

## Condensed matter

- study of "materials" and "matter"
- study of complex systems.
- branching out:
  - Cold atomic systems
  - artificial quantum system
  - Complex data networks

→ Since 1970, field theory → Wilson renormalization

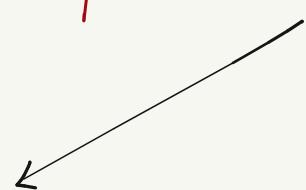
→ Anderson - Higgs mechanism



superconductivity (BCS theory) in 1950 → Goldstone mechanism

→ Experiment driven

Central problem:  $\hat{H} = \sum_i \frac{\hat{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq i'} \frac{q_i q_{i'}}{|\vec{r}_i - \vec{r}_{i'}|}$



Solve it in macroscopic situation.

↓  
Quantum many-body Hamiltonian is complex!

e.g. spin  $\pm 1$ : Hilbert space:  $2^n$ !

→ Reductionalist versus emergent.

Broken symmetry, excitations, topological defects



- Landau paradigm. The presence or absence of a certain symmetry element  
in a state of matter is almost never ambiguous.

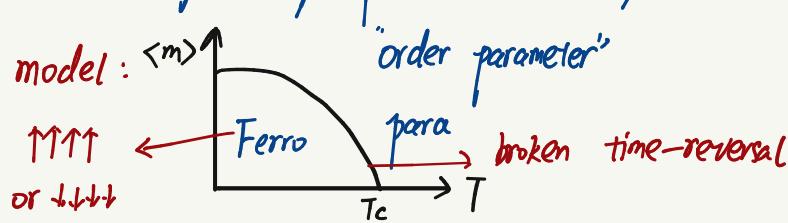
- High symmetry phases signify disorder

phase transition. ⇒ appearance of order parameter.

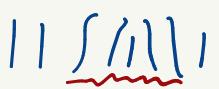
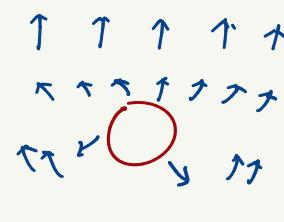
- Low symmetry phases identify "order"

All conventional (except topological) phase of  
matter can be identified by broken symmetry.

- Ising model:  
or  $\uparrow\downarrow\uparrow\downarrow$



• Common states

phase	Broken symmetry	order parameter	excitation (Boson)	topo defects
Ferro	time-reversal	magnetization	spin-waves (magnons)	domain wall
Nematic	Rotational	$\langle \vec{n} \rangle$		disclinations
crystal	translational	$\rho$ (density)	phonons (Boson)	dislocation 
superfluid	gauge-invariance $\psi \rightarrow e^{i\theta} \psi$	$\langle \psi \rangle = \int n_0 e^{-i\theta}$ ground state number	phonons and rotors (electrons in super conductor)	vortices 

• Crystal lattice :

the ground state of a Hamiltonian -

lattice: a set of points :  $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$ ,  $n_i = 0, \pm 1, \pm 2, \dots$   
 $\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$  linearly independent.

Space-group symmetry  $\Rightarrow$  lattice translation, point group (rotation, reflection)

is periodic  $\{\vec{R}\} = \{\vec{R} + \vec{a}\}$

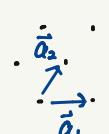
1D lattice: only one kind

2D lattice:  $\vec{a}_1, \vec{a}_2$

①  $(1,0), (0,1) \Rightarrow \frac{\pi}{2}$  rotation symmetry, square lattice

how many?: only 5 lattices.

② rectangular: lose  $\frac{\pi}{2}$  rotation symmetry.

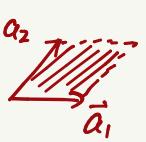
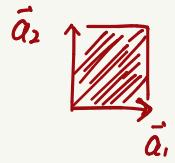
③ triangular:   $\vec{a}_1 = (1,0)$ ,  $\vec{a}_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$   $\frac{\pi}{3}$  rotation

④ centered rectangular:  lose  $\frac{\pi}{3}$  rotation

⑤ arbitrary  $\vec{a}_1, \vec{a}_2$

### 3D lattice: Bravais Lattices

primitive vectors define a "unit cell":



$$\text{Volume: } V_c = |(\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_3| \quad (3D)$$

Wigner-Seitz cell (conventional choice of unit cell):

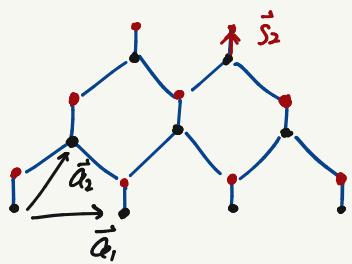
find the part of lattice closest to any lattice point



- crystal structure is a lattice plus a "basis".

every atom in crystal is on  $\left\{ \begin{array}{l} \vec{R}_n \text{ (a lattice point)} \\ \vec{s}_m, m=B \text{ for } B^{\text{th}} \text{ atoms in the basis.} \end{array} \right.$

honey-comb:  $\Rightarrow$  graphene's structure



add basis vectors to triangular

$$\left\{ \begin{array}{l} \vec{s}_1 = \alpha(0,0) \\ \vec{s}_2 = \alpha(0, \frac{1}{\sqrt{3}}) \end{array} \right.$$

- The reciprocal lattice:

A crystal lattice is invariant under some translation:

$$\vec{T} = u_1 \vec{a}_1 + u_2 \vec{a}_2 + u_3 \vec{a}_3, u_1, u_2, u_3 \text{ integer}$$

$$\Rightarrow f(\vec{r}) = f(\vec{r} + \vec{T}) \quad (\text{periodic condition})$$

ensures Fourier expansion:  $f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G} \cdot \vec{r}}$

$$f(\vec{r} + \vec{T}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G} \cdot \vec{r}} \underbrace{|e^{i\vec{G} \cdot \vec{T}}|}_{e^{i\vec{G} \cdot \vec{T}}} \rightarrow e^{i\vec{G} \cdot \vec{T}} = 1$$

To find  $\vec{G}$ ,  $\vec{G} = v_1 \vec{b}_1 + v_2 \vec{b}_2 + v_3 \vec{b}_3$ , then  $\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij} \Rightarrow \left\{ \begin{array}{l} \vec{G} \cdot \vec{T} = 2\pi(v_1 u_1 + v_2 u_2 + v_3 u_3) \\ \vec{b}_i = \frac{2\pi}{V_c} \vec{a}_i \times \vec{a}_c \end{array} \right. \Rightarrow \left\{ \begin{array}{l} \vec{b}_1 = \frac{2\pi(\vec{a}_2 \times \vec{a}_3)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \\ \text{Volume of unit cell} \end{array} \right.$

- reciprocal of reciprocal is real space lattice.

- Consider a set of points constituting a Bravais lattice  $\vec{R}$ , and a plane wave incident on the lattice,  $e^{i\vec{k}\cdot\vec{r}}$
- For a general  $\vec{k}$ , such a plane wave will not have the [periodicity of the lattice]!

- But certain  $\vec{k}$  will:

reciprocal lattice vectors,  $\vec{k} = \vec{G}$  (important for scattering experiment)

- first Brillouin zone is the Wigner-Seitz cell in reciprocal space.

e.g. 3D simple cubic

$$\left\{ \begin{array}{l} \vec{a}_1 = a\hat{x} \\ \vec{a}_2 = a\hat{y} \\ \vec{a}_3 = a\hat{z} \end{array} \right. \Rightarrow \left\{ \begin{array}{l} \vec{b}_1 = \frac{2\pi}{a}\hat{x} \\ \vec{b}_2 = \frac{2\pi}{a}\hat{y} \\ \vec{b}_3 = \frac{2\pi}{a}\hat{z} \end{array} \right. \quad V_{BZ} = |(\vec{b}_1 \times \vec{b}_2) \cdot \vec{b}_3|$$

$\downarrow$

$$-\frac{\pi}{a} < k_i < \frac{\pi}{a}, \quad i=x,y,z$$

- excitation of lattice - phonon.

Note: electronic state in a periodic crystal lattice.

For example, the ions may give rise to a periodic potential for electrons' "feel".

Schrödinger equation:  $-\frac{\hbar^2}{2m} \nabla^2 \psi + \underbrace{V(x)}_{\text{periodic}} \psi(x) = E \psi(x)$ .

recall: For a particle in a box.  $\psi_k(x) = A \sin(kx)$ .  $E = \frac{\hbar^2 k^2}{2m}$ ,  $k = \frac{n\pi}{a}$ ,  $n=1,2,3, \dots$



For a periodic potential, the solution to Schrödinger equation is:

⇒ Bloch Theorem:  $\psi_k(\vec{r}) = \underline{u}_k(\vec{r}) e^{i\vec{k}\cdot\vec{r}}$

Bloch function:  $u_k(\vec{r}) = u_k(\vec{r} + \vec{R})$

- The eigen function of time-dependent Schrödinger equation for a periodic potential are a [plane wave times a periodic function].

- In 1D (non-degenerate),

$\dots \xrightarrow{a} \cdot \cdot \cdot (N \text{ sites})$

PBC  $\Rightarrow$  lattice becomes a ring. }  $\Rightarrow$  Solution:  $\psi(x+a) = C\psi(x)$ ,  $C$  is constant.  
 potential  $\Rightarrow V(x) = V(x+sa)$

goes once along the ring:

Trial form:  $\psi(x+Na) = C^N \psi(x)$ , But wavefunction has to  
 $N$  lattices. be single-valued.

$$\text{Then } C = e^{i2\pi s/N}, s = 0, 1, \dots, N-1$$

$$\Rightarrow \psi(x) = \underline{u(x)} e^{i \frac{2\pi s x}{Na}}, s = 0, 1, \dots, N-1.$$

(note  $u(x)$  has the periodicity as lattice).

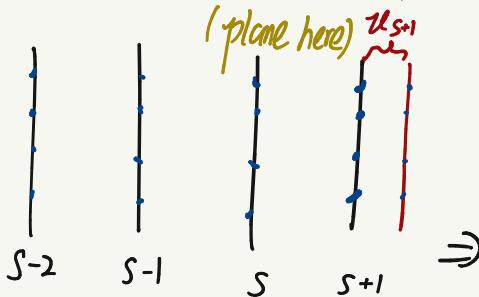
Note: •  $\hbar k$  is "crystal momentum", not in real.

- regions where no Bloch function solutions called "forbidden" Band
  - Bloch function allows for simple approximate descriptions of quasiparticle excitations.
  - classical and quantum waves  $\Rightarrow$  lattice vibrations  $\Rightarrow$  phonon
- $\Rightarrow$  elementary excitation: wave motion (e.g. sound waves macroscopically) microscopically,

atoms on crystal  $\vec{R}_0$  is the equilibrium.

$$\Rightarrow \vec{R} = \vec{R}_0 + \vec{u} \xrightarrow{\text{deviation:}} \text{assume small } u, \frac{m}{a} \ll 1.$$

- Start with classical dynamics:  $u_s$  is the displacement of each plane.



Assumption of interaction: nearest neighbor

$$F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s)$$

$\Rightarrow$  harmonic approximation,

(3D)

$\rightarrow$  Coupled equation

- Solve the Coupled E.O.M.

$$M \frac{d^2 u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s)$$

assume,  $\vec{u}_s = u e^{i(\vec{k} \cdot \vec{r}_s - \omega t)}$

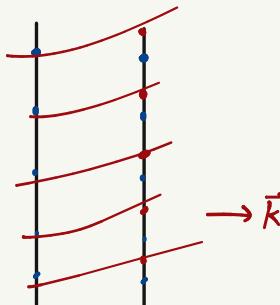
- "normal mode" analysis
- expansion in running waves.

Note: in high dimensions,

can have transverse wave.

$\Rightarrow$  in 3D, one longitudinal wave

and two transverse modes



plugging in,  $\begin{cases} -M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s) \\ u_{s\pm 1} = u e^{i\omega t} e^{iska} e^{\pm ika} \end{cases}$

$$\Rightarrow -M\omega^2 u e^{iska} = C u (e^{i(s+1)ka} + e^{i(s-1)ka} - 2e^{iska})$$

$$\Rightarrow \omega^2 M = -C (e^{ika} + e^{-ika} - 2) = 2C(1 - \cos ka)$$

$$\omega^2 = \frac{2C}{M}(1 - \cos ka) = \frac{4C}{M} \sin^2 \frac{ka}{2} \Rightarrow \omega(k) = \sqrt{\frac{4C}{M}} \left| \sin \frac{ka}{2} \right| \quad (\text{Dispersion relation})$$

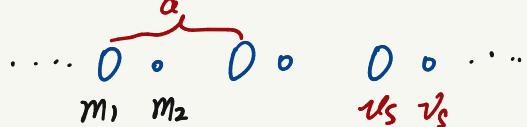
Decouple is processed by normal mode.

For small  $k$ ,  $\omega \rightarrow v k \Rightarrow$  sound wave (long wave length)  $\Rightarrow v = \sqrt{\frac{Ca^2}{M}}$   
(Continuum approximation)

at  $k = \pm \frac{\pi}{a}$ ,  $v_s = v e^{\pm i s \pi}$ : standing waves  $\rightarrow v_g = \frac{dv}{dk} \Big|_{\pm \frac{\pi}{a}} = 0$   
(boundary)

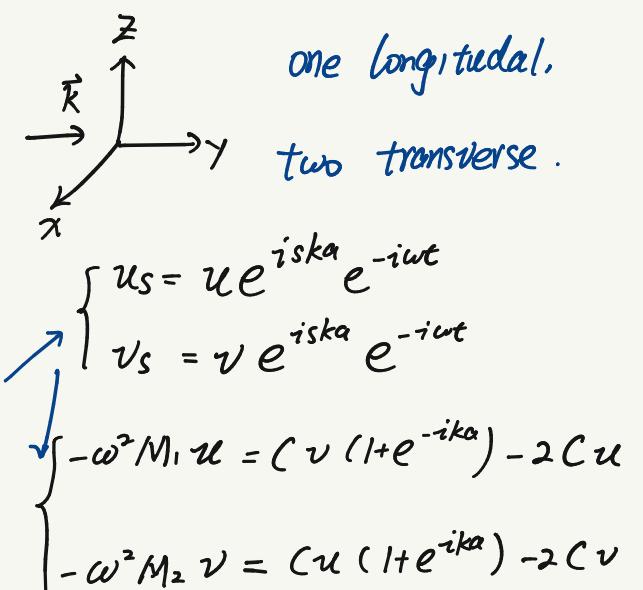
Note: in  $D > 1$ , must label both  $\vec{k}$  and polarization  $\lambda$ :

For two atoms in one unit cell, in 1D



EOM: neighbor and harmonic.

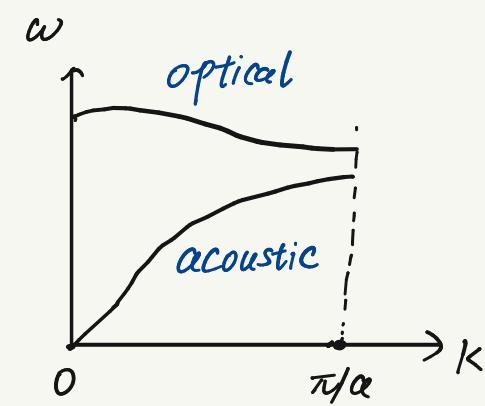
$$\begin{cases} M_1 \frac{d^2 u_s}{dt^2} = C(v_s + v_{s-1} - 2v_s) \\ M_2 \frac{d^2 v_s}{dt^2} = C(u_{s+1} + u_s - 2u_s) \end{cases}$$



For homogeneous linear equation,

have a solution only if  $\det A = 0$

$\downarrow$   
matrix of coefficient.



$$\begin{vmatrix} 2C - M_1 \omega^2 & -C(1 + e^{-ika}) \\ -C(1 + e^{ika}) & 2C - M_2 \omega^2 \end{vmatrix} = 0 \Rightarrow \text{two solution}$$

limit : 1)  $ka \ll 1$ ,  $\cos ka \approx 1 - \frac{1}{2}k^2 a^2$

$$2) \quad ka \approx \pm \pi. \quad \begin{cases} \omega^2 = \frac{2C}{M_1} \\ \omega^2 = \frac{2C}{M_2} \end{cases}$$

(3D)

- in a crystal with  $p$  atoms per unit cell,

$\begin{cases} 3 \text{ acoustical modes.} \rightarrow \text{center of mass} \\ 3(p-1) \text{ optical modes.} \rightarrow \text{relative motion.} \end{cases}$

- Quantum mechanics of lattice vibration

real space  $\rightarrow$  momentum space  
(decoupled)

In QM.  $\begin{cases} \vec{u}(\vec{R}) \text{ becomes operators.} \\ \vec{p} = m\dot{\vec{u}} \end{cases}$

- model of quantum lattice vibration due to Einstein.

Consider each atom on the lattices as independent oscillator (non-interacting)

In the linear case,  $\hat{H} = \sum_{\lambda, \vec{R}} \left[ \frac{\hat{p}^2(\vec{R})}{2m} + \frac{1}{2}m\omega_E^2 \hat{u}^2(\vec{R}) \right]$ ,  $\omega_E$  is constant  
 $\lambda = 1, 2, 3$   $\downarrow$  sum of 3N independent oscillators.

Solution:  $\hat{H} = \sum_{\lambda, \vec{R}} \hbar\omega_E (\hat{a}_\lambda^\dagger(\vec{R}) \hat{a}_\lambda(\vec{R}) + \frac{1}{2}) = \sum_{\lambda, \vec{R}} \hbar\omega_E (\hat{n}_\lambda(\vec{R}) + \frac{1}{2})$  (in number basis)

$\hat{a}_\lambda^\dagger(\vec{R}_k)$  creates an excitation at  $\vec{R}_k$

Commutator (Boson):  $[\hat{a}_\lambda(\vec{R}), \hat{a}_{\lambda'}^\dagger(\vec{R}')] = \delta_{\vec{R}, \vec{R}'} \delta_{\lambda, \lambda'}$ . (second quantization)

$\Rightarrow$  Einstein phonons  $\rightarrow$  optical branch  $\rightarrow \omega_E \approx \text{constant}$ ,  $E = (n + \frac{1}{2})\hbar\omega_E$   
(localized at lattices)

$\sum |n_{\lambda_1}(\vec{R}_1), n_{\lambda_2}(\vec{R}_2), n_{\lambda_3}(\vec{R}_3), \dots n_{\lambda_N}(\vec{R}_N)\rangle$

Fock space.

- more generally: the displacement are coupled.

1D:  $\mathcal{H} = \sum_{s=1}^N \left[ \frac{p_s^2}{2m} + \frac{1}{2} C (u_{s+1} - u_s)^2 \right]$  (nearest neighbor)

make Fourier transformation,

$$u_s = \frac{1}{\sqrt{N}} \sum_k u_k e^{iksa}, \quad p_s = \frac{1}{\sqrt{N}} \sum_k p_k e^{iksa}.$$

in momentum space:

$$\Rightarrow \mathcal{H} = \sum_k \frac{p_k p_{-k}}{2m} + \frac{1}{2} m \omega^2(k) u_k u_{-k}$$

$\Rightarrow$  (creator and annihilator  $\alpha$  "running wave" of vector  $\vec{k}$ ,

3D case:

Hamiltonian:  $\mathcal{H} = \sum_{\vec{k}} \hbar \omega(\vec{k}) (\alpha_{\lambda}^+(\vec{k}) \alpha_{\lambda}(\vec{k}) + \frac{1}{2})$  (uncoupled)!

come from "how many modes a wave vector":

$\lambda$  stands for polarization  $\begin{cases} 3 \text{ acoustic} \\ 3p3 \text{ optical} \end{cases}$

$\alpha_{\lambda}^+(\vec{k})$  is labeled by  $\vec{k}, \lambda$ . (p atoms in a cell)

note:  $\hbar \vec{k}$  is crystal momentum

Thermal effects of phonons Canonical ensemble:  $\langle \hat{A} \rangle = \frac{\text{Tr} [\hat{A} e^{-\beta \hat{H}}]}{\text{Tr} [e^{-\beta \hat{H}}]}$

each phonon has a probability of being excited at a given temperature  $T$ ,

what is the energy of all the phonons being excited:  $U = \sum_{\vec{k}\lambda} \hbar \omega_{\lambda}(\vec{k}) \langle \hat{n}_{\vec{k}\lambda} + \frac{1}{2} \rangle$

$$\langle \hat{n}_{\vec{k}\lambda} \rangle = \frac{\sum_n n e^{-\beta E_n}}{\sum_n e^{-\beta E_n}} = \frac{\sum_n n e^{-\beta \hbar \omega_{\lambda}(\vec{k}) (n + \frac{1}{2})}}{\sum_n e^{-\beta \hbar \omega_{\lambda}(\vec{k}) (n + \frac{1}{2})}}, \quad \sum_n e^{-\lambda n} = \frac{1}{1 - e^{-\lambda}}$$

(trace in number basis.)

$$\text{no chemical potential. } \Rightarrow \langle \hat{n}_{\vec{k}\lambda} \rangle = \frac{1}{e^{\frac{\hbar \omega_{\lambda}}{k_B T}} - 1} = \frac{e^{-\lambda}}{(1 - e^{-\lambda})^2}$$

$$\Rightarrow \text{specific heat } C_v = \frac{\partial U}{\partial T} \Big|_v . \text{ classical case: } k_B T \gg \hbar \omega : e^{\frac{\hbar \omega_{\lambda}}{k_B T}} \approx 1 + \frac{\hbar \omega_{\lambda}}{k_B T}$$

$$\left\{ \begin{array}{l} U_{\text{classical}} \approx \sum_{\vec{k}\lambda} \hbar \omega_{\lambda} \frac{1}{\hbar \omega_{\lambda}} k_B T = k_B T \sum_{\vec{k}\lambda} 1 = k_B T (3N) p \\ C_v = \frac{\partial U}{\partial T} \Big|_v = 3N k_B p \Rightarrow \text{Dulong and Petit law.} \end{array} \right.$$

Low temperature limit :

$$C_V = \frac{\partial}{\partial T} \sum_{k\lambda} \frac{\hbar\omega_{k\lambda}}{e^{\beta\hbar\omega_{k\lambda}/k_B T} - 1}$$

deal it  
in the form of integral

$$\sum_k \rightarrow \frac{V}{(2\pi)^3} \int d^3k \quad \left( \frac{(2\pi)^3}{V} \right)$$

volume of B.Z.)

$$= V \frac{\partial}{\partial T} \sum_{B.Z.} \int \frac{d^3k}{(2\pi)^3} \frac{\hbar\omega_{k\lambda}(k)}{e^{\beta\hbar\omega_{k\lambda}(k)/k_B T} - 1}$$

1) Forget the basis

2) assume same dispersions for  $3Np$  modes  
(linear :  $\omega = ck$  (acoustic branch!!))

3) Extend the limit of integration from  $k=0 \rightarrow \infty$ .

$$= V \frac{\partial}{\partial T} \sum_{B.Z.} \int \frac{d^3k}{(2\pi)^3} \frac{\hbar ck}{e^{\beta\hbar ck/k_B T} - 1}$$

$$= V \frac{\partial}{\partial T} \sum_{B.Z.} \int \frac{4\pi k^2 dk}{(2\pi)^3} \frac{\hbar ck}{e^{\beta\hbar ck/k_B T} - 1}$$

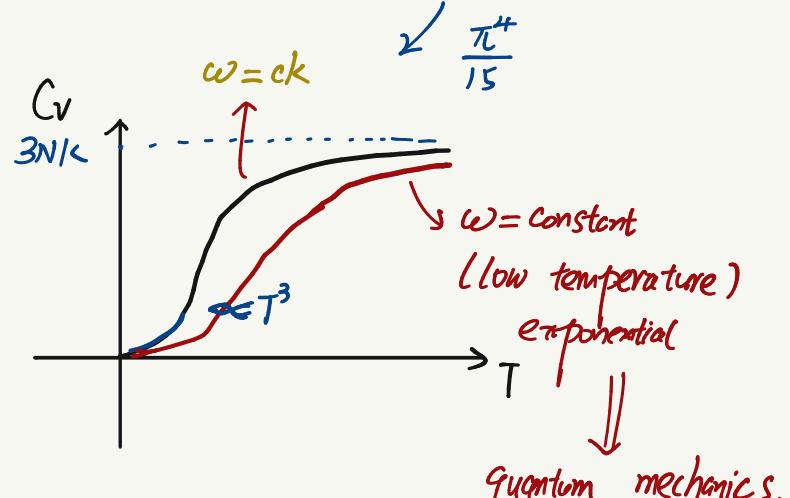
take  $\beta\hbar ck = x = \frac{\hbar ck}{k_B T}$

$$= V \frac{\partial}{\partial T} \sum_{B.Z.} \frac{4\pi}{(2\pi)^3} \int_0^\infty \left(\frac{k_B T}{\hbar c}\right)^2 x^2 \frac{k_B T x}{e^x - 1} \left( \frac{T k_B}{\hbar c} dx \right) = V \frac{\partial}{\partial T} \frac{(k_B T)^4}{(\hbar c)^3 (2\pi)^2} \left[ \int_0^\infty \frac{x^3 dx}{e^x - 1} \right]$$

↓

$$C_V \approx V \frac{\partial}{\partial T} \left( \frac{\pi^2}{10} \frac{(k_B T)^4}{(\hbar c)^3} \right) = V \frac{2\pi^2}{5} k_B \left( \frac{k_B T}{\hbar c} \right)^3$$

↓ Debye law.



• BEC : Macroscopic quantum phenomena

- Superconductivity → BCS (1957)
- Superfluidity
- BEC → experiment 1995