January 14, 2020

① Phonons
② X-Ray
③ Electronic properties

RESPONSE FUNCTION → how do measurements

P	R	F
X	X	S
V	J	σ
$\underline{D}$	$\underline{E}$	
$\underline{H}$	$\underline{B}$	
Q	T	c_v

$$p \rightsquigarrow \boxed{} \rightsquigarrow R$$

$$R = F(p)$$

GOAL = What is F? Build a model that give the response

In principal we can do everything with quantum mechanic.
TASK → build models for $R = F(p) = A\,p$ $\quad A \simeq \frac{R}{P}$ LINEAR APPROXIMATION

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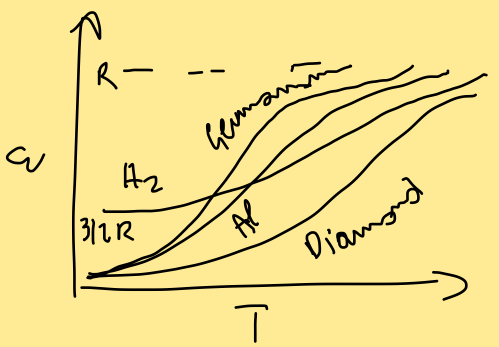
c_v $\quad Q \rightarrow \boxed{?} \rightarrow T$ $\quad$ What is inside the box? Model



TERMODYNAMICS
- axiomatic theory
- not based on a model
- avogadro law → connection the macroscopic behaviour with the micro

WHICH IS THE CONNECTION BETWEEN Q–T?

ZERO PRINCIPLE

Something hot – something cold in contact → reach equilibrium

STATE → U, V, M, $M_1, \dots, M_f$
↓ internal energy
→ # partical of chemical components

I need to make a choice = U or S, then the other variables are correlated

THERMAL CONTACT → two materials in contact exchange heat

THERMAL EQUILIBRIUM → the state does not change (dynamical eq.)

T → in Kelvin $\quad \boxed{A}\ T_A \quad \boxed{B}\ T_B \quad \longrightarrow \quad \boxed{\begin{matrix} A \\ B \end{matrix}}\ T_{AB} \qquad T_A \leq T_{AB} \leq T_B$

FIRST PRINCIPLE

Perpetuum motion does not exist $\rightarrow$ GENERALIZATION OF ENERGY CONSERVATION

$\exists\, U : \alpha, \beta$ at equilibrium $\quad E = U(\beta) - U(\alpha)$

INTERNAL ENERGY

$E = W + Q \qquad$ W work done, Q heat supplied

$W + Q = \Delta U$ or $\quad dU = đW + đQ$

eg. $đW = -PdV \quad đW = \underline{E}\cdot d\underline{P} \quad đW = \underline{H}\cdot d\underline{H}$

SECOND PRINCIPLE

heat flows spontaneously from high-T to low-T

it is not possible the opposite.

$\exists\, S$, ENTROPY, extensive variable

- during arbitrary ADIABATIC PROCESS (no heat exchange

$$Q_{\alpha\to\beta} = 0 \rightarrow S(\beta) \geq S(\alpha)$$

$$đQ = 0 \rightarrow dS \geq 0$$

CARNOT CYCLE $\quad dS \geq \dfrac{đQ}{T}$

if transformation reversible $\quad dS = \dfrac{đQ}{T}$

THIRD PRINCIPLE

Related to QM

"The S of all perfect crystal at T=0 is always the same = a constant that we assume to be 0"

QUESTION: HOW TO CONNECT T WITH Q

$$\xrightarrow[đQ]{Q} \boxed{?} \xrightarrow[dT]{T}$$

$$\left(\frac{đQ}{dT}\right)_V = \left(\frac{\partial U}{\partial T}\right)_V = C_V$$

$$đQ + đW = dU$$

$$đQ - PdV = dU$$

Principle of TD are at constant V?

?

STATE VARIABLE

REALITY $\rightarrow$ not constant V

$C_V \rightarrow C_p$

eg. $\Delta Q = I^2 R \Delta t$

January 16, 2020

- $C_p \sim C_v$
- CM phase space
- SM Boltzmann
- SM Equipartition
- Dulong - Petit

$\left.\begin{matrix} \\ \\ \\ \\ \end{matrix}\right\}$ Classical physics

---

$$\xrightarrow{P} \boxed{} \xrightarrow{R} \qquad \left(\frac{đQ}{dT}\right)_{V,N} = C_{V,N}$$

$$F(P) = R \qquad đQ + đW = dU$$

LINEAR APPROXIMATION $\qquad đQ = TdS$

Let's be little bit more precise on the C_V definition: in principle I can also define $C_{P,N}$ and relates it with $C_{V,N}$

$$\left(\frac{đQ}{dT}\right)_{P,N} = C_{P,N}$$

$$C_{P,N} = C_{V,N} + \left(\frac{\partial V}{\partial T}\right)_{P,N}\left[\left(\frac{\partial U}{\partial V}\right)_{T,N} + P\right]$$

ISOTER. COMPRESSIBILITY $\quad k_{T,N} = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{T,N}$

THERMAL EXPANSIVITY $\quad \alpha_{P,N} = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{P,N}$

We can combine all together and we obtain:

$$\boxed{k_{T,N}\left(C_{P,N} - C_{V,N}\right) = TV\alpha^2_{P,N}} \longrightarrow \boxed{C_v \sim C_p}$$

NB Water has very high specific heat = this is the reason of life on earth

I feel cold when I touch metal because conduction is high

MODEL = Box full of particle

What we know for moving from mechanics (one system at the time) to statistical mechanics (avogadro number of same systems)? clarify the concept of phase space.

PHASE SPACE

Hamiltonian mechanics allow to go from CLASSICAL to QUANTUM mechanics.

HM $\rightarrow$ position and momenta as INDIPENDET VARIABLES

$\underline{r}_1, \underline{r}_2, \dots, \underline{r}_N$ POSITIONS
$\underline{p}_1, \underline{p}_2, \dots, \underline{p}_N$ MOMENTA

In HM I need only momenta = first order differential equation

$q_1, q_2 \dots q_{3N}$
$p_1, p_2, \dots p_{3N}$ $\rightarrow (q_1 q_2 \dots q_{3N}\ p_1 p_2 \dots p_{3N}) \rightarrow \Gamma$ PHASE SPACE

$\dim \Gamma = 2N_f$ $\quad N_f$ degree of freedom

Which equation do I have? No forces, ENERGY

$H(q_1 q_2 \dots q_{3N}\ p_1 p_2 \dots p_{3N}, t)$

not all systems

$H = T + V$

$$\boxed{\begin{cases} \dot{q}_i = \dfrac{\partial H}{\partial p_i} \\ \dot{p}_i = -\dfrac{\partial H}{\partial q_i} \end{cases}}$$

HAMILTON EQUATIONS

Kinetic energy is not related to the positions $\frac{1}{2}mv^2 = \frac{p^2}{2m} = T$

$\dot{p} = -\dfrac{\partial H}{\partial q_i} = -\dfrac{\partial V}{\partial q_i} \longrightarrow$ Nothing less than the second law of Newton

$$\{f,g\} = \sum_i \left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} \right)$$ POSSION BRACKETS

I can use poisson brackets to rewrite the Hamilton equations

$$\boxed{\begin{aligned} \dot q_i &= \{q_i, H\} \\ \dot p_i &= \{p_i, H\} \end{aligned}}$$

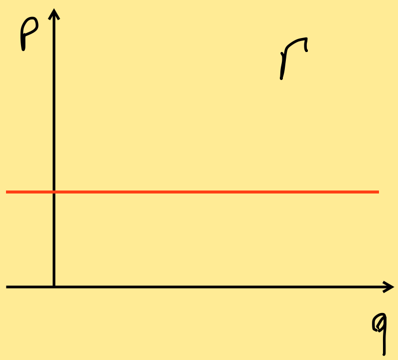
- usefull when we will do harmonic oscillator
- quantization

EX: FREE PARTICLE

$$H = \frac{p^2}{2m} = \frac{p_1^2 + p_2^2 + p_3^2}{2m}$$

$N = 1$ dim $\Gamma = 6$

$(q_1 q_2 q_3 p_1 p_2 p_3)$



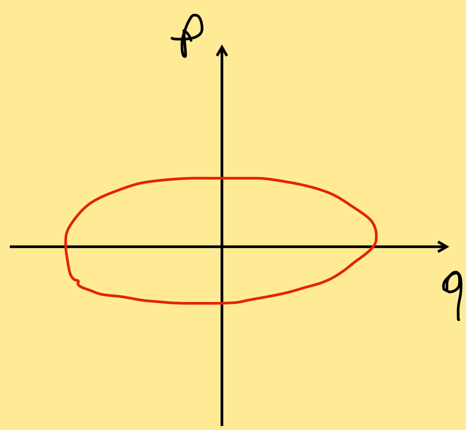
$$\begin{cases} \dot q_i = \dfrac{\partial H}{\partial p_i} = \dfrac{p_i}{m} \longrightarrow p_i = m \dot q_i \\ \dot p_i = -\dfrac{\partial H}{\partial q_i} = 0 \longrightarrow \text{Momentum is conserved: no forces!} \end{cases}$$

EX: HARMONIC OSCILLATOR

$$H = \frac{p^2}{2m} + \frac{1}{2} k q^2 \qquad \omega^2 = \frac{k}{m}$$

$$\begin{cases} \dot q_i = \dfrac{\partial H}{\partial p_i} = \dfrac{p_i}{2m} \\ \dot p_i = -\dfrac{\partial H}{\partial q_i} = -kq \end{cases} \longrightarrow \begin{aligned} q &= q_0 \cos \omega t \\ p &= p_0 \sin \omega t \end{aligned}$$

Hooke force

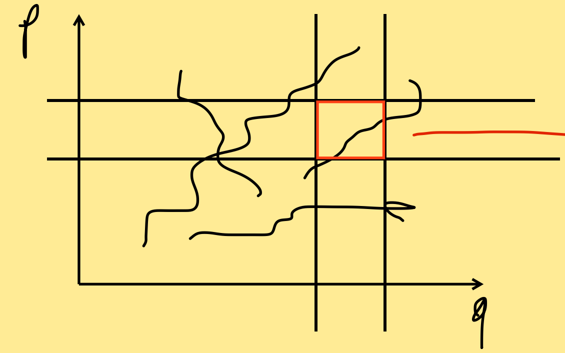


I have phase space now.

Now I have to introduce the concept of ENSAMBLE

ENSAMBLE → each particle different initial conditions

To many particle → I need to consider averages



$H(q_1 q_2 \cdots q_{3N} P_1 P_2 \cdots P_{3N})$

$\to dq_1 dq_2 \cdots dq_{3N} \, dp_1 dp_2 \cdots dp_{3N}$

N particles in total

n_i particles in each cell

EQUILIBRIUM → something that maximize the probability to find a particle

ONLY ONE CELL $\quad \binom{N}{n_i} = \dfrac{N!}{n_i!(N-n_i)!}$

ALL THE COMBINATION FOR ALL CELL $\quad P = \binom{N}{n_1}\binom{N-n_1}{n_2}\binom{N-n_1-n_2}{n_3} \cdots = \dfrac{N!}{n_1!\,n_2!\,n_3!\cdots}$

I have to maximize P, if at EQUILIBRIUM

there is something missing:

- N remain the same $\sum_i n_i = N$
- Energy conservation $\sum_i n_i E_i = E$

$\Big\}$ TWO CONSTRAIN TO IMPOSE

TRICK: I work on $\log P$ instead of P

$$F[\{n_i\}, \alpha, \beta] = \ln P - \alpha\left(\sum_i n_i - N\right) - \beta\left(\sum_i n_i E_i - E\right)$$

Lagrange mult.

I need to comput $\dfrac{\partial F}{\partial n_i} = 0$.

NB. $\ln P = \ln(N!) - \sum_i \ln(n_i!)$

$\ln n! = \sum_1^n \ln n \sim \int_1^n \ln x \, dx =$

STEARLIN APPROX.

$\ln P = N \ln N - N - \sum_i (n_i \ln n_i - n_i)$

$$\frac{\partial F}{\partial n_i} = 0 = -\ln n_i \cancel{-1} \cancel{+1} - \alpha - \beta E_i$$

$$\boxed{\begin{aligned} n_i &= \exp(-\alpha - \beta E_i) \\ &= A\, e^{-\beta E_i} \end{aligned}}$$

This is a discrete formulation, I can do also the continuous formulation

$$dn = A e^{-\beta H(q,p)}$$

$$\int dn = N$$

$$A = \frac{1}{\int e^{-\beta H} dp_1 dp_2 \cdots dp_{3N} \, dq_1 dq_2 \cdots dq_{3N}}$$

BOLTZMANN DISTRIBUTION FUNCTION

What is β? $\beta = \frac{1}{k_B T}$, interpreted a posteriori

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We need to count what happens to n_i when H is quadratic in T and V = we can derive the EQUIPARTITION THEOREM.

January 21, 2020

- CM
- CM + SM + TD

Today

- Equipartition
- CM
- QM

Next

- QM Ethan
- Article on Einstein

$C_p = \left(\frac{đQ}{dT}\right)_{P,N}$ $\quad C_v = \left(\frac{đQ}{dT}\right)_{V,N} = \left(\frac{\partial U}{\partial T}\right)_{V,N}$

$đQ + đW = dU$

$đW = -PdV = \phi$

$\boxed{C_p \simeq C_T \text{ SOLID}}$

RESPONSE

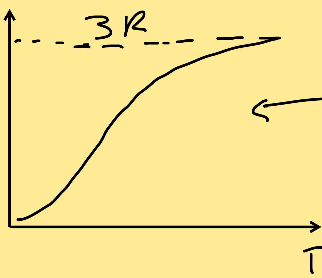
$F(P) = R$

$\downarrow$

C_V

SM

C_V



DOULONG PETIT

ENSAMBLE

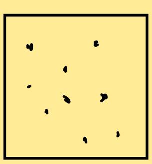
$d\mu = \frac{1}{A} e^{-\beta H(q,p)}$ $\quad H(q,p)$

$C_V = \left(\frac{\partial U}{\partial T}\right)_V = 3R$

$U = 3RT$

EQUIPARTITION

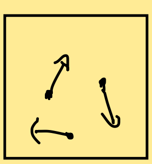
$U = \int_\Gamma H(q,p)\, d\mu$

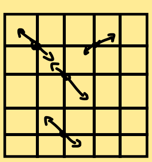


GAS

$H = \frac{p^2}{2m}$

BOTH QUADRATIC HAMILTONIANS





SOLID

$\sum_i \frac{p_i^2}{2m} + \frac{k q_i^2}{2}$

$H = H(q_1 q_2 q_3 \dots p_1 p_2 \dots) = \sum_i (b_j p_j^2 + a_j q_j^2)$

$U = \langle H \rangle \longrightarrow \frac{\int b_i p_i^2 d\mu}{\int d\mu} = \frac{\int_\Gamma b_j p_j^2 e^{-\beta H} dq_1 dq_2 \dots dp_1 dp_2 \dots}{\int_\Gamma e^{-\beta H} dq_1 dq_2 \dots dp_1 dp_2 \dots}$

$= \frac{\int_\Gamma dp_j\, e^{-\beta b_j p_j^2} b_j p_j^2}{\int_\Gamma dp_j\, e^{-\beta b_j p_j^2}}$

$= b_j \frac{1}{2\beta b_j} = \frac{1}{2\beta} = \frac{1}{2} k_B T$

$\boxed{\text{EQUIPARTITION THEOREM OF ENERGY}}$

NB $\prod_{k \neq j} \frac{\int e^{-\beta b_k p_k^2} dp_k}{\int e^{-\beta b_k p_k^2} dp_k} = 1$

$\int e^{-(ax)^2} x^2 dx = \frac{\sqrt{\pi}}{4a^3}$

$\int e^{-(ax)^2} dx = \frac{\sqrt{\pi}}{2a}$

$H = \frac{p^2}{2m} = \frac{p_x^2 + p_y^2 + p_z^2}{2m} = \frac{3}{2} k_B T$

$H = \sum_i \frac{p_i^2}{2m} + \frac{k q_i^2}{2} = 6 N_A \frac{1}{2} k_B T = 3RT$

$R = N_A k_B$

I can do this for every quadratic Hamiltonian that I know.

$\frac{\int a_j q_j^2 d\mu}{\int d\mu}$

C_V is not a function of T! PROBLEM!
I am not so off... $T \to \infty$, $C_V \to 3R$
For now the approximations are: quadratic Hamiltonian

$$\boxed{C_V = \left(\frac{\partial U}{\partial T}\right)_N = 3R \quad \text{DOULONG - PETIT MODEL}}$$

Classically we cannot explain the T dependence of C_V: we introduce QUANTUM MECHANICS.

1° POSTULATE → the wave function ψ describes the state of the system

$$\psi(\underline{r}_1, \underline{r}_2, \dots, \underline{r}_f, t)$$

$$\psi^* \psi \, d\tau = \psi^* \psi \, d\underline{r}_1 d\underline{r}_2 \dots d\underline{r}_f \longrightarrow \int \psi^* \psi \, d\tau = 1$$

2° POSTULATE → From classical physics to quantum
classically we can always define an operator as function of positions and momenta.

$$\begin{cases} \underline{r}_i \to \hat{\underline{r}}_i \\ \underline{p}_i \to i\hbar \dfrac{\partial}{\partial \underline{r}_i} = -i\hbar \underline{\nabla}_i \end{cases} \qquad \hbar = \frac{h}{2\pi}$$

ARE THE SAME THING

Eg. $H = \dfrac{p^2}{2m} \longrightarrow \hat{H} = -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2}$

$$H = \frac{\underline{p}^2}{2m} \longrightarrow \hat{H} = -\frac{\hbar^2}{2m}\nabla^2$$

$$\{f, g\} \longrightarrow \frac{1}{i\hbar}[\hat{f}, \hat{g}]$$

$$\{q, p\} = \frac{\partial q}{\partial q}\frac{\partial p}{\partial p} - \cancel{\frac{\partial q}{\partial p}\frac{\partial p}{\partial q}} = 1$$

$[\hat{q}, \hat{p}] = i\hbar$ $\quad (\hat{q}\hat{p} - \hat{p}\hat{q})\psi = \left(-x\left(i\hbar\frac{\partial}{\partial x}\right) - \left(-i\hbar\frac{\partial}{\partial x}\right)x\right)\psi$

$$= -i\hbar x\frac{\partial \psi}{\partial x} + i\hbar\frac{\partial}{\partial x}(x\psi)$$

$$= \cancel{-i\hbar x\frac{\partial \psi}{\partial x}} + i\hbar\frac{\partial x}{\partial x} + \cancel{i\hbar\frac{\partial \psi}{\partial x}} = i\hbar$$

3° POSTULATE → Eigenvalue problem

$\hat{\mu}\psi = m\psi$ $\quad$ m are the possible value that $\hat{\mu}$ can assume apply on ψ

$$\hat{\mu} = \left(\underline{r}_i - i\hbar\frac{\partial}{\partial \underline{r}_i}; t\right)$$

EG. $\hat{H}\psi = E\psi$ Schrodinger equation at the stationary state

4° POSTULATE → The time evolution of the system is determine by the Schrodinger equation

$$H\psi = i\hbar\frac{\partial}{\partial t}\psi$$

FREE - PARTICLE MODEL

$H = \frac{p^2}{2m}$ $\quad H\psi = i\hbar\frac{\partial}{\partial t}\psi$

$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2$ $\quad -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ $\quad \psi(\underline{r}, t)$

$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = i\hbar\frac{\partial\psi}{\partial t}$ $\quad \psi(x,t) = \varphi(x)\phi(t)$

Solved by separate the variable

$$-\frac{\hbar^2}{2m}\phi(t)\frac{\partial^2\varphi}{\partial x^2} = i\hbar\,\varphi(x)\frac{\partial\phi}{\partial t}$$

$$\frac{-\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial^2 x}}{\varphi(x)} = i\hbar\frac{\partial\phi}{\partial t} \longrightarrow$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial^2 x} = E\varphi \qquad \varphi(x) = Be^{ikx}$$

$$i\hbar\frac{\partial\phi}{\partial t} = E\phi \qquad \phi(t) = Ae^{-i\omega t}$$

$$\omega:\ i\hbar(-i\omega) = E$$

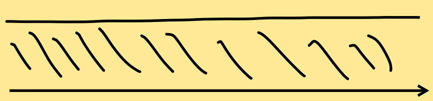
$$\boxed{E = \hbar\omega = \frac{h}{\cancel{2\pi}}\cancel{2\pi}\,\nu = h\nu \quad \text{EINSTEIN RELATION}}$$

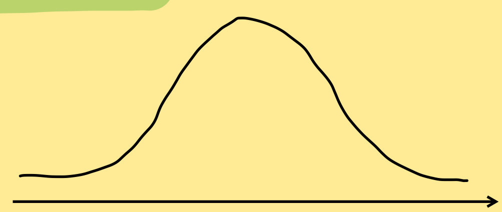
$$E = \frac{\hbar^2}{2m}k^2 \qquad k = \frac{2\pi}{\lambda}$$

$$\hbar k = p = \frac{h}{\cancel{2\pi}}\frac{\cancel{2\pi}}{\lambda} = \frac{h}{\lambda} \longrightarrow \begin{array}{l} p\lambda = h \\ \lambda = \frac{h}{p} \end{array}$$

PROBLEM Free-electron model gives a φ that is NOT NORMALIZABLE

→ SOLUTION = WAVE-PACKETS





February 25, 2020

SUMMARY

DP $\longrightarrow$ + QM Einstein model

Coupled $\longrightarrow$ normal modes

TODAY

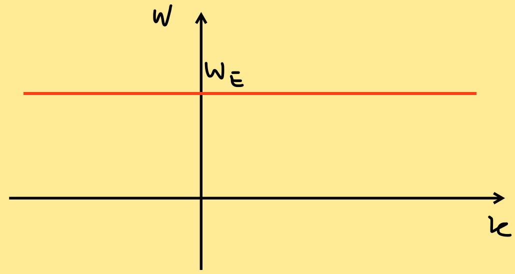
QM

Quasi particles

DOS

$$U = \hbar\omega_E\left(n_{BE}(\omega, T) + \frac{1}{2}\right) 3N_A$$

this point



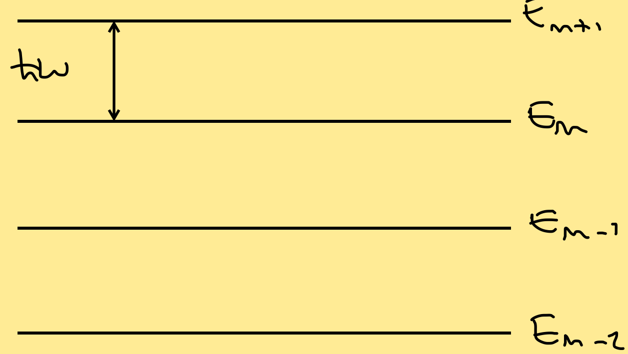
EINSTEIN MODEL

$$U = \sum_{n,\underline{k}} \hbar\omega_n(\underline{k})\left(n_{BE} + \frac{1}{2}\right)$$

$$\psi_n(x,t) = |n\rangle \qquad H|n\rangle = E_n|n\rangle \qquad H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$$

$$[\hat{x},\hat{p}] = i\hbar \qquad [\hat{x},\hat{H}] = \frac{i\hbar}{m}\hat{p}$$

$$\begin{cases} (E_n - E_k)\langle k|\hat{x}|n\rangle = \dfrac{i\hbar}{m}\langle k|\hat{p}|n\rangle \\ (E_n - E_k)\langle k|\hat{p}|n\rangle = -im\hbar\omega^2\langle k|\hat{x}|n\rangle \end{cases}$$



$$E_n = \hbar\omega(n + c)$$

II QUANTIZATION

NB. In a non-relativistic regime, it does not add nothing: it is only another notation.

$$-im\omega \begin{cases} (E_m - E_k)\langle k|\hat{x}|m\rangle = \frac{i\hbar}{m}\langle k|\hat{p}|m\rangle \\ (E_m - E_k)\langle k|\hat{p}|m\rangle = -im\hbar\omega^2\langle k|\hat{x}|m\rangle \end{cases} +$$

$$(-im\omega)(E_m - E_k)\langle k|x|m\rangle + (E_m - E_k)\langle k|p|m\rangle = (-im\omega)\frac{i\hbar}{m}\langle k|p|m\rangle - im\hbar\omega^2\langle k|x|m\rangle$$

$$(E_m - E_k)\langle k|\underbrace{p - im\omega x}_{a}|m\rangle = \hbar\omega\langle k|\underbrace{p - im\omega x}_{a}|m\rangle$$

$a \to$ destroies exitations (quasi particles)
$a^+ \to$ adds exitations

$(p - im\omega x)^* = (p + im\omega x)$
$a \neq a^+ \to$ not observable (2nd postulate QM)

Let's see some properties of a

$\langle m-1|a|m\rangle = \lambda_m = \sqrt{m}$ $\qquad a|m\rangle = \sqrt{m}|m-1\rangle$

$\langle m|a^+|m-1\rangle = \lambda^*_m = \sqrt{m}$ $\qquad a^+|m-1\rangle = \sqrt{m}|m\rangle$

LOWERING AND RAISING OPERATORS

In II quantization each exitation corresponds to a quantum of energy.

Let's understand the ZERO-POINT ENERGY.

$a|0\rangle = (p - im\omega x|0\rangle = 0|0\rangle$ (by definition) $\longrightarrow (p + im\omega x)(p - im\omega x)|0\rangle = (p^2 + im\omega[x,p] + m^2\omega^2x^2)|0\rangle$

$$2m\left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 - \frac{1}{2}\hbar\omega\right)|0\rangle = 0$$

$$H|0\rangle = \frac{1}{2}\hbar\omega|0\rangle$$

The absence of exitation have an energy because of indetermination principle.

NB. $E_m = \hbar\omega\left(m + \frac{1}{2}\right)$

In order to simplify how we write H

$$\left.\begin{aligned}(p-im\omega x)\frac{1}{\sqrt{2m\hbar\omega}} &= \sqrt{\frac{m\omega}{2\hbar}}\,x+i\frac{p}{\sqrt{2m\hbar\omega}} = a\\ (p+im\omega x)\frac{-i}{\sqrt{2m\hbar\omega}} &= \sqrt{\frac{m\omega}{2\hbar}}\,x-i\frac{p}{\sqrt{2m\hbar\omega}} = a^+\end{aligned}\right\}\quad \boxed{\begin{aligned}&[a,a^+]=1\\ &H=\left(a^+a+\tfrac{1}{2}\right)\hbar\omega\end{aligned}}$$

$\hat{N} = a^+a \rightarrow$ how many exitations I have in the system

$$\hat{N}|n\rangle = a^+a\,|n\rangle = n|n\rangle$$

$$a = \begin{pmatrix} 0 & 1 & & & \\ & 0 & \sqrt{2} & & \\ & & 0 & \sqrt{3} & \\ & & & 0 & \sqrt{4} \\ & & & & \ddots \end{pmatrix} \qquad a^+ = \begin{pmatrix} 0 & & & & \\ 1 & 0 & & & \\ & \sqrt{2} & 0 & & \\ & & \sqrt{3} & 0 & \\ & & & \sqrt{4} & \ddots \end{pmatrix} \qquad N = \begin{pmatrix} 1 & & & & \\ & 2 & & & \\ & & 3 & & \\ & & & 4 & \\ & & & & \ddots \end{pmatrix}$$

Now I want to write H for more than one oscillator = a family of oscillators

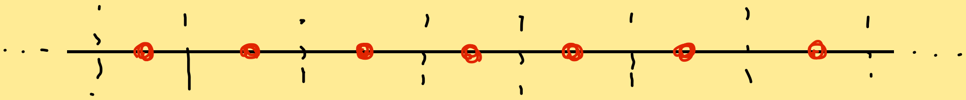
$$H = \sum_{n\underline{k}} \hbar\omega_{n\underline{k}}\left(a^+_{n\underline{k}}\,a_{n\underline{k}} + \frac{1}{2}\right)$$

Now I have to count the particles differently

$$|n_1\, n_2\, n_3 \dots \rangle = \sum (a_1^+)^{n_1}(a_2^+)^{n_2}\dots|0\rangle$$ FOCK SPACES $\rightarrow$ direct product of H spaces

LINEAR CHAIN OF OSCILLATORS

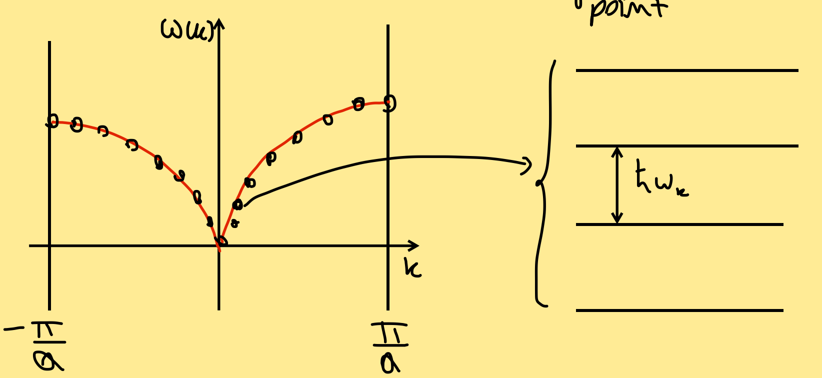
$$H=\sum_n \frac{p_n^2}{2m}+\frac{1}{2}J\left(2u_n^2-u_nu_{n+1}-u_nu_{n-1}\right)$$



$$a_k=\frac{1}{\sqrt{N}}\sum_n e^{-ikna}\left[\left(\frac{m\omega(k)}{2\hbar}\right)^{1/2}u_n+i\sqrt{\frac{1}{2\hbar m\omega(k)}}\,p_n\right]$$

$$a_k^+=\frac{1}{\sqrt{N}}\sum_n e^{ika}$$

We have a ladder for each k point



$$[a_k,a_{k'}^+]=\delta_{kk'}$$

$$[a_{k'},a_k]=[a_k^+,a_{k'}^+]=0$$

$$H=\sum_k \hbar\omega(k)\left(a_k^+a_k+\frac{1}{2}\right)$$

$$E(k')=\underbrace{\langle 0|a_{k'}}_{\langle k'|}H\underbrace{a_{k'}^+|0\rangle}_{|k'\rangle}$$

Now, instead of do a sum I want to do an integral

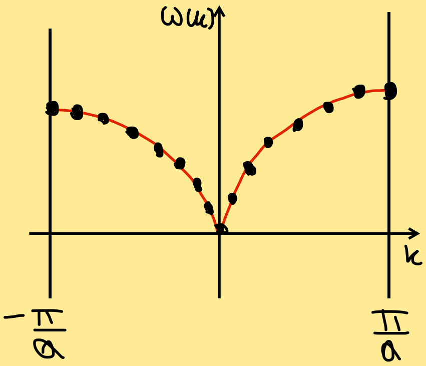
$$U\sim\int\hbar\omega\, g(\omega)\, n_{BE}(\omega T)\,d\omega \longrightarrow \int d\omega\ \text{DOS}$$ How many states have for each ω

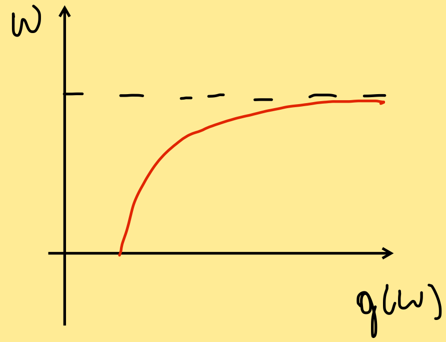
$$g(\omega)\to v\left(\frac{d\omega}{dk}\right)^{-1}$$

$$\omega(k)=2\left(\frac{J}{m}\right)^{1/2}\sin\left(\frac{ka}{2}\right) \qquad k=\frac{2\pi}{a}\frac{m}{N} \qquad \rho(k)=\frac{N}{\frac{2\pi}{a}}=\frac{Na}{2\pi}$$

$$\begin{cases} dn=\rho(k)\,dk \\ dn=\frac{1}{2}g(\omega)\,d\omega\end{cases} \rightarrow \frac{Na}{2\pi}dk=\frac{1}{2}g(\omega)d\omega$$

$$g(\omega)=\frac{Na}{\pi}\frac{dk}{d\omega}=\frac{Na}{\pi}\left(\frac{d\omega}{dk}\right)^{-1} \rightarrow \boxed{g(\omega)=\frac{1}{\pi a}\left(\frac{m}{J}\right)^{1/2}\frac{1}{\cos\left(\frac{ka}{2}\right)}}$$





February 27, 2020

SUMMARY

· QUASI-PARTICLE = PHONONS (BOSONS)
(QUASI-MOMENTUM $\underline{k}$)

· DP → Einstein → Normal modes → acustic phonons →
→ Debye Interpolation scheme

CM	QM	CM	$\omega_n(\underline{k})$	$\omega(\underline{k}) = v_s(\underline{k})$	$\int_0^{\omega_D} g(\omega)d\omega = 3N$
SM	SM $\begin{cases} FD \\ BE \end{cases}$		Periodicity		
			PBC		
			(WS/BZ, RL)		
			DOS: $g(\omega)$		

C_v → the only vibrations that I can have at low T are the acustic one

$$U_\circ = \int \hbar\omega\, g(\omega)\, n_{BE}(\omega,T)\,d\omega + U_0 \qquad g(\omega) \equiv DOS$$

$$\rightarrow k = \frac{2\pi}{a}\frac{m}{N} \qquad g(k) = \left(\frac{\frac{2\pi}{a}}{N}\right)^{-1} = \frac{Na}{2\pi}$$

$$\rightarrow \frac{Na}{2\pi}d\underline{k} = \frac{1}{2}g(\omega)d\omega \qquad g(\omega) = \frac{Na}{\pi}\left(\frac{d\omega}{d\underline{k}}\right)^{-1} = \frac{2L}{\pi a}\left(\frac{4J}{m} - v^2\right)^{1/2}$$

We have to develop the theory for $k \to 0$ = we want to see if when $T \to 0$ the $C_v \to 0$ in a qube way = in order to not loose everything, I have to introduce Debye model.

DOS

We want to generalize the DOS

$$\sum_{n\underline{k}} f_m(\underline{k}) \quad \frac{V}{(2\pi)^3}\sum_m \int d\underline{k}\, f(\underline{k}) \longrightarrow \int g(\omega)\,d\omega\, f(\omega)$$

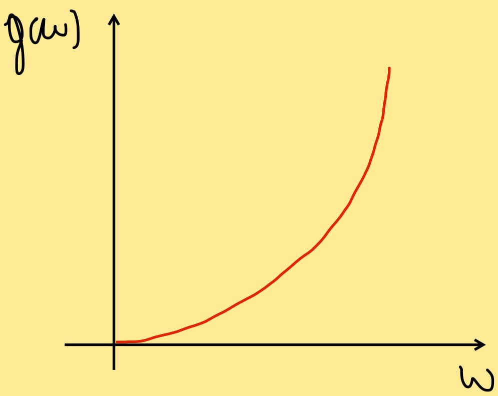
Mathematically = use the property of Dirac delta –

$$\int_{BZ} \delta(\omega'-\omega(\underline{k}))\, g(\underline{k})\, d\underline{k} \doteq g(\omega') \qquad \delta(\omega'-\omega(\underline{k})) = \begin{cases} \infty & \omega'=\omega(\underline{k}) \\ 0 & \omega'\neq\omega(\underline{k}) \end{cases}$$

$$\rho(\underline{k}) = \frac{V}{(2\pi)^3} \qquad g(\omega') = \int_{BZ} \delta(\omega'-\omega(\underline{k}))\,\rho(\underline{k})\,d\underline{k} \qquad \underline{v}_s|\underline{k}| = \omega = v_s\sqrt{k_1^2+k_2^2+k_3^2}$$

$$k^2 = \frac{\omega^2}{v_s^2} \qquad 2k\,dk = \frac{2\omega\,d\omega}{v_s^2} \longrightarrow dk = \frac{d\omega}{v_s}$$

$$dn = g(\omega)d\omega = \frac{V}{(2\pi)^3}4\pi k^2 dk = \frac{V}{(2\pi)^3}4\pi\frac{\omega^2}{v_s^3}d\omega = \frac{V}{2\pi^2}\frac{\omega^2}{v_s^3}d\omega$$



$$\boxed{g(\omega) = \frac{V}{2\pi^2}\frac{\omega^2}{v_s^3}}$$

Now we want to compute the C_V

$$x = \frac{\hbar\omega}{k_BT} \qquad dx = \frac{\hbar}{k_BT}d\omega$$

$$\hbar^3\omega = \frac{1}{\hbar^2}(k_BT)^3 x^3$$

$$U = U_0 + \frac{V}{2\pi^2}\frac{1}{v_s^3}\int_0^\infty \hbar\omega^3 \frac{1}{e^{\frac{\hbar\omega}{k_BT}}-1}\,d\omega$$

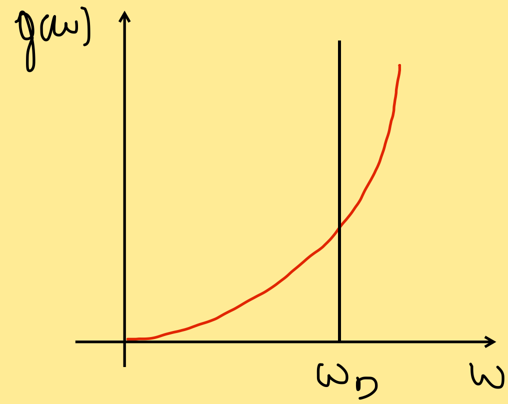
$$= U_0 + \frac{V}{2\pi^2}\frac{1}{v_s^3}\frac{(k_BT)^4}{\hbar^3}\underbrace{\int_0^\infty \frac{x^3}{e^x-1}\,dx}_{\frac{\pi^4}{15}}$$

$$U = U_0 + \frac{V}{2\pi^2}\frac{1}{v_s^3}\frac{(k_B T)^4}{\hbar^3}\frac{\pi^4}{15}$$

$$\left(\frac{\partial U}{\partial T}\right)_V = C_V \sim T^3$$ → fixed problem at lower T
→ now problem at high T

NB. I have to interpolate between this model and Einstein = this is the contribution of Debye -

ω_D → cutoff frequency when you have enough energy



ω_D → I know how many vibrations I have in the system = 3N

$$U = U_0 + \frac{V}{2\pi^2}\frac{1}{v_s^3}\int_0^{\infty \to \omega_D} \hbar\omega^3 \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}\, d\omega$$

$$3 \cdot \frac{1}{v_s^3} \longrightarrow \frac{2}{v_T^3} + \frac{1}{v_L^3} \qquad g(\omega) = \frac{V}{2\pi^2}\left(\frac{2}{v_T^3} + \frac{1}{v_L^3}\right)\omega^2$$

$$\int_0^{\omega_D} \omega^2 d\omega = \left[\frac{V}{2\pi^2}\left(\frac{2}{v_T^3} + \frac{1}{v_L^3}\right)\right] 3N = \frac{\omega_D^3}{3} \longrightarrow \omega_D = \left(9N\left[\frac{V}{2\pi^2}\left(\frac{2}{v_T^3} + \frac{1}{v_L^3}\right)\right]\right)^{1/3}$$

$$g(\omega) = \frac{9N}{\omega_D^3}\omega^2$$

$$U = U_0 + \frac{9N}{\omega_D^3}\int_0^{\omega_D} \frac{\hbar\omega^3}{e^{\frac{\hbar\omega}{k_B T}} - 1}\, d\omega$$

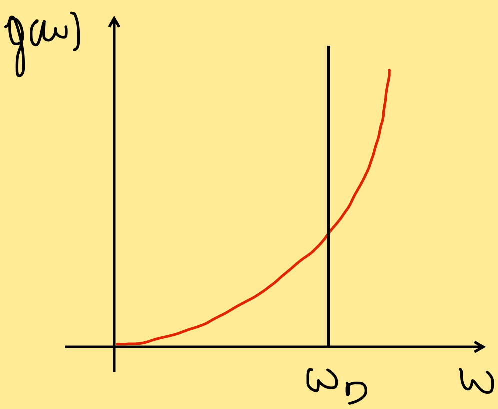
$$\frac{\Theta_D}{T} = \frac{\hbar\omega_D}{k_B T} \longrightarrow \Theta_D = \frac{\hbar\omega_D}{T}$$ ≡ DEBYE TEMPERATURE

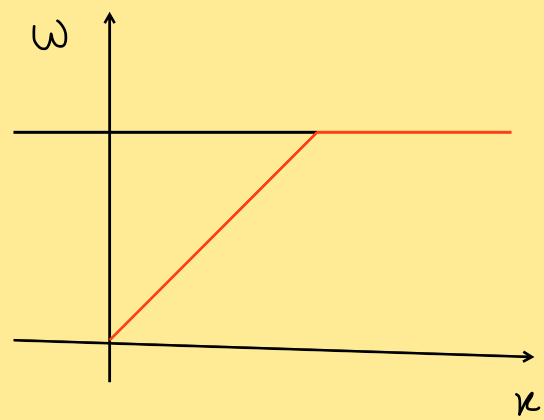
$$\frac{\partial U}{\partial T} = \frac{9N}{\omega_D^3} \int_0^{\frac{\theta_D}{T}} \frac{\hbar\omega\, e^{\frac{\hbar\omega}{k_BT}} \frac{\hbar\omega}{k_BT}\frac{1}{T^2}}{\left(e^{\frac{\hbar\omega}{k_BT}}-1\right)^2}\, d\omega$$

$$= \frac{9N}{\omega_D^3}\frac{k_B^3T^2}{\hbar^2}\frac{k_BT}{\hbar}\int_0^{\frac{\theta_D}{T}} \frac{x^4 e^x}{(e^x-1)^2}\,dx = C_V$$

$$\int_0^{\frac{\theta_D}{T}} \frac{x^4 e^x}{(e^x-1)^2}\,dx \underset{\substack{T\to\infty \\ x\to 0}}{\sim} \int_0^{\frac{\theta_D}{T}} \frac{x^4(1+x)}{x^2}\,dx \sim \int_0^{\frac{\theta_D}{T}} x^2\,dx \sim \left(\frac{\theta_D}{T}\right)^3 \frac{1}{3}$$

$$C_V \underset{T\to\infty}{\sim} \left(\frac{\theta_D}{T}\right)^3 \frac{1}{3}\frac{9N}{\omega_D^3}\frac{k_B^3T^2}{\hbar^2}\frac{k_BT}{\hbar} \sim \text{const} = 3R$$





NB. Now we close the story = we are able to catch the two limits ($T\to 0$, $T\to\infty$), but not in the middle.
We studied only harmonic oscillations, not anharmonic = a solid will never melt only with harmonic oscillations.