{e^{-\epsilon/k_B T}}{1 + e^{-\epsilon/k_B T}}$$



The above figure shows that probability ~~of~~ for a randomly selected impurity atom to be in excited state goes to zero as T goes to zero.

At all temperatures, $\underline{p(1) + p(0) = 1}$.