

10/03/25

Lecture 18

Acoustic Phonons as Goldstone Modes

It can be shown that the Acoustic phonons (low energy) are the Goldstone modes of a crystal lattice & the optical modes are the Higgs modes of the lattice.

Consider the lattice hamiltonian which has N -atoms & every atom is coupled with others by springs. The hamiltonian has the form,

$$H_{\text{crystal}} = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i,j} J_{ij} (u_i - u_j)^2$$

' u_i ' are deviations of the atom from their equilibrium position. J_{ij} is the coupling b/w i^{th} & j^{th} atom. p_i are the conjugate momenta to u_i .

The kinetic energy term is trivial and won't give any excitation. It is the spring like coupling which leads to the phonon excitations.

Observe that the Crystal Hamiltonian is independent of the location of the crystal, but only deviations of the atoms from the equilibrium positions will matter. Thus it has continuous translation symmetry.

To get the phonon dispersion relation, we focus on the potential energy (Interaction part).

$$H_{\text{int.}} = \frac{1}{2} \sum_{i,j} T_{ij} (u_i - u_j)^2$$

To get the dispersion relation we go to the momentum space & diagonalize the Hamiltonian.

$$u_q = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{i\vec{q} \cdot \vec{r}} \underbrace{u_{\vec{r}}}_{\text{real space derivation of } r^{\text{th}} \text{ atom}}$$

$$\Rightarrow u_{\vec{r}} = \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{-i\vec{q} \cdot \vec{r}} u_{\vec{q}}$$

$$\Rightarrow u_i - u_j = \frac{1}{\sqrt{N}} \sum_{\vec{q}} \left[e^{-i\vec{q} \cdot \vec{r}_i} - e^{-i\vec{q} \cdot \vec{r}_j} \right] u_{\vec{q}}$$

$$= \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{-i\vec{q} \cdot \vec{r}_i} \left[1 - e^{-i\vec{q} \cdot (\vec{r}_j - \vec{r}_i)} \right] u_{\vec{q}}$$

$R_{ij} = \vec{r}_j - \vec{r}_i$

$$= \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{-i\vec{q} \cdot \vec{r}_i} \left[1 - e^{-i\vec{q} \cdot \vec{R}_{ij}} \right] u_{\vec{q}}$$

$$\Rightarrow u_i - u_j = \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{-i\vec{q} \cdot \vec{r}_i} \left[1 - e^{-i\vec{q} \cdot \vec{R}_{ij}} \right] u_{\vec{q}}$$

$$\Rightarrow (u_i - u_j)^2 = \frac{1}{N} \sum_{\vec{q}, \vec{q}'} \left[e^{-i(\vec{q} + \vec{q}') \cdot \vec{r}_i} \left[1 - e^{-i\vec{q} \cdot \vec{R}_{ij}} \right] \right. \\ \left. \times \left[1 - e^{-i\vec{q}' \cdot \vec{R}_{ij}} \right] u_{\vec{q}} u_{\vec{q}'} \right]$$

Thus the H_{int} in q -space becomes

$$H_{int} = \frac{1}{2N} \sum_{i,j} J_{ij} \sum_{\vec{q}, \vec{q}'} \left[e^{-i(\vec{q} + \vec{q}') \cdot \vec{r}_i} \left[1 - e^{-i\vec{q} \cdot \vec{R}_{ij}} \right] \right. \\ \left. \times \left[1 - e^{-i\vec{q}' \cdot \vec{R}_{ij}} \right] u_{\vec{q}} u_{\vec{q}'} \right]$$

$$\sum_{i,j} = \sum_{\vec{r}_i} \sum_{\vec{r}_j} = \sum_{\vec{r}_i} \sum_{\vec{R}_{ij}} \\ \vec{r}_j \rightarrow \vec{R}_{ij}$$

$$\Rightarrow H_{int} = \frac{1}{2} \sum_{\vec{R}_{ij}} J_{ij} \sum_{\vec{q}, \vec{q}'} u_{\vec{q}} u_{\vec{q}'} \left[1 - e^{-i\vec{q} \cdot \vec{R}_{ij}} \right] \\ \times \left[1 - e^{-i\vec{q}' \cdot \vec{R}_{ij}} \right] \\ \times \underbrace{\frac{1}{N} \sum_{\vec{r}_i} e^{-i(\vec{q} + \vec{q}') \cdot \vec{r}_i}}_{\delta(\vec{q} + \vec{q}')}]$$

$$\Rightarrow H_{int} = \frac{1}{2} \sum_{\vec{R}_{ij}} J_{ij} \sum_{\vec{q}} u_{\vec{q}} u_{-\vec{q}} \left[1 - e^{-i\vec{q} \cdot \vec{R}_{ij}} \right] \\ \times \left[1 - e^{i\vec{q} \cdot \vec{R}_{ij}} \right]$$

$$(1 - e^{-i\vec{q} \cdot \vec{R}_{ij}})(1 - e^{i\vec{q} \cdot \vec{R}_{ij}}) \\ = 1 + 1 - 2 \cos(\vec{q} \cdot \vec{R}_{ij}) \\ = 2 [1 - \cos(\vec{q} \cdot \vec{R}_{ij})]$$

$$\Rightarrow H_{int} = \sum_{\vec{R}_{ij}} J_{ij} \sum_{\vec{q}} u_{\vec{q}} u_{-\vec{q}} [1 - \cos(\vec{q} \cdot \vec{R}_{ij})]$$

$$H_{int} = \sum_{\vec{q}} \left[\sum_{\vec{R}_{ij}} J_{ij} [1 - \cos(\vec{q} \cdot \vec{R}_{ij})] \right] u_{\vec{q}} u_{-\vec{q}}$$

$$\text{Let } J(\vec{q}) = \sum_{\vec{R}_{ij}} J_{ij} [1 - \cos(\vec{q} \cdot \vec{R}_{ij})]$$

$$\Rightarrow H_{int} = \sum_{\vec{q}} J(\vec{q}) u_{\vec{q}} u_{-\vec{q}}$$

This is the diagonalized Hamiltonian in q -space.

If $J_{ij} = J$ same for nearest bonds zero for further bonds, then in 3 dimensions,

$$J(\vec{q}) = [1 - \cos(aq_x)] + [1 - \cos(aq_y)] + [1 - \cos(aq_z)]$$

$a \Rightarrow$ lattice spacing

The Partition function is given by

$$Z = \int \prod_i d\mathbf{u}_i e^{-\beta H_{\text{int.}}(\{\vec{r}_i\})}$$

↳ Configurational integral to be precise

In q -space it is,

$$Z = \int \left(\prod_{\vec{q}} d\mathbf{u}_{\vec{q}} \right) e^{-\beta H_{\text{int}}(q)}$$

↳ q -space
Hamiltonian

$$= \int \left(\prod_{\vec{q}} d\mathbf{u}_{\vec{q}} \right) e^{-\beta \sum_{\vec{q}} f(\vec{q}) \mathbf{u}_{\vec{q}} \mathbf{u}_{-\vec{q}}}$$

$$\Rightarrow Z = \prod_{\vec{q}} \left[\int d\mathbf{u}_{\vec{q}} e^{-\beta f(\vec{q}) \mathbf{u}_{\vec{q}} \mathbf{u}_{-\vec{q}}} \right]$$

Here each term in the product is an independent partition func. corresponding to a particular mode given by $\vec{q}$. So each $\vec{q}$ mode acts as an individual excitation which corresponds to phonons.

Moreover the $u_{\vec{q}} \neq u_{-\vec{q}}$ are complex conjugates of each other since

$$u_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{i\vec{q} \cdot \vec{r}} u_{\vec{r}}$$

$$u_{\vec{q}}^* = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{-i\vec{q} \cdot \vec{r}} \underbrace{u_{\vec{r}}}_{\text{real}}$$

$$u_{\vec{q}}^* = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{i(-\vec{q}) \cdot \vec{r}} u_{\vec{r}}$$

$$\Rightarrow \boxed{u_{\vec{q}}^* = u_{-\vec{q}}}$$

$$\begin{aligned} \text{Let } Z_{\vec{q}} &= \int du_{\vec{q}} e^{-\beta g(\vec{q})} u_{\vec{q}} u_{-\vec{q}} \\ &= \int du_{\vec{q}} e^{-\beta g(\vec{q})} |u_{\vec{q}}|^2 \end{aligned}$$

$$\text{Let } |u_{\vec{q}}|^2 = a_{\vec{q}}^2 + b_{\vec{q}}^2$$

$$\Rightarrow Z_{\vec{q}} = \int_{-\infty}^{\infty} da_{\vec{q}} \int_{-\infty}^{\infty} db_{\vec{q}} \underbrace{e^{-\beta g(\vec{q})} (a_{\vec{q}}^2 + b_{\vec{q}}^2)}_{\text{two independent Gaussians}}$$

$$\Rightarrow \boxed{Z_{\vec{q}} = \frac{\pi}{\beta g(\vec{q})}}$$

To find $\langle u_q u_{\vec{q}'} \rangle$ & $\langle u_i u_j \rangle$

These are the Correlation functions.

$$u_i = \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{-i\vec{q} \cdot \vec{r}_i} u_{\vec{q}}$$

$$u_i u_j = \frac{1}{N} \sum_{\vec{q}, \vec{q}'} e^{-i(\vec{q} \cdot \vec{r}_i + \vec{q}' \cdot \vec{r}_j)} u_{\vec{q}} u_{\vec{q}'}$$

$$\langle u_i u_j \rangle = \frac{1}{N} \sum_{\vec{q}, \vec{q}'} e^{-i(\vec{q} \cdot \vec{r}_i + \vec{q}' \cdot \vec{r}_j)} \langle u_{\vec{q}} u_{\vec{q}'} \rangle$$

Now the Hamiltonian has translation invariance, so if all $\vec{r}_i \rightarrow \vec{r}_i + \vec{a}$.
i.e. if we apply a global translation, then the physics shouldn't change

i.e.

$$\langle u(\vec{r}_i) u(\vec{r}_j) \rangle = \langle u(\vec{r}_i + \vec{a}) u(\vec{r}_j + \vec{a}) \rangle$$

is needed, this is possible only if $\langle u(\vec{r}_i) u(\vec{r}_j) \rangle$ is a function of $\vec{r}_i - \vec{r}_j$. This is possible only if $\langle u_{\vec{q}} u_{\vec{q}'} \rangle = \delta_{\vec{q} \vec{q}'} \langle u_{\vec{q}} u_{-\vec{q}} \rangle$

$$\Rightarrow \langle u_i u_j \rangle = \frac{1}{N} \sum_{\vec{q}} e^{-i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} \langle u_{\vec{q}} u_{-\vec{q}} \rangle$$

Now

$$\langle u_{\vec{q}} u_{-\vec{q}} \rangle = \frac{\int du_{\vec{q}} u_{\vec{q}} u_{-\vec{q}} e^{-\beta f(\vec{q})} u_{\vec{q}} u_{-\vec{q}}}{Z_{\vec{q}}}$$

Again using $u_{\vec{q}} u_{-\vec{q}} = |u_{\vec{q}}|^2$
 & $|u_{\vec{q}}|^2 = a_{\vec{q}}^2 + b_{\vec{q}}^2$ we get

$$\langle u_{\vec{q}} u_{-\vec{q}} \rangle = \frac{\int da_{\vec{q}} db_{\vec{q}} (a_{\vec{q}}^2 + b_{\vec{q}}^2) e^{-\beta f(\vec{q})} (a_{\vec{q}}^2 + b_{\vec{q}}^2)}{Z_{\vec{q}}}$$

$$= \frac{\int da_{\vec{q}} db_{\vec{q}} a_{\vec{q}}^2 e^{-\beta f(\vec{q})} (a_{\vec{q}}^2 + b_{\vec{q}}^2)}{Z_{\vec{q}}} + \frac{\int da_{\vec{q}} db_{\vec{q}} b_{\vec{q}}^2 e^{-\beta f(\vec{q})} (a_{\vec{q}}^2 + b_{\vec{q}}^2)}{Z_{\vec{q}}}$$

$$= \frac{2 \left[\sqrt{\frac{\pi}{\beta f(\vec{q})}} \frac{\sqrt{\pi}}{2 [\beta f(\vec{q})]^{3/2}} \right]}{\frac{\pi}{\beta f(\vec{q})}} = \frac{1}{\beta f(\vec{q})}$$

$$\Rightarrow \langle u_{\vec{q}} u_{-\vec{q}} \rangle = \frac{1}{\beta f(\vec{q})}$$

$$\text{or } \langle u_{\vec{q}} u_{\vec{q}'} \rangle = \frac{\delta_{\vec{q}, -\vec{q}'}}{\beta f(\vec{q})}$$

$$\Rightarrow \langle u_i u_j \rangle = \frac{1}{N} \sum_{\vec{q}} e^{-i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} \frac{1}{\beta f(\vec{q})}$$

We can convert the sum to an integration as follows,

$$\langle u_i u_j \rangle = \frac{k_B T}{(2\pi)^d} \int_{B.Z.} d^d q \frac{e^{-i\vec{q} \cdot \vec{r}_{ij}}}{f(\vec{q})}$$

Thus $\langle u_i u_j \rangle$ is given by the inverse fourier transform of $\left[\frac{k_B T}{f(\vec{q})} \right]$

$$\& \langle u_i^2 \rangle = \frac{k_B T}{(2\pi)^d} \int \frac{d^d q}{f(\vec{q})}$$

The total energy is given by

$$E = - \frac{\partial}{\partial \beta} \log(Z)$$

$$\log(Z) = \sum_{\vec{q}} \log(Z_{\vec{q}})$$

where Z_q was found to be

$$Z_q = \frac{\pi}{\beta g(q^2)} \Rightarrow \log(Z_q) = \log \left[\frac{\pi}{\beta g(q^2)} \right]$$

$$\Rightarrow E = \sum_{\vec{q}} \frac{\partial}{\partial \beta} \left[\log(\beta) - \log \left(\frac{\pi}{g(q^2)} \right) \right]$$

$$= \sum_{\vec{q}} \frac{1}{\beta} = K_B T \sum_{\vec{q}} (1)$$

$$\Rightarrow E = N K_B T$$

$$\text{Per phonon energy } \varepsilon_q = K_B T$$

Per phonon
energy

Note that we are dealing with classical hamiltonian without any quantum picture. Thus this model is for very high T

q-Potts Model

(in d-dimensions)

The potts model hamiltonian is given by,

$$H = -J \sum_{\langle i, j \rangle} \delta(s_i, s_j)$$

where $s_i = \{q \text{ number of distinct objects}\}$

$$Z = \text{Trace} \left[e^{\beta J \sum_{\langle i, j \rangle} \delta(s_i, s_j)} \right]$$

$$\text{Let } K = \beta J$$

$$\Rightarrow Z = \text{Trace} \left[\prod_{\langle i, j \rangle} e^{K \delta(s_i, s_j)} \right]$$

when $s_i = s_j$ the term is e^K

when $s_i \neq s_j$ then the term is 1

$$\Rightarrow e^{K \delta(s_i, s_j)} = 1 + \delta(s_i, s_j) [e^K - 1]$$

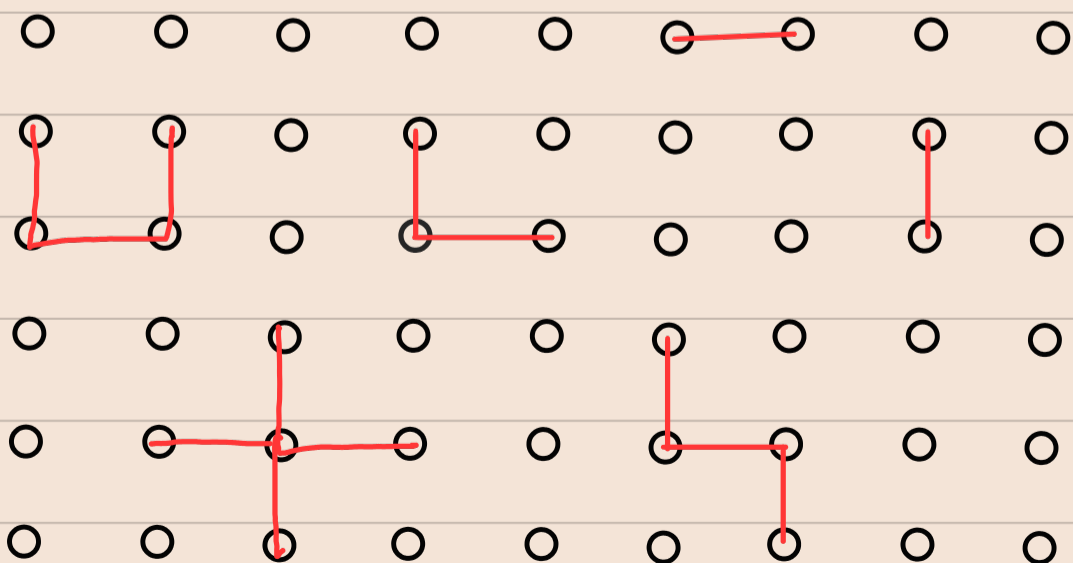
$$\text{Let } v = e^K - 1$$

$$\Rightarrow Z = \text{Trace} \left[\prod_{\langle i,j \rangle} (1 + v \delta(s_i, s_j)) \right]$$

$$Z = \text{Trace} \left[1 + v \sum_{\langle i,j \rangle} \delta(s_i, s_j) + v^2 \sum_{\langle i,j \rangle \times \langle k,l \rangle} \delta(s_i, s_j) \delta(s_k, s_l) + \dots \right]$$

This is an expansion of partition function in increasing orders of 'v'.

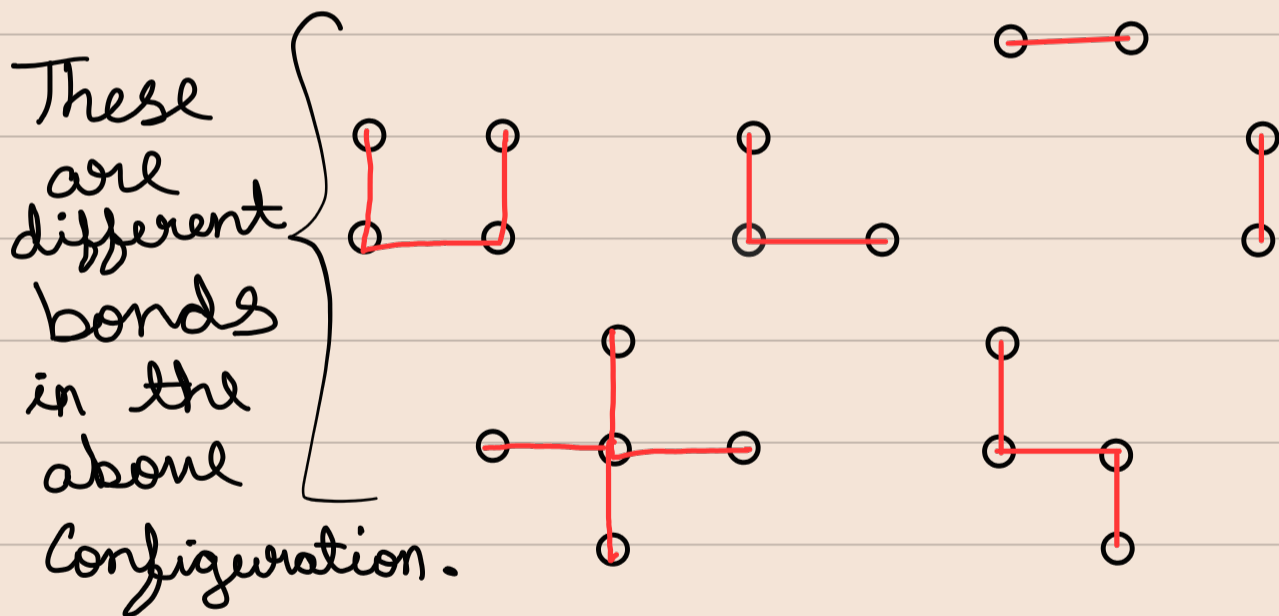
This partition function can be visualized as follows. Consider a d-dimensional lattice & whenever there is $s_i = s_j$ for neighbours we denote it with a bond.



This some random configuration of bonds

Whenever there is a bond b/w two nearby lattice sites, it implies the $S_i = S_j$ corresponding to them & it contributes to the 'Z' by a factor of '2'.

We define a cluster as the set of sites connected by bonds. And if a site has no bond, then it is its own individual cluster.



There are a total of 14 bonds in this config. And number of sites connected by bonds are 20. Then the number of clusters are given by

$$N_s - 14 = 54 - 14 = 40.$$

Let $\{G\} \Rightarrow$ Set of all possible configurations

$n(G) \Rightarrow$ No: of clusters in a configuration 'G'.

$b(G) \Rightarrow$ No: of bonds in the configuration 'G'.

The no. of clusters & No: of bonds are related by,

$$\underline{n(G) = N_s - b(G)}$$

where $N_s \Rightarrow$ total number of sites.

Now each cluster gives a factor of 'q' as the summation of S_i can take 'q' terms & each bond contributes to 'v' in partition function.

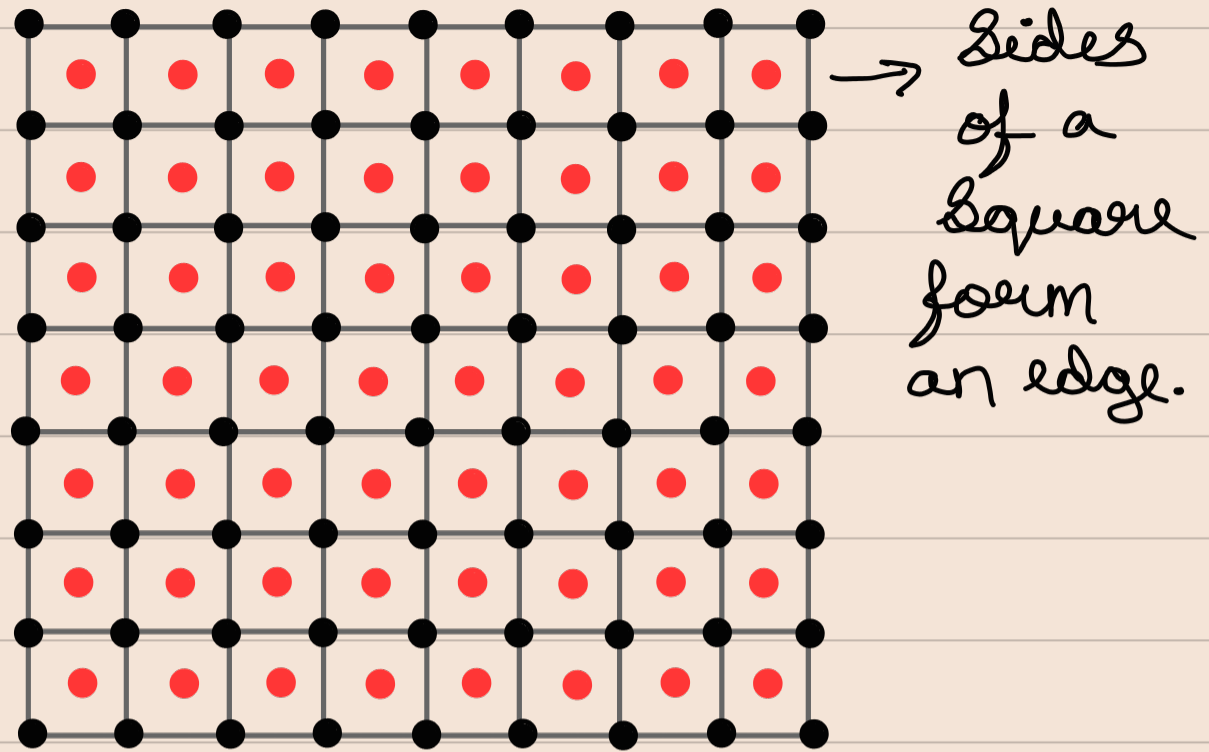
Thus the partition function can be equivalently written as

$$Z = \sum_{\{G\}} q^{n(G)} v^{b(G)}$$

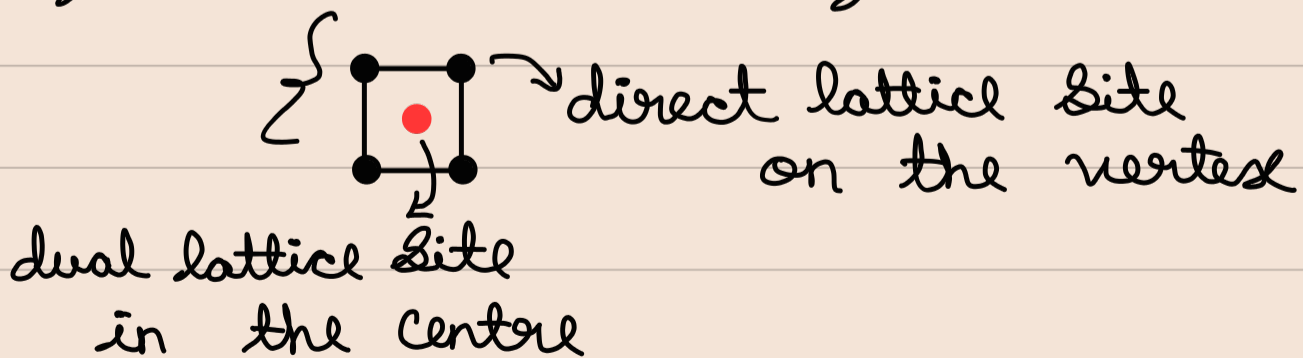
This is an exact relation, which matches with the partition function of the random cluster model. & 'q' appears as weight factor for each cluster. This relation holds for any lattice & any dimensions.

The critical temperature & phase transition can be exactly found without going to the complete analysis. Rather by mapping the q-potts model of a particular lattice with its dual we get a particular temperature where the q-potts & its dual are equivalent. This corresponds to the critical temp.

Dual lattice for Square lattice



The dual lattice for a square lattice is another square lattice. If the vertices of all squares are the locations of sites of direct lattice, then the collection of all the centers of a square will form the dual.



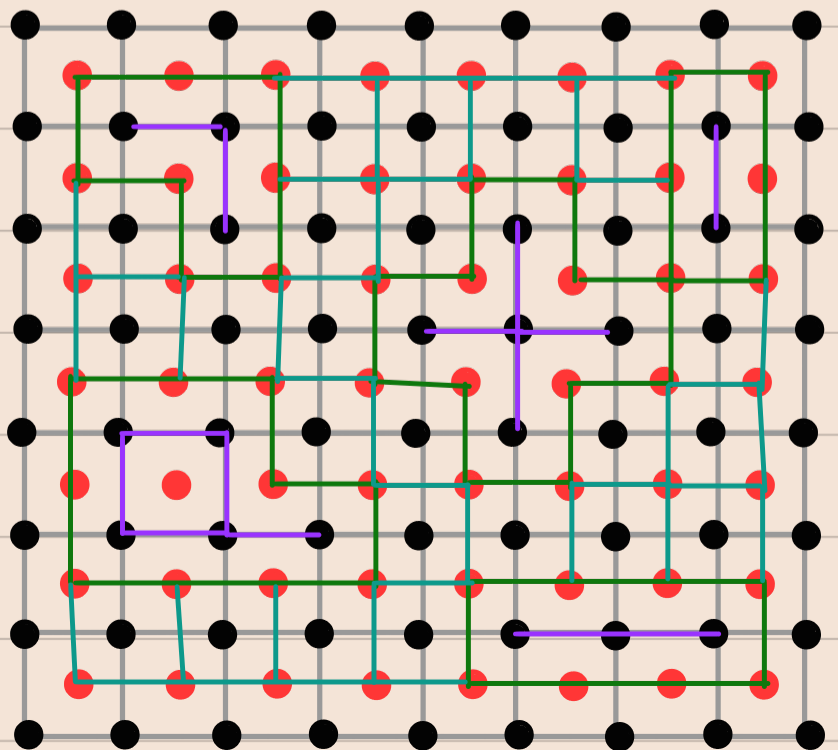
The Potts model on dual lattice is got as follows,

Consider a random configuration of bonds of a square lattice got by joining the black dots (vertices). For this configuration we draw dual lattice of centers of squares. For every group of real lattice sites & also for every isolated real lattice site (basically around every cluster in real lattice), we draw bonds around them in dual lattice, such that no dual lattice bond cuts the real lattice bonds. Thus the dual bonds always form a circuit or a closed path around every cluster.

— This is a bond on real lattice sites

— This is a bond in dual lattice sites around a group of real lattice sites which form cluster

— This is a bond in dual lattice around isolated single site in real lattice.

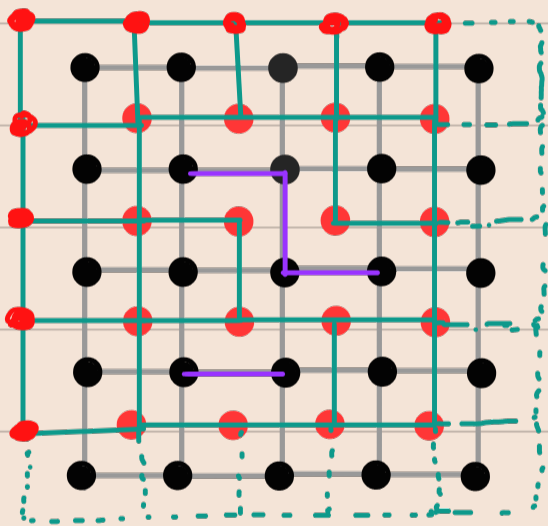


Now the dual configuration has $b(D)$ number of bonds $\neq$ the number of dual circuits will be $C(D) = N_s - b(D)$ (same as that of direct lattice). $C(D) = n(G)$

By construction we have

$$b(D) + b(G) = E$$

where $E \Rightarrow$ all possible edges on the direct/real lattice.



$$n(G) = 21$$

$$C(D) = 21$$

↓
(Periodicity of lattice)

$$N_s = 25$$

$$b_G = 4 \text{ (Purple lines)}$$

$$b_D = 36 \text{ (green lines)}$$

$$b_G + b_D = 40$$

all possible edges in real/direct lattice of N_s sites.

N_s sites are distributed into

$N_x \times N_y$ along x & y direction

No: sites along x -line

→ No: of sites along y -line

Usually $N_x = N_y$ for Square lattice. There are $N_x - 1$ horizontal edges in a x -line of N_x points. Similarly $N_y - 1$ vertical edges in a y -line of N_y points. But there are also N_x number of vertical edges along x -line & N_y number of horizontal edges along y -line. Thus total no. of edges is given by

$$E = (N_x - 1)N_y + (N_y - 1)N_x$$

$$\Rightarrow E = N - N_y + N - N_x = 2N - N_x - N_y$$

In above figure $N_x = N_y = 5$.

There are 5×4 vertical edges & 4×5 horizontal edges.

$$\Rightarrow \underline{E = 20 + 20 = 40}$$

Thus we have the relations

$$b(G) + b(D) = E$$

$$n(G) = c(D)$$

$$\Rightarrow Z_{\text{real lattice}} = \sum_{\{G\}} q^{n(G)} v^{b(G)}$$

$$= \sum_{\{D\}} q^{c(D)} v^{[E - b(D)]}$$

Use Euler relation relating

$$c_D + N_s = b(D) + n(D)$$

$$\Rightarrow Z_{\text{dual}} = \sum_{\{D\}} q^{(b(D) + n(D) - N_s)} v^{[E - b(D)]}$$

$$Z_{\text{dual}} = \frac{v^E}{q^{N_s}} \sum_{\{D\}} q^{n(D)} \left(\frac{q}{v} \right)^{b(D)}$$

$\frac{v^E}{q^{N_s}}$ is a constant for a given lattice & model.

Even though $\mathcal{Z}$ is dependent on temperature, the variables of different configurations is $n(D) \neq b(D)$.

Thus the resultant $\mathcal{Z}_{\text{dual}}$ is also a q -potts model but for the dual lattice of $\mathcal{Z}_D = \frac{q}{\mathcal{Z}}$

$$\Rightarrow \mathcal{Z}_D \mathcal{Z} = q$$

$$\Rightarrow (e^{B_D J} - 1) (e^{B J} - 1) = q$$

- If B is very small (T is large) then B_D is very large (T_D is small)
- If B is very large (T is small) then B_D is very small (T_D is large).

Thus the dual- q -potts is mapped to inverse temperature given by $(e^{B_D J} - 1) (e^{B J} - 1) = q$.

Thus if the real potts model describes a low temperature phase, then the dual potts model describes a phase of high temperature, and vice versa.

Hence, that temperature where dual & real potts model map to itself has to be the phase transition or the critical temperature.

$$\Rightarrow \text{when } T_{\text{critical}}^{\text{real}} = T_{\text{critical}}^{\text{dual}} = T_c$$

$$\text{we get } v_c^2 = q \Rightarrow e^{B_c J} - 1 = \sqrt{q}$$

$$\Rightarrow B_c J = \ln(1 + \sqrt{q})$$

$$\Rightarrow \boxed{T_c = \frac{J}{k_B \ln(1 + \sqrt{q})}}$$

This is an exact result for the critical temperature for potts model in 2D Square lattice.

The Self dual point of temperature is the critical temperature ' T_c ' which distinguishes low temperature phase & high temperature phase. At ' T_c ' the low & high temp. phases are equivalent & the system is invariant under the duality transformation. This reflects the symmetry b/w the ordered & disordered phases at the phase transition, where neither phase behaviour dominates & both are equivalent.