Thu 4 May

25 89 40

Debye model of solids

- transform coupled atoms into non-interacting phonons

Phonon gas → Planck spectrum

$$\langle E\rangle \propto \int_0^{\omega_{max}} \frac{\omega^3}{e^{\beta\hbar\omega}-1}\,d\omega \qquad x = \beta\hbar\omega = \frac{\hbar\omega}{T}$$

$$x_{max} \propto \omega_{max}/T$$

$$\langle E\rangle \propto T^4 \int_0^{T_D/T} \frac{x^3}{e^x-1}\,dx \qquad \text{Debye temp } T_D \propto \sqrt[3]{N/V}$$

High-T: $\frac{T_D}{T} \ll 1$ → integrating over $0 \le x \ll 1$

$$e^x - 1 \approx x$$

$$\langle E\rangle \propto T^4 \int_0^{T_D/T} \frac{x^3}{x}\,dx \propto T^4\left(\frac{T_D}{T}\right)^3 \propto T$$

$$C_V = \frac{\partial}{\partial T}\langle E\rangle = \text{const.}$$

same as Einstein solid

Low-T $\frac{T_D}{T} \gg 1$ $\quad \int_0^{T_D/T} \frac{x^3}{e^x-1}\,dx \to \Gamma(4)\,\zeta(4) = 6\left(\frac{\pi^4}{90}\right) = \text{const.}$

$$\langle E\rangle \propto T^4 \to C_V \propto T^3 \checkmark$$

Electron (fermion) gas

$$\langle E\rangle_F \propto \int_0^\infty F(E)\,E^{3/2}\,dE = \int_0^\infty \frac{E^{3/2}}{e^{\beta(E-\mu)}+1}\,dE \qquad u = F(E),\quad dv = E^{3/2}\,dE$$

$$\int_a^b u\,dv = \underbrace{uv\Big|_a^b}_{0} - \int_a^b v\,du$$

$$\langle E\rangle_F \propto \int_0^\infty \left(\frac{-dF}{dE}\right) E^{5/2}\,dE \qquad \frac{-d}{dE}\left(e^{\beta(E-\mu)}+1\right)^{-1} = \frac{\beta e^x}{(e^x+1)^2}$$

$$x = \beta(E-\mu)$$

$$\langle E\rangle_F \propto \int_0^\infty \frac{e^x}{(e^x+1)^2} E^{5/2}\, d(\beta E) = \int_{-\beta\mu \to -\infty}^{\infty} \frac{e^x}{(e^x+1)^2} \underbrace{E^{5/2}}_{x}\, dx$$

$$x \ll -1 : \quad \frac{e^x}{(e^x+1)^2} = \frac{e^x}{1} \ll 1$$

$$x \gg 1 : \quad \frac{e^x}{(e^x+1)^2} = \frac{e^x}{e^{2x}} = \frac{1}{e^x} \ll 1$$

$\to$ Integrand peaked around $x=0 \leftrightarrow E=\mu$

Taylor: $$E^{5/2} = \mu^{5/2} + \frac{5}{2}(E-\mu)\mu^{3/2} + \frac{15}{8}(E-\mu)^2\mu^{1/2} + \dots$$
$$= \mu^{5/2} + \frac{5}{2} x T \mu^{3/2} + \frac{15}{8}(xT)^2 \mu^{1/2}$$

$$\langle E\rangle_F \approx \underbrace{A\int_{-\infty}^{\infty} \frac{e^x}{(e^x+1)^2}\,dx}_{\text{not in } C_V} + B\underbrace{\int_{-\infty}^{\infty} \frac{\cancel{xTe^x}}{(e^x+1)^2}\,dx}_{0} + CT^2\int_{-\infty}^{\infty} \frac{x^2 e^x}{(e^x+1)^2}\,dx$$

$$C_V = \frac{\partial}{\partial T}\langle E\rangle_F \propto T \checkmark$$

<u>Lattices</u>

Cubic $\to$ square in <u>2d</u> coord #: 2d $\to$ 4

Coord. # is number of nearest neighbours

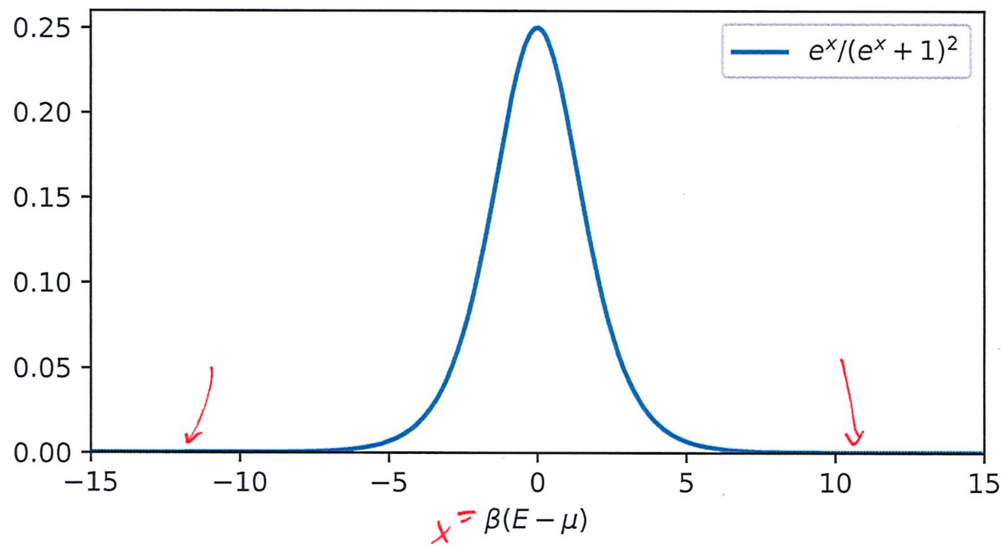
Honeycomb coord # is $d+1 \to 3$

Triangular (A_d^*) coord # is $2(d+1) \to 6$

Kagome (2d) coord # = 4 but not square

Generalize Ising model $$E = -\underbrace{J}_{\text{interaction strength}} \sum_{\langle jk\rangle} s_j s_k + \underbrace{\cancel{h}}_{0} \sum_n s_n$$

What are ground states (and order params)
for $J>0$ and $J<0$
w/ n.n. pairs from square, honeycomb, triangular lattices?

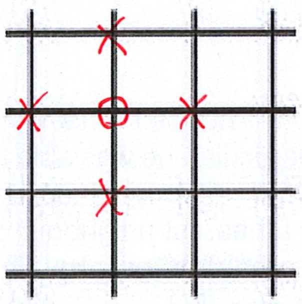


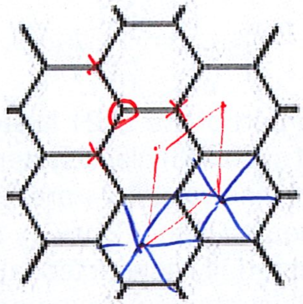
0.25
0.20
0.15
0.10
0.05
0.00
−15
−10
−5
0
5
10
15
$e^x/(e^x+1)^2$
$x = \beta(E-\mu)$

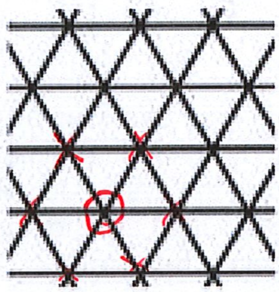
MATH327: Statistical Physics, Spring 2023
Tutorial activity — Lattices

In the lectures we are focusing on simple cubic lattices with periodic boundary conditions, but other lattice structures play important roles in both nature and mathematics. Some of the remarkable electronic properties of graphene, for example, are due to its two-dimensional honeycomb lattice structure, while more elaborate three-dimensional lattices play central roles in the search for materials exhibiting high-temperature superconductivity.

The figure below shows three simple two-dimensional lattices, each of which has a different **coordination number** — the number of nearest neighbours for each site (with periodic boundary conditions). We have already seen that the square lattice has coordination number $C = 2d = 4$, and generalizes to simple cubic and hyper-cubic lattices in higher dimensions.

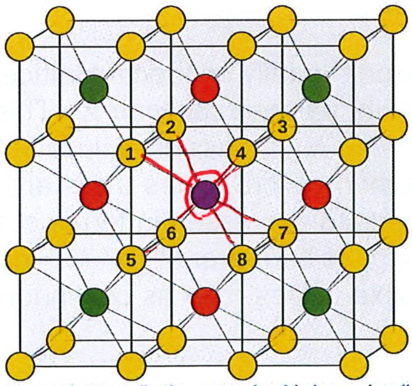




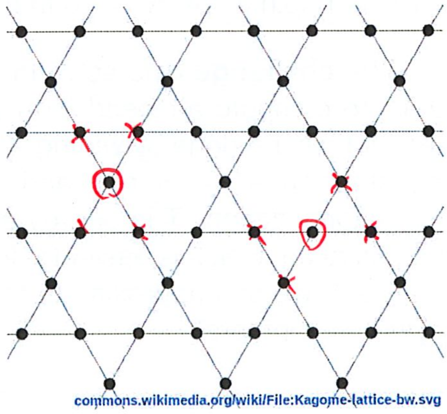


The honeycomb lattice of graphene has a smaller coordination number $C = d + 1 = 3$, and generalizes to 'hyper-diamond' lattices in higher dimensions. Finally, the triangular lattice essentially fills in the middle of each honeycomb cell, leading to coordination number $C = 2(d + 1) = 6$. Its higher-dimensional generalizations are known as A_d^* lattices, of which the simplest example is the three-dimensional body-centered cubic lattice shown below. Also shown below is the 'kagome' lattice, which has the same $C = 4$ as the square lattice, illustrating that the coordination number is insufficient to completely characterize a lattice.

A_3^* (bcc)



msestudent.com/body-centered-cubic-bcc-unit-cell



commons.wikimedia.org/wiki/File:Kagome-lattice-bw.svg

Fully connected lattice / complete graph

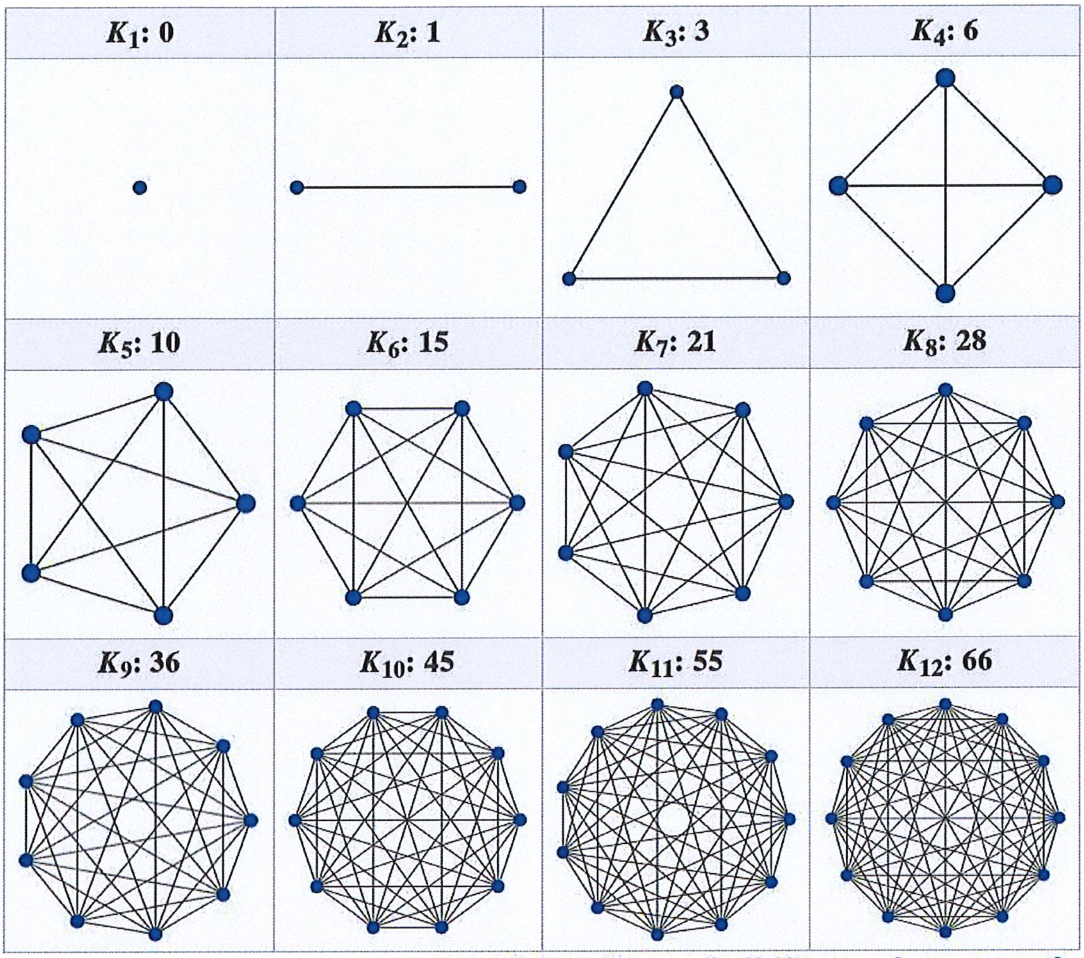
$$E = -\frac{J}{N} \sum_{j<k} S_j S_k - H \sum_n S_n = \frac{-J}{2N} \sum_{j \neq k} S_j S_k - H \sum_n S_n$$

Solve → closed-form expression for part. func. Z

Organize as sum over magnetizations

$$Z = \sum_{m=-1}^{1} (\dots) \rightarrow \int_{-1}^{1} (\dots)\, dm$$

find E in terms of m



en.wikipedia.org/wiki/Complete_graph