Statistical Mechanics Exam

Marks distribution: 10 + 9+ 9 + 12

Instructions: Some of the problems could involve tedious algebra. Please ensure that you take utmost care in carrying out the algebra. Getting the correct final result is important. Also for your own benefit, in some cases you may want to check the consistency of the final answer by analyzing the problem in more than one way.

1. Consider a cylinder of radius a, kept vertically, containing N molecules of a monatomic gas. m is the mass of each atom, g is the acceleration due to gravity, and T is the temperature of the gas. The upper end of the cylinder is closed with a piston of weight w. In the equilibrium situation the piston is at a height h above the lower end of the cylinder. The height h is large so that the effect of the gravitational pull on the atoms cannot be ignored. The temperature is sufficiently large so that we can use classical statistical mechanics.

   a) Beginning with the definition of the canonical partition function, find an expression for the free energy F of the system as a function of a, N, m, g, h.

   b) Using the result of part a), and the equation $dF = -dW - SdT$ where dW is the work done by the system, and S is the entropy of the system, calculate the net force exerted by the gas on the piston, i.e. calculate the weight w in terms of a, N, m, g, h.

   c) Calculate the equilibrium density of atoms at a height x above the bottom of the cylinder.

2. Consider a one dimensional ideal monatomic Bose gas containing N atoms each of mass m, confined in a periodic box of length L. Find the temperature T at which the fraction f of the total number of particles will be in the ground state, assuming that $f << 1$ but $fN >> 1$. T should be determined in terms of N, L, f and m. (Note that you need to do this calculation for large but finite L and N.)

3. Consider a two dimensional classical gas containing N atoms each of mass m, which interact with each other via a potential $v(\vec{r}_i, \vec{r}_j)$ of the form

$$\begin{aligned} v(\vec{r}_i, \vec{r}_j) &= v_0 \quad \text{for} \quad |\vec{r}_i - \vec{r}_j| \le a \\ &= v_1 \quad \text{for} \quad a < |\vec{r}_i - \vec{r}_j| \le b \\ &= 0 \quad \text{for} \quad |\vec{r}_i - \vec{r}_j| > b\,. \end{aligned}$$

The gas is confined to a box of area A. Calculate the correction to the equation of state of the system, i.e. to the ratio $PA/(NkT)$, to order (N/A). Note that for a two dimensional gas, P is the force per unit length exerted by the gas on the one dimensional boundary of the two dimensional box.

4. Consider a one dimensional Ising model with $2N$ sites, with variable s_i at the i-th site taking values ± 1 and satisfying periodic boundary condition $s_{i+2N} \equiv s_i$. The energy associated with a given configuration is given by

$$E = -J \sum_{i=1}^{2N} s_i s_{i+1} - A \sum_{i=1}^{2N} s_i s_{i+2}\,.$$

Calculate the free energy per site of this model in the thermodynamic limit to first order in A.

Hint: You may find it useful to work with N new variables (s_{2i-1}, s_{2i}) with $1 \le i \le N$. The new variable takes four possible values.

13/2/06

Electron in a magnetic field B along z

$$E = \underbrace{\frac{eB\hbar}{mc}\left(j+\tfrac{1}{2}\right)}_{E_{xy} = E'} + \underbrace{\frac{p_z^2}{2m}}_{= E_z}$$

These are the Landau levels

For each j, there are ∞ no. of states.

$\rightarrow \infty$ degeneracy (infinite volume limit)

Q) If we put the system in a finite box what happens to the degeneracy?

Take a box of length L_3 in the z-direction & L_1, L_2 in x, y direction.

Suppose $N(j)$ is the number of states for energy level j.

(Implicitly assuming the volume is large)

final result will not depend on a cubic or cyl. box in the large V limit

No. of states between E' and $E' + dE'$

$$= N(j) \times \frac{dE'}{\frac{eB\hbar}{mc}}$$

$$= \frac{mc}{eB\hbar} N(j)\, dE'$$

H.O. wavefns fall off exponentially & most of them won't be affected in the large V limit even if we confine them in a box

The ones with very large excitations will be affected in a box - but not in $V \to \infty$ limit

So there will still be degeneracy on confinement within a box

For $B = 0$, we have free particles

No. of states between E' & $E' + dE'$

in the range $dp_x\, dp_y$

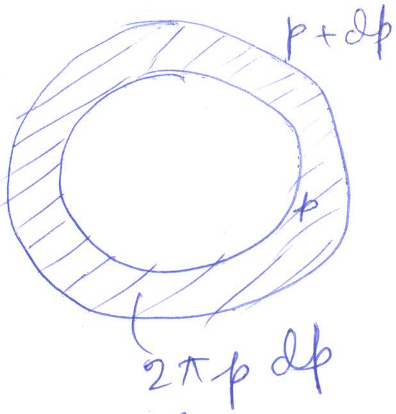
$$= \frac{L_1}{2\pi\hbar} dp_x \cdot \frac{L_2}{2\pi\hbar} dp_y = \frac{L_1 L_2}{h^2} dp_x\, dp_y$$

$p' = \sqrt{p_x^2 + p_y^2}$

$$\boxed{p_x = \frac{2\pi\hbar}{L_1} n_x}$$

# of states betn p' & $p'+dp'$

$$= \frac{L_1 L_2}{h^2} 2\pi p'\,dp'$$



# of states of energy between E' and $E'+dE'$ ← $\frac{L_1 L_2}{h^2} 2\pi m\,dE'$

$E' = p'^2/2m$

$dE' = \frac{p'dp'}{m}$

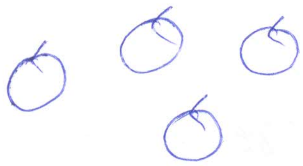
you should get back this ans. on putting $B=0$ in $\frac{mc}{eB\hbar} N(j)\,dE'$

$$\frac{\cancel{m}c}{eB\hbar} N(j) = \frac{L_1 L_2}{h^2} 2\pi \cancel{m}$$

$$N(j) = L_1 L_2 \frac{eB}{ch} \quad \text{for small } B$$

Correct result for finite B (area A must be large)

(also)



[$N(j)$ → degeneracy of a Landau level. The proportionality to L_1L_2 reflects the fact that the projection of the e^- orbit onto the xy-plane can be centred anywhere in the plane without changing the energy. Thus when the ext. field is turned on, the energy spectrum associated with the motion in the xy-plane changes from a continuous spectrum to a discrete one, & the level spacing & degeneracy ↑ with the ext. field.]

otherwise the degeneracy won't be there

HUANG p.255 ⇒

classically, the orbits can be centred around various places - provided you are not close to the wall — when we quantise it, the no. of states $\propto$ area

→ count the no. of non-overlapping orbits (though classically you have a continuum — an infinite # of orbits

Smaller B ⇒ larger orbit

Balancing Lorentz force by centrifugal force

Classically, particle doesn't know about the box provided it doesn't intersect the box — Q. mechanically it's not true — there is a shift in the energy level $\propto \frac{1}{\text{area of box}}$

Effect of electron spin

$\longrightarrow$ introduce a new quantum no. s which takes value ± 1.

There is a new contribution to E which is $-\mu_0 B s$

μ_0: magnetic moment of the electron

$$\mathcal{H} = \frac{eB\hbar}{mc}\left(j+\tfrac{1}{2}\right) + \frac{p_z^2}{2m} - \mu_0 B s$$

Degeneracy $N(j) = L_1 L_2 \frac{eB}{ch}$

$$\sum_{\substack{\text{single particle}\\ \text{states}}} \longrightarrow \int \frac{L_3}{h}\, dp_z \sum_{j=0}^{\infty} {}^{N(j)} \sum_{s=\pm 1}$$

$$\frac{L_3}{h}\left(\frac{L_1 L_2}{ch}\, eB\right) = \frac{eBV}{ch^2}$$

it will affect all the energy levels in the same way — lift either up or down $\rightarrow$ so same degeneracy

Recall for non-interacting particles

~~$\ln \mathcal{Q} = \sum_n \ln(1+ z$~~

$$\ln \mathcal{Q} = \sum_n \ln\left(1 + z e^{-\beta e_n}\right)$$

e_n: energy of $|n\rangle$

$\sum_n$: over single particle states $|n\rangle$

$$\bar{N} = z \frac{\partial}{\partial z} \ln \mathcal{Q} = \sum_n \frac{z e^{-\beta e_n}}{1 + z e^{-\beta e_n}}$$

$$N = \frac{eBV}{h^2 c} \int dp_z \sum_{j=0}^{\infty} \sum_{s=\pm 1} \underbrace{\frac{z e^{-\beta\left\{\frac{p_z^2}{2m} - \mu_0 B s + e|B|\hbar/mc\,(j+\frac{1}{2})\right\}}}{1 + z e^{-\beta\left\{\frac{p_z^2}{2m} - \mu_0 B s + \frac{e|B|\hbar}{mc}(j+\frac{1}{2})\right\}}}}$$

(1) monotone increasing fn. of z
(2) $\to 0$ as $z \to 0$
(3) $\to \infty$ as $z \to \infty$

$\overset{\text{this}}{\underset{\text{means}}{\Longrightarrow}}$ unique soln. for z for every N.

Consider low density approximation

N/V small $\Longrightarrow$ z small

The integral is very complicated to solve – so we use various approxmns.

$$\frac{N}{V} \simeq \frac{eBz}{h^2c}\int dp_z \sum_{j=0}^{\infty}\sum_{s=\pm1} e^{-\beta\left(\frac{p_z^2}{2m} - \mu_0 Bs + \frac{eB\hbar}{mc}(j+1/2)\right)}$$

Implicitly taken $B > 0$

We should have written $|B|$ $\because$ B can be +ve or −ve – bcos $\omega^2 = \frac{e^2B^2}{\hbar^2c^2}$

$$\ln \mathcal{Q} = \sum_n \ln\left(1 + z e^{-\beta e_n}\right) \simeq z\sum_n e^{-\beta e_n}$$

$$= z\,\frac{eBV}{h^2c}\int dp_z \sum_{j=0}^{\infty}\sum_{s=\pm1} e^{-\beta\left(\frac{p_z^2}{2m} - \mu_0 BS + \frac{eB\hbar}{mc} \times (j+1/2)\right)}$$

$$= V\,\frac{N}{V}$$

$$\ln \mathcal{Q} = z\,\frac{eBV}{h^2c}\left(\int dp_z\, e^{-\beta p_z^2/(2m)}\right)\left(\sum_{j=0}^{\infty} e^{-\beta\frac{eB\hbar}{mc}(j+1/2)}\right)\left(\sum_{s=\pm1} e^{\beta\mu_0 Bs}\right)$$

$$= z\,\frac{eBV}{h}\sqrt{\frac{2\pi m}{\beta}}\;\frac{e^{-\beta\frac{eB\hbar}{2mc}}}{1 - e^{-\beta\frac{eB\hbar}{mc}}} \times \left(e^{\beta\mu_0 B} + e^{-\beta\mu_0 B}\right)$$

$$\Rightarrow \ln \mathcal{Q} = z \frac{eBV}{h^2 c} \sqrt{\frac{2\pi m}{\beta}} \frac{1}{2 \sinh\left(\frac{\beta e B \hbar}{2mc}\right)} \times 2 \cosh(\beta \mu_0 B)$$

$$= z \frac{eBV}{h^2 c} \sqrt{\frac{2m\pi}{\beta}} \frac{\cosh(\beta \mu_0 B)}{\sinh\left(\frac{\beta e B \hbar}{2mc}\right)}$$

$\bar{N} =$ "

$\ln \mathcal{Q} = \bar{N}$ true only in the low z approximations

Magnetization of a given particle

$= \left(-\frac{\partial e^{(i)}}{\partial B}\right)$ single particle energy

$$\mathcal{Q} = \sum_N \sum_{\substack{\text{all} \\ N \text{ particle} \\ \text{states}}} e^{-\beta \sum_{i=1}^{N} e_i} z^N$$

sum over all particles in a given ensemble

Total magnetization

$$= \left(-\frac{\partial\left(\sum e_i(B)\right)}{\partial B}\right)$$

$$\left(\frac{\partial \mathcal{Q}}{\partial B}\right)_{z,\beta} = + \sum_N \sum_{\substack{\text{all } N \\ \text{particle} \\ \text{states}}} \left(-\beta \sum_i \frac{\partial e_i}{\partial B}\right) z^N e^{-\beta \sum_i e_i(B)}$$

$$= \frac{1}{\mathcal{Q}} \left(\frac{\partial \mathcal{Q}}{\partial B}\right)_{z,\beta} = \beta \mathcal{M}$$ → total magnetization

$$\ni \left(\frac{\partial \ln \mathcal{Q}}{\partial B}\right)_{z,\beta} = \beta \mu$$

Magnetization / unit volume is

$$M = \frac{\mu}{V} = \frac{1}{V\beta}\left(\frac{\partial \ln \mathcal{Q}}{\partial B}\right)_{z,\beta}$$

$\rightarrow$ fn. of N, β, V & B

This can be thought of a a fn. of N, V & β bcos z can be eliminated in terms of N & V

$$\text{Susceptibility} = \left(\frac{\partial M}{\partial B}\right)_{V,N,\beta}$$

We'll calculate susceptibility at $B=0$.

But M must be calculated keeping z fixed otherwise you will get a triviality

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Keep up to quadratic terms in B (in $\ln \mathcal{Q}$ — because we need $\frac{\partial^2 \ln \mathcal{Q}}{\partial B^2}$ & other terms won't contribute for $B=0$)

$$\ln \mathcal{Q} = z \cdot \frac{\cancel{eB}V}{h^2 \cancel{c}}\sqrt{\frac{2m\pi}{\beta}} \; \frac{1 + \frac{1}{2}\beta^2\mu_0^2 B^2 + O(B^4)}{\frac{\beta \cancel{e B}\hbar}{2m\cancel{c}}\left\{1 + \frac{1}{3!}\left(\frac{\beta e B \hbar}{2mc}\right)^2 + O(B^4)\right\}}$$

$$= z\frac{V}{h^2}\,\frac{2m}{\beta\hbar}\sqrt{\frac{2m\pi}{\beta}}\left\{1 + \frac{1}{2}\beta^2\mu_0^2B^2 + O(B^4)\right\}$$

$$\times \left\{1 - \frac{1}{6}\left(\frac{\beta e B\hbar}{2mc}\right)^2 + O(B^4)\right\}$$

$$= 2z\frac{V}{h^3}\left(\frac{2m\pi}{\beta}\right)^{3/2}\left\{1 + \frac{1}{2}\beta^2\mu_0^2B^2 - \frac{1}{6}\left(\frac{\beta e B \hbar}{2mc}\right)^2 + O(B^4)\right\}$$

$$\bar{N} = 2z \frac{V}{h^3}\left(\frac{2m\pi}{\beta}\right)^{3/2}\left\{1 + \frac{1}{2}\beta^2\mu_0^2 B^2 - \frac{1}{6}\left(\frac{\beta e B \hbar}{2mc}\right)^2 + O(B^4)\right\}$$

Magnetization per ~~unit~~ unit volume

$$M = \frac{1}{V\beta}\frac{\partial \ln Q}{\partial B}$$

$$= \frac{1}{V\beta}\underbrace{2z\frac{V}{h^3}\left(\frac{2m\pi}{\beta}\right)^{3/2}}_{\bar{N}\{1+O(\beta^2)\}} 2B\left\{\frac{1}{2}\beta^2\mu_0^2 - \frac{1}{6}\left(\frac{\beta e \hbar}{2mc}\right)^2 + O(B^2)\right\}$$

The alignment of e^- spin with the ext. field gives rise to paramag. whereas the orbital motions of the e^-'s give rise to diamag.

$$= \frac{1}{V\beta}\bar{N}\, 2B\left\{\frac{1}{2}\beta^2\mu_0^2 - \frac{1}{6}\beta^2\left(\frac{e\hbar}{2mc}\right)^2\right\}$$

$$M = \frac{\bar{N}}{V}\beta B\left\{\mu_0^2 - \frac{1}{3}\left(\frac{e\hbar}{2mc}\right)^2\right\}$$

$$\chi = \left(\frac{\partial M}{\partial B}\right)_{\beta,\bar{N},V}$$

$$= \frac{\bar{N}}{V}\frac{1}{KT}\left\{\mu_0^2 - \frac{1}{3}\left(\frac{e\hbar}{2mc}\right)^2\right\}$$

2 terms of opposite sign

Paramagnetism (comes from explicit magnetic moment of the ~~system~~ particles)

Diamagnetism (comes from orbital motion of the charged particle in a magnetic field)

Due to electric charge

Classically there is no diamagnetism — clear from the '$\hbar$' factor in the expression for χ in $\hbar \to 0$ limit so it doesn't survive classically

15/2/06

Lattice vibration

One dimensional lattice with N atoms.

N = odd (for simplicity)

Periodic boundary conditions:-

$(N+1)$th atom = 1^{st} atom

o o o o o o o o o o o o
1 2 3 4

We assume a 1-D theory so that atoms can vib. only along ...

y_n: displacement of the nth atom from its mean position

$$\text{Kinetic energy} = \frac{m}{2}\sum_{n=1}^{N} \dot{y}_n^2$$

m = mass of each atom

Potential energy (nearest neighbour interaction)

$$V = \frac{K}{2}\sum_{n=1}^{N}\left(y_n - y_{n+1}\right)^2$$

P.E. can depend only on the rel. disp. of nearest neighbours assumption – another assumption is V is quadratic in rel. disp.

For small vib., quadratic term is the dominant term

We consider only nearest neighbour int.

$\frac{1}{2}K\left(y_N - y_{N+1}\right)^2$ is the term for $n=N$

[Doesn't affect bcos it is one unphysical term among n-terms in thermodyn. limit. But adding this term simplifies life – otherwise why should we include a term containing int. betw. Nth & 1^{st} atom? For it is unphysical]

nearest ~~neighbour~~ neighbour int.

$$\phi_s = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{2\pi i n s/N} y_n \qquad s = 0, 1, \ldots, (N-1)$$

This is a discrete fourier transfm.

$$\Rightarrow y_n = \frac{1}{\sqrt{N}}\sum_{s=0}^{N-1} e^{-2\pi i n s/N}\phi_s$$

Φ_s is complex

$$\Phi_s^* = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{-2\pi i n s/N} y_n = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{2\pi i N/N} e^{-2\pi i n s/N} y_n = \Phi_{N-s} y_n$$

$$\Phi_s^* = \Phi_{N-s} \qquad \Phi_N = \Phi_0$$

$\Rightarrow \Phi_0$ is real

Φ_s & Φ_{N-s} for $s \neq 0$ are complex conjugates.

Can take Φ_0 and Φ_s for $s = 1, 2, \ldots, \frac{N-1}{2}$ as independent variables.

Ex. Check that the kinetic term

$$= m \sum_{s=1}^{\frac{N-1}{2}} \dot{\Phi}_s^* \dot{\Phi}_s + \frac{m}{2} \dot{\Phi}_0^2$$

$$\text{Potential Energy} = K \sum_{s=1}^{\frac{N-1}{2}} \left| e^{\frac{2\pi i s}{N}} - 1 \right|^2 \Phi_s^* \Phi_s$$

In the thermodyn. limit N even or odd makes no diff.

$$\Phi_s = \frac{1}{\sqrt{2}}\left(X_s + i \Psi_s\right)$$

$$L = \sum_{s=1}^{(N-1)/2} \left\{ \frac{1}{2} m \dot{X}_s^2 - \frac{K}{2}\left(2 - 2\cos\frac{2\pi s}{N}\right) X_s^2 \right\} + \sum_{s=1}^{(N-1)/2} \left\{ \frac{1}{2} m \dot{\Psi}_s^2 - \frac{K}{2}\left(2 - 2\cos\frac{2\pi s}{N}\right)\Psi_s^2 \right\} + \frac{1}{2} m \dot{\Phi}_0^2$$

Define $\xi_r = X_r$ for $1 \leq r \leq \frac{N-1}{2}$

$\xi_{-r} = \Psi_r$ for $1 \leq r \leq \frac{N-1}{2}$

$$L = \sum_{r=-\frac{N-1}{2}}^{\frac{N-1}{2}} \left\{ \frac{1}{2} m \dot{\xi}_r^2 - \underbrace{\frac{K}{2}\left(2 - 2\cos\frac{2\pi r}{N}\right)}_{\frac{m}{2}\omega_r^2 \;\; 4\sin^2\left(\frac{\pi r}{N}\right)} \xi_r^2 \right\}$$

$$\omega_r^2 = \frac{K}{m}$$

$\therefore \quad \omega = 2 \left| \sin \frac{\pi r}{N} \right| \sqrt{K/m}$

Conjugate momentum:

$$\Pi_r = \frac{\partial L}{\partial \dot{\xi}_r} = m \dot{\xi}_r$$

$$\mathcal{H} = \sum_r \Pi_r \dot{\xi}_r - L$$

$$= \sum_{r=-\frac{N-1}{2}}^{\frac{N-1}{2}} \left\{ \frac{\Pi_r^2}{2m} + \frac{1}{2} m \omega_r^2 \xi_r^2 \right\}$$

Quantization $\Rightarrow$ Energy eigenstates are labelled by

$$\left\{ n_{-\frac{N-1}{2}}, n_{-\frac{N-1}{2}+1}, \ldots, n_{\frac{N-1}{2}} \right\}$$

a Collection of H.O. Quantise them

$$E = \sum_{r=-\frac{N-1}{2}}^{\frac{N-1}{2}} \hbar \left(n_r + 1/2 \right) \omega_r$$

$$= \hbar \sum_r n_r \omega_r + \underbrace{\frac{1}{2} \hbar \sum_r \omega_r}_{\text{constant}}$$

This const. term plays no role in thermodynamics — adding a const. term to energy plays no role in thermodyn.

$$\Rightarrow E = \sum_r \hbar n_r \omega_r + E_0$$

$n_r = 0, 1, 2, \ldots$

Reinterprete this as a gas of non-interacting bosons with single particle energy levels given by $\hbar\omega_1, \hbar\omega_2, \hbar\omega_3, \ldots$

$\uparrow$ n_1 particles, $\uparrow$ n_2, $\uparrow$ n_3

this system has the same quantum energy states as the lattice system

Imagine this as Bosons in some quantum potential whose energy levels are given by

Total energy $= \hbar \sum_r n_r \omega_r$

these particles are called phonons

these are fictitious particles — not real particles

Partition fn. entirely characterised by energy levels

$$\ln \mathcal{Q} = -\sum_{r} \ln\left(1 - z e^{-\beta\hbar\omega_r}\right)$$

Quantum statistics same for both systems — reinterpretation

$\rightarrow$ grand canonical partition fn. of a gas of free particles

mapped the original problem of quantising lattice vib. to that of a multiparticle system of boson gas of non-int. particle

total no. of particles $= \sum n_r$

Now what do do with $z = e^{\beta\mu}$?

No. of phonons not fixed $\rightsquigarrow$ same situation as photons

no. of phonons not conserved — any small int. in the lattice is going to change it

$\Rightarrow$ recipe: set $\mu = 0$, $z = 1$.

So do set $\mu = 0$ as for the case of photons

$\rightarrow$ can calculate all thermodynamic quantities.

mode s

* Interpretation of the index s:-

$$y_n = \frac{1}{\sqrt{N}} \sum_{s=0}^{N-1} e^{-2\pi i n s/N} \phi_s$$

Consider a configuration:

$\phi_{s_0} \neq 0$

$\phi_s = 0$ for all $s \neq s_0$

$$y_n = \frac{\phi_{s_0}}{\sqrt{N}} e^{-2\pi i n s_0/N}$$

Equilibrium position of n^{th} atom is

$x_n = n\underbrace{a}_{\text{lattice spacing}}$

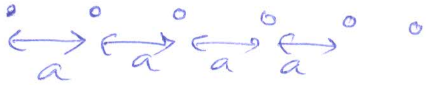
* $s = 0$ case corr. to a H.O. that will give free particle energy states bcos it involves only ϕ_0^2

factorise the $s = 0$ part

$$\Rightarrow y_n = \frac{\phi_{s_0}}{\sqrt{N}} e^{-2\pi i x_n s_0 / (Na)}$$

Na = L = (total length)

$$= \frac{\phi_{s_0}}{\sqrt{N}} e^{-2\pi i x_n s_0 / L}$$



$$y = \frac{\phi_{s_0}}{\sqrt{N}} e^{-2\pi i x_n s_0 / L}$$

$$= \frac{\phi_{s_0}}{\sqrt{N}} e^{-2\pi i x_n / \lambda}$$

$$\lambda = \frac{L}{s_0}$$ wavelength of the oscillatory wave

The particular mode of vibs labelled by ϕ_{s_0} has the interpretation of having an wavelength L/s_0

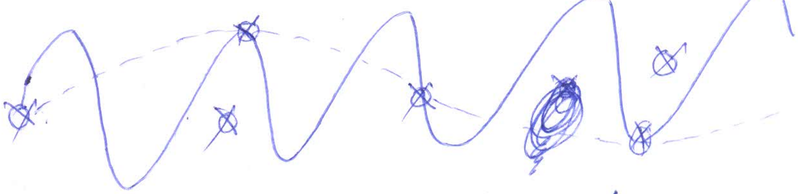
$$1 \le s_0 \le N$$

$$\boxed{\frac{L}{N} \le \lambda \le L}$$

$\frac{L}{N}$ = a

Taking the upper bound as N, rather N-1, is easier for analysis

Can't have a wavelength larger than the size of the box of the box
- we have periodic B.C.
- integer no. of things should fit into the lattice



$$\lambda = 4/5\, a$$

Particles at nodes don't get displaced

(Taking λ smaller than a is equiv. to taking a λ larger than a)

$$2a = 2\tfrac{1}{2}\lambda = \tfrac{5}{2}\lambda$$
$$\Rightarrow \lambda = \tfrac{4}{5}a$$

there are allowed values of λ less than a which don't satisfy quantisation condn.

Define

$$p_r = \frac{2\pi\hbar}{\lambda_r} = \frac{2\pi\hbar}{L} r = \frac{h}{L} r$$

$\rightarrow$ momentum associated with rth mode.

$$e_r = \hbar\omega_r = \hbar\, 2\sqrt{\frac{K}{m}}\left|\sin\frac{\pi r}{N}\right|$$

this mom. is diff. from the conjugate mom. defined earlier

$$\cancel{= \sqrt{K}} \quad \cancel{= 2\hbar\sqrt{K/m}\,\sin\left(\frac{\pi a\, p_r}{N}\right)}$$

for our purpose we'll treat p_r's as just only labels

$$\Rightarrow e_r = 2\hbar\sqrt{K/m}\,\sin\left(\frac{\pi L p_r}{N\hbar}\right)$$

$$= 2\hbar\sqrt{K/m}\left|\sin\left(\frac{\pi a\, p_r}{\hbar}\right)\right|$$

But the total physical mom. carried by the state is indeed

$$\sum n_r p_r$$

$$\underset{\text{for small } p_r}{\simeq} 2\hbar\sqrt{K/m}\,\frac{\pi a|p_r|}{\hbar}$$

$$= \sqrt{K/m}\; a\,|p_r|$$

You can think phonons are destroyed at the boundaries — or switch on a little cubic term which can change the phonon no.

The quadratic term doesn't change phonon no. as we have diagonalised this & got an e.state which won't change with time

this has no '$\hbar$' term & should have some classical interpretation

$$\lambda_r = \frac{L}{r}$$

$$\omega_r = 2\sqrt{K/m}\left|\sin\frac{\pi r}{N}\right|$$

$$\simeq 2\sqrt{\frac{K}{m}}\,\frac{\pi r}{N}$$

$$\text{Frequency } \nu_r = \frac{\omega_r}{2\pi} = \sqrt{K/m}\;\, r/N$$

$$\underbrace{\nu_r\lambda_r}_{c_s} = \sqrt{K/m}\;\frac{r}{N}\;\frac{L}{r} = \sqrt{K/m}\; a$$

$c_s \to$ velocity of sound wave

$$\therefore\; e_r = c_s|p_r| \quad (\text{for small } p_r)$$

similar to that of photon - only c replaced by c_s

When you take ħ large or small ~~when~~ then you are to specify what things you are keeping fixed

$$p_r = \frac{h}{L} r$$

$$\sum_r \Rightarrow \frac{L}{h} \int dp$$ in thermodynamic limit

→ same counting that we got for particles

particle nature of wave means ħ large ~~keep~~ keeping other attributes fixed & wave nature of wave for ħ→0

similarly, particle nature of particle - - -

$$-\frac{N-1}{2} < r \leq \frac{N-1}{2}$$

$$-\frac{N-1}{2} \frac{h}{L} \leq p \leq \frac{N-1}{2} \frac{h}{L}$$

$$|p| \leq \frac{h}{2} \frac{N}{L} \rightarrow \boxed{p_{max}}$$ in thermodynamic limit

this is a finite no. — this is the kind of constraint we didn't have for photons

Also $\epsilon_r = c_s |p_r|$ only for small p_r

No. of ~~modes~~ allowed values of p (no. of single particle states) $\boxed{\text{modes}}$

$$= \frac{L}{h} \int_{-p_{max}}^{p_{max}} dp = \frac{L}{h} \cdot 2p_{max}$$

$$= \frac{L}{h} \cdot \frac{Nh}{L} = N$$

Pathria (176) → for wavelengths shorter than λ_{min}, it would be meaningless to speak of a wave of atomic displacements.

Changing variables from y_n to Φ_s — make sure no. of degrees of freedom is the same ($=N$)

Though here we are dealing in the language of particles & single particle states

No. of states for particles ~~(N no)~~ is indeed ∞ — but here we have mapped the prob. into single particle states

16/2/06

3 dim - lattice

A lattice point (n_1, n_2, n_3) — integers

Displacements:

$$y^1(n_1,n_2,n_3),\ y^2(n_1,n_2,n_3),\ y^3(n_1,n_2,n_3)$$

$$L = \sum_{n_1,n_2,n_3} \frac{1}{2} m \sum_{i=1}^{3} \left(\dot{y}^i(n_1,n_2,n_3)\right)^2 - \sum_{n_1,n_2,n_3} \underbrace{\sum_{s_1,s_2,s_3}}_{\text{nearest nbrs.}} \sum_{i,j=1}^{3} \left\{ y^i(n_1+s_1, n_2+s_2, n_3+s_3) - y^i(n_1,n_2,n_3)\right\} \left\{ y^j(n_1+s_1,n_2+s_2,n_3+s_3) - y^j(n_1,n_2,n_3)\right\} K_{ij}$$

Eqm. is stable $\downarrow$ so K_{ij} is a +ve definite matrix

You can choose K_{ij} to be sym. bcos antisym. part will give vanishing contribution

$$y^i(n_1,n_2,n_3) = \frac{1}{\sqrt{N}} \sum_{\lambda_1,\lambda_2,\lambda_3} e^{(2\pi i n_1\lambda_1/N_1 + 2\pi i n_2\lambda_2/N_2 + 2\pi i n_3\lambda_3/N_3)} \times \phi^i(\lambda_1,\lambda_2,\lambda_3)$$

$N = N_1 N_2 N_3$

(n_1,n_2,n_3), (n_1+N_1, n_2, n_3), (n_1, n_2+N_2, n_3), (n_1,n_2,n_3+N_3) are same points.

Substitute & analyze in the same way.

Treat $\phi^i(\lambda_1,\lambda_2,\lambda_3)$ as new coordinates.

$$H = \sum_{\lambda_1,\lambda_2,\lambda_3} H_{\lambda_1,\lambda_2,\lambda_3}\left(\vec{\phi}_{\lambda_1,\lambda_2,\lambda_3}, \dot{\vec{\phi}}_{\lambda_1,\lambda_2,\lambda_3}\right)$$

$\downarrow$

Kinetic term + Potential term quadratic in $\vec{\phi}_{\lambda_1,\lambda_2,\lambda_3}$ $\Downarrow$ (can be made into) sum of 3 independent harmonic oscillators

Prop. of this fourier exp. $\downarrow$ decouple terms containing $\lambda_1, \lambda_2, \lambda_3$

(with) Angular frequencies

$\omega^1(\lambda_1,\lambda_2,\lambda_3)$, $\omega^2(\lambda_1,\lambda_2,\lambda_3)$, $\omega^3(\lambda_1,\lambda_2,\lambda_3)$

General state is labelled by

$n^i_{\lambda_1,\lambda_2,\lambda_3}$

~~occupancy no. of~~ Excitation level of the harmonic oscillator with angular frequency $\omega^i_{\lambda_1,\lambda_2,\lambda_3}$

$$E = \sum_{i=1}^{3} \sum_{\lambda_1,\lambda_2,\lambda_3} \underbrace{n^i_{\lambda_1,\lambda_2,\lambda_3}}_{\text{integers}} \hbar\, \omega^i_{\lambda_1,\lambda_2,\lambda_3}$$

index i indicates that a single atom has 3 vibrational modes

$p_1 = 2\pi\hbar \frac{\lambda_1}{L_1}$, $p_2 = 2\pi\hbar\, \lambda_2/L_2$, $p_3 = 2\pi\hbar\, \lambda_3/L_3$

$\vec{p} = (p_1, p_2, p_3)$ will be interpreted as the momentum of the single particle state.

$e^i(\vec{p})$

$\Downarrow$ (can be interpreted as)

Energy of a single particle state of momentum $\vec{p}$.

For every $\vec{p}$ we have 3 different types of states $i = 1, 2, 3$

$\Rightarrow$ 3 different polarization states of the phonon.

In the generic case, we'll get diff. relations bet. $e^i(\vec{p})$ & p^i depending on i

$$\bar{E} = -\frac{\partial}{\partial \beta} \ln Q = \frac{3N}{\beta} = 3NkT$$

Just like the classical system of 3N H.O.'s

No surprise bcos at high temp. Bose stat. should coincide with normal classical statistics

vel. of sound diff. in diff. dirns — or it depends on diff. polarisation

$\sqrt{\sin^2 \frac{k\pi}{N}}$

Remove the region R & can int. over all space bcos any $\vec{p}$ is restricted to small values

Low temperature

β is large

contribution comes for small $e_i(\vec{p}) \xRightarrow{\text{means}}$ small $\vec{p}$

$$e_i = \sqrt{c_{ijk}\, p_j\, p_k}$$

$\Downarrow$ constants which could depend on the lattice

$$\ln Q \simeq -\frac{V}{h^3} \int_R d^3p \sum_{i=1}^{3} \ln\left(1 - e^{-\beta\sqrt{c_{ijk} p_j p_k}}\right)$$

$$\simeq -\frac{V}{h^3} \int d^3p \sum_{i=1} \ln (\;\text{''}\;)$$

$$p_i = \frac{u_i}{\beta}$$

$$\ln Q = -\frac{V}{h^3}\frac{1}{\beta^3} \underbrace{\int d^3u \sum_{i=1}^{3} \ln\left(1 - e^{-\sqrt{c_{ijk} u_j u_k}}\right)}_{-C}$$

$\hookrightarrow$ related to the lattice

$$= +C\frac{V}{h^3}\frac{1}{\beta^3}$$

$$\bar{E} = -\frac{\partial}{\partial \beta} \ln Q = \frac{3CV}{h^3}\frac{1}{\beta^4} = \frac{3CV}{h^3} k^4 T^4$$

c_v = specific heat / volume

$$= \frac{1}{V}\left(\partial E / \partial T\right)_V = \frac{12C}{h^3} k^4 T^3$$

At low temperature,

specific heat of a lattice $\simeq T^3 \times$ constant

Specific heat of free electrons $\simeq T \times$ constant

Total specific heat : $AT^3 + BT$

at low temperature

At sufficiently low temp., sp. heat decreases linearly with T as BT is the dominant term then

N $2\pi i n s/N$

Proof $\phi_s = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{2\pi i n s/N} y_n$

$$\sum_{s=0}^{N-1} \phi_s e^{-2\pi i n' s/N} = \frac{1}{\sqrt{N}} \sum_{s=0}^{N-1} \sum_{n=1}^{N} e^{2\pi i s/N (n-n')} y_n$$

$$= \frac{1}{\sqrt{N}} \sum_{s=0}^{N-1} y_{n'} + \frac{1}{\sqrt{N}} \sum_{s=0}^{N-1} \sum_{\substack{n=1 \\ n\neq n'}}^{N} e^{2\pi i s/N (n-n')} y_n$$

$$= \frac{N}{\sqrt{N}} y_{n'} + \frac{1}{\sqrt{N}} \sum_{\substack{n=1 \\ n\neq n'}}^{N} e^{2\pi i (n-n')} \left(\frac{1-e^{2\pi i (n-n')}}{1-e^{2\pi i (n-n')/N}} \right) y_n$$

finite geometric series

$$= \sqrt{N} y_{n'} + \frac{1}{\sqrt{N}} \sum_{\substack{n=1 \\ n\neq n'}}^{N} e^{2\pi i (n-n')} \cancel{\frac{(1-1)}{1-e^{(\ )}}} y_n$$

0

$$\therefore y_{n'} = \frac{1}{\sqrt{N}} \sum_{s=0}^{N-1} \phi_s e^{-2\pi i n' s/N}$$

H.W.

$$T = \frac{m}{2} \sum_{n=1}^{N} \dot{y}_n^2 \Rightarrow \frac{2T}{m} = \frac{1}{N} \sum_{n=1}^{N} \sum_{s=0}^{N-1} \dot{\phi}_s e^{-2\pi i n s/N} \sum_{s'=0}^{N-1} \dot{\phi}_{s'} e^{-2\pi i n s'/N}$$

$$\Rightarrow \frac{2T}{m} = \frac{1}{N} \sum_{n=1}^{N} \sum_{s=0}^{N-1} \sum_{s'=0}^{N-1} \dot{\phi}^*_{N-s} e^{2\pi i n (N-s)/N} \dot{\phi}_{s'} e^{-2\pi i n s'/N}$$

$$= \frac{1}{N} \sum_{n} \sum_{s'} \sum_{l=N}^{1} \dot{\phi}^*_l e^{2\pi i n l/N} \dot{\phi}_{s'} e^{-2\pi i n s'/N}$$

Putting $N-s = l$

$$\cancel{= \frac{1}{N} \sum_n \sum_{s=0}^{N-1} \sum_{l=1}^{N} \dot{\phi}_s \dot{\phi}^*_l e^{2\pi i n (l-s)/N}}$$

$$\cancel{= \frac{1}{N} \sum_n \sum_{l=1}^{N} \dot{\phi}_0 \dot{\phi}^*_l e^{2\pi i n l/N} + \frac{1}{N} \sum_n \sum_{s=0}^{N-1}}$$

$$\Rightarrow \frac{2T}{m} = \frac{1}{N}\sum_{n=1}^{N}\sum_{s=0}^{N-1}\sum_{l=1}^{N} \dot\phi_s \dot\phi_l^* e^{2\pi i n(l-s)/N}$$

$$= \frac{1}{N}\sum_{n=1}^{N}\left(\dot\phi_0 + \sum_{s=1}^{N-1}\dot\phi_s e^{-2\pi i n s/N}\right)\left(\dot\phi_N^* e^{2\pi i n} + \sum_{l=1}^{N-1}\dot\phi_l^* e^{2\pi i n l/N}\right)$$

$$= \frac{1}{N}\sum_{n=1}^{N}\left[\dot\phi_0^2 + \sum_{l=1}^{N-1}\dot\phi_0\dot\phi_l^* e^{2\pi i n l/N} + \sum_{s=1}^{N-1}\dot\phi_0\dot\phi_s e^{-2\pi i n s/N} + \sum_{s=1}^{N-1}\sum_{l=1}^{N-1}\dot\phi_s\dot\phi_l^* e^{2\pi i n(l-s)/N}\right]$$

$\because \phi_0 = \phi_N$ = real

$$= \dot\phi_0^2 + \frac{\dot\phi_0}{N}\sum_{l=1}^{N-1}\dot\phi_l^*\sum_{n=1}^{N} e^{2\pi i n l/N} + \frac{\dot\phi_0}{N}\sum_{s=1}^{N-1}\dot\phi_s\sum_{n=1}^{N} e^{-2\pi i n s/N} + \frac{1}{N}\sum_{s=1}^{N-1}\dot\phi_s\dot\phi_s^*$$

Now, $\displaystyle\sum_{n=1}^{N} e^{2\pi i n l/N} = e^{2\pi i l/N}\frac{(1-e^{2\pi i})}{1-e^{2\pi i l/N}} = 0$

$$\therefore \frac{2T}{m} = \dot\phi_0^2 + \frac{N}{N}\sum_{s=1}^{\frac{N-1}{2}}\dot\phi_s\dot\phi_s^* + \frac{N}{N}\sum_{s=\frac{N-1}{2}+1}^{N-1}\dot\phi_s\dot\phi_s^*$$

Putting $N-s=l$

s	$\frac{N+1}{2}$	$N-1$
l	$\frac{N-1}{2}$	1

$$= \frac{N}{N}\sum_{l=\frac{N-1}{2}}^{1}\dot\phi_{N-s}\dot\phi_{N-s}^*$$

$$= \frac{N}{N}\sum_{l=1}^{\frac{N-1}{2}}\dot\phi_s^*\dot\phi_s$$

$$= \dot\phi_0^2 + 2\sum_{s=1}^{\frac{N-1}{2}}\dot\phi_s\dot\phi_s^*$$

$N - \frac{N-1}{2} - 1$
$= \frac{2N - N + 1}{2} - 1$
$= \frac{N+1}{2} - 1$
$= \frac{N-1}{2}$

$$\Rightarrow \frac{2T}{m} = \dot\phi_0^2 + \sum_{s=1}^{\frac{N-1}{2}}\dot\phi_s\dot\phi_s^*$$

$$\Rightarrow \boxed{T = \frac{m}{2}\dot\phi_0^2 + m\sum_{s=1}^{\frac{N-1}{2}}\dot\phi_s\dot\phi_s^*}$$