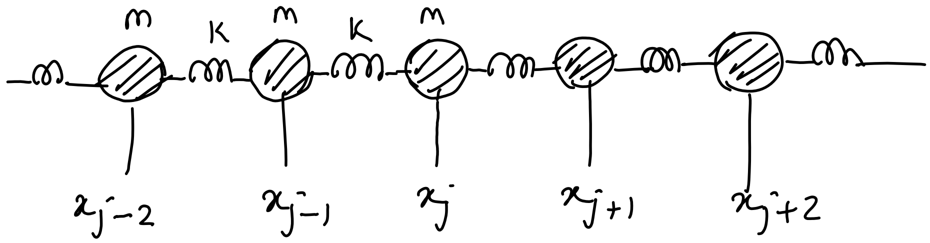
Crystal Vibrations : Phonons

Session 26 – 28

Note Title 3/14/2008



$$H = T + U$$

$$T = \sum_j \frac{\hat{p}_j^2}{2m}$$

relative displacement

$$U = \sum \frac{1}{2} k(\Delta x)^2 = \frac{k}{2} \sum (\Delta x)^2 = \frac{k}{2} \sum_j \left(2x_j^2 - x_j x_{j+1} - x_j x_{j-1}\right)$$

for N atoms in the crystal, we have :

$$\hat{H} = \sum_{j=1}^{N} \frac{\hat{p}_j^2}{2m} + \frac{k}{2} \sum_{j=1}^{N} \left(2x_j^2 - x_j x_{j+1} - x_j x_{j-1}\right)$$

Define new operators $\hat{a}_q$ and $\hat{a}_q^+$:

$$\begin{cases} \hat{a}_q = \dfrac{1}{\sqrt{N}} \displaystyle\sum_j^N \left(\frac{m\omega_q}{2\hbar}\right)^{1/2} \underbrace{e^{-iqjL}} \left(\hat{x}_j + \frac{i\hat{p}_j}{m\omega_q}\right) \\ \hat{a}_q^+ = \dfrac{1}{\sqrt{N}} \displaystyle\sum_j^N \left(\frac{m\omega_q}{2\hbar}\right)^{1/2} \underbrace{e^{iqjL}}_{\text{Bloch phase factor}} \left(\hat{x}_j - \frac{i\hat{p}_j}{m\omega_q}\right) \end{cases}$$

ω_q to be defined $\Rightarrow$

$$\begin{cases} \hat{x}_j = \dfrac{i}{\sqrt{N}} \displaystyle\sum_q^N \left(\frac{\hbar}{2m\omega_q}\right)^{1/2} e^{iqjL} \left(\hat{a}_q + \hat{a}_{-q}^+\right) \\ \hat{p}_j = \dfrac{-i}{\sqrt{N}} \displaystyle\sum_q^N \left(\frac{m\hbar\omega_q}{2}\right)^{1/2} e^{iqjL} \left(\hat{a}_q - \hat{a}_{-q}^+\right) \end{cases}$$

Note: $[\hat{a}_q, \hat{a}_q^\dagger] = 1$ as before.

Substitute $\hat{x}_j$ & $\hat{p}_j$ in H to get:

$$\hat{H} = -\frac{1}{4}\sum_q \hbar\omega_q (a_q - a_{-q}^\dagger)(a_{-q} - a_q^\dagger)$$

$$+\frac{1}{4}\sum \frac{\hbar}{\omega_q} \underbrace{\frac{k}{m}(2 - e^{iqL} - e^{-iqL}}_{\equiv \omega_q^2})(a_q + a_{-q}^\dagger)(a_{-q} + a_q^\dagger)$$

$$\hat{H} = \frac{1}{4}\sum_q \hbar\omega_q \Big[\underbrace{(a_q + a_{-q}^\dagger)(a_{-q} + a_q^\dagger) - (a_q - a_{-q}^\dagger)(a_{-q} - a_q^\dagger)}_{\text{Simplify to get} = 4a_q^\dagger a_q + 2}\Big]$$

$$\boxed{\hat{H} = \sum_q \hbar\omega (a_q^\dagger a_q + \tfrac{1}{2})}$$

This is the sum of independent harmonic oscillators each with frequency $\omega(q)$:

q: wavevector ($q = \frac{2\pi}{\lambda}$ λ: wave length)

ω_q: Corresponding frequency

As before the number operator is: $\boxed{\hat{N}_q = \hat{a}_q^\dagger \hat{a}_q}$

And the Corresponding energy for this wavevector is:

$$\boxed{E_n = \hbar\omega_q (n + \tfrac{1}{2})}$$

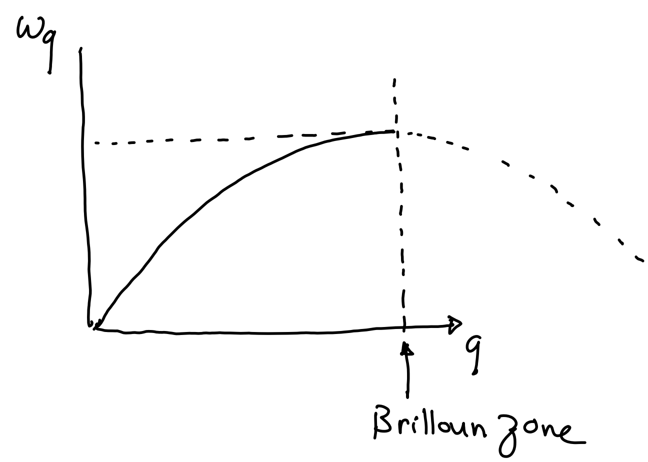
n here is the Phonon occupation number in the wavevector q.

(Phonon has zero spin and is boson like photon)

Here we defined:

$$\omega_q^2 = \frac{k}{m}\left(2 - e^{iqL} - e^{-iqL}\right)$$

$$= \frac{k}{m}\left(2 - 2\cos qL\right) = \frac{2k}{m}\left(1 - \cos qL\right)$$



Fermions and Bosons

For N interacting particle, the general form of the Hamiltonian is:

$$\hat{H} = \sum_j^N \frac{\hat{p}_j^2}{2m_j} + \sum_j^N \hat{V}_j(x_j) + \underbrace{\sum_{j,k}^{j>k} \hat{V}_{j,k}(x_j - x_k)}_{\text{Two body interaction}}$$

Schrodinger equ.:

$$\hat{H}\,\psi(x_1, x_2, \dots x_N, t) = i\hbar \frac{\partial}{\partial t}\psi(x_1, x_2, \dots x_N, t)$$

$|\psi(x_1, x_2, \dots x_N)|^2 dx_1 dx_2 \dots dx_N$ is the probability of finding the particle 1 in x_1 to x_1+dx_1 and particle 2 in x_2 to x_2+dx_2, etc.

This is a single multiparticle wavefunction that describes the state of the N-particle system.

The difficulty of solving this Schrödinger equation is due to the interacting term $\sum \hat{V}_{jk}(x_j - x_k)$. If we ignore this term, the problem is easy as we can separate the variables:

$$\hat{H} = \sum_{j}^{N} \frac{p_j^2}{2m_j} + V(x_j) = \sum_{j}^{N} H_j \quad \Rightarrow$$

$$\Psi(x_1, x_2, x_3 \cdots x_N) = \Psi(x_1)\Psi(x_2)\cdots\Psi(x_N) \quad \Rightarrow$$

$$H_1\Psi(x_1) = E_1\Psi(x_1) \longrightarrow E_1, \Psi(x_1)$$

$$H_2\Psi(x_2) = E_2\Psi(x_3) \longrightarrow E_2, \Psi(x_2)$$

$$\vdots$$

$$H_N\Psi(x_N) = E_N\Psi(x_N) \longrightarrow E_N, \Psi(x_3)$$

$$\Rightarrow \begin{cases} E = E_1 + E_2 + \cdots E_N \\ \Psi = \Psi(x_1)\Psi(x_2)\cdots\Psi(x_N) \end{cases}$$

We will assume the interaction term is small and ignore it here.

Symmetry of indistinguishable particles

Electrons are all the same in a material. They are indistinguishable. Photons & Phonons are also indistinguishable, but they have a major distinction as compared with electrons:

Electron $\longrightarrow$ fermion

Phonon, photon $\longrightarrow$ Boson

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fermion : half-odd-integer spin

Boson : integer spin.

Electron: $S = \pm \frac{1}{2}$

Photon: $S = \pm 1$

Phonon: $S = 0$

Fermions obey the Pauli Exclusion principle:

"No identical fermions may occupy the same state"

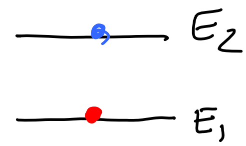
<u>Recall</u>: Symmetry $\Longrightarrow$ Even or odd parity

Consider two particles at positions x_1, x_2: (non-interacting)

$$\hat{H}\,\psi(x_1,x_2) = E\,\psi(x_1,x_2)$$

$$\psi(x_1,x_2) = \psi(x_1)\,\psi(x_2) \Rightarrow$$

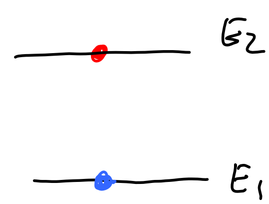
$$\begin{cases} H_1\,\psi(x_1) = E_1\,\psi(x_1) \\ H_2\,\psi(x_2) = E_2\,\psi(x_2) \end{cases}$$



where $\hat{H} = \hat{H}_1 + \hat{H}_2$

$$\rightarrow \quad \hat{H}\,\psi(x_1,x_2) = (E_1+E_2)\,\psi(x_1,x_2)$$

Since the particles are identical, we should be able to interchange (permute) them without affecting the total energy:



In other word, if we apply permutation operator the energy doesn't change. So the permutation operator must commute with H:

$$[\hat{P}_{12}, \hat{H}]\,\psi = (P_{12}H - HP_{12})\,\psi$$

$$= \hat{P}_{12}\hat{H}\,\psi(x_1,x_2) - \hat{H}\hat{P}_{12}\,\psi(x_1,x_2)$$

$$= E\,P_{12}\,\psi(x_1,x_2) - \hat{H}\,\psi(x_2,x_1)$$

$$= E\,\psi(x_2, x_1) - E\,\psi(x_2, x_1)$$

$$= 0$$

$$[\hat{P}_{12}, \hat{H}] = 0$$

Theorem:

For two commuting commutato, there exists at least a simoltaneous eigenstate.

If ψ is the simoltaneous eigenstate of H & P_{12}:
Let's apply interchang two time, we should return to the intial state:

$$\psi(x_1, x_2) \xrightarrow{P_{12}} \psi(x_2, x_1) \xrightarrow{P_{12}} \psi(x_1, x_2)$$

$$P_{12}\,\psi(x_1, x_2) = \lambda\,\psi(x_1, x_2)$$

$$P_{12}P_{12}\,\psi(x_1, x_2) = \lambda\,P_{12}\,\psi(x_1, x_2)$$

$$= \lambda^2\,\psi(x_1, x_2) = \psi(x_1, x_2)$$

$$\Rightarrow \lambda = \pm 1$$

So $P_{12}\,\psi(x_1, x_2) = \pm\,\psi(x_1, x_2) = \psi(x_2, x_1)$

So ψ is either symmetric or antisymmetric.

Fermions : Antisymmetric ψ_a

Bosons : Symmetric ψ_s

For two particle :

$$\psi_s = \frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2) + \psi_2(x_1)\right]$$

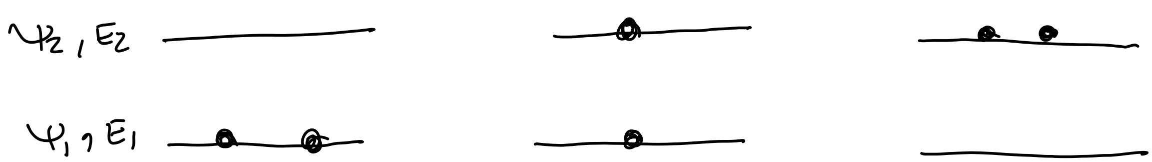
$$\psi_a = \frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)\right]$$

columns : particle

$$= \frac{1}{\sqrt{2}}\begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) \\ \psi_2(x_1) & \psi_2(x_2) \end{vmatrix}$$

Rows : state

Boson :

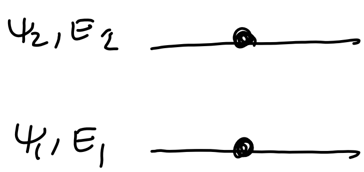


$\psi(x_1, x_2) = \psi_1(x_1)\psi_1(x_2) \to E = E_1 + E_1$

$\frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1)\right] \to E = E_1 + E$

$\psi_2(x_1)\psi_2(x_2) \to E = E_2 + E_2$

Fermion :



$$\psi(x_1, x_2) = \frac{1}{2}\left[\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2) + \psi_2(x_1)\right]$$

$$\downarrow$$

$$E = E_1 + E_2$$

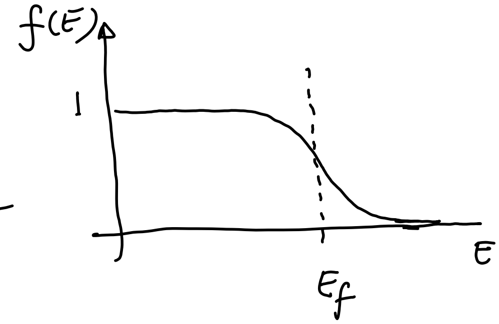
for N fermions, the ground state wave function is:

$$\Psi_a(x_1, x_2, \cdots x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) & \cdots & \psi_1(x_N) \\ \psi_2(x_1) & \psi_2(x_2) & \cdots & \psi_2(x_N) \\ \vdots & & & \\ \psi_N(x_1) & & & \psi_N(x_N) \end{vmatrix}$$

Fermi–Dirac distribution

Energy distribution of fermions obeys the F–D distribution:

$$f(E) = \frac{1}{1 + e^{\frac{E-\mu}{k_B T}}}$$



μ : Chemical potential

chemical potential is the chang in total energy if a particle is added to the system:

$$\mu = \frac{\partial E}{\partial N}$$ at constant antropy and volume

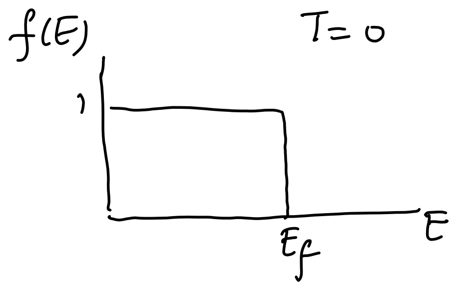
Number of electrons:

$$n = \int \underset{\substack{\uparrow \\ \text{spin}}}{2} f(E, E_f) \frac{d^3k}{(2\pi)^3}$$

Or equally:

$$n = \int_0^\infty D(E) f(E)\, dE$$

At $T=0$:



$\hookrightarrow k_f \qquad E_f = \frac{\hbar^2 k_f^2}{2m}$

$$n_{T=0} = \int \frac{2}{(2\pi)^3} d^3k$$

$$= \int_0^{k_f} \frac{2}{(2\pi)^3} 4\pi k^2 \sin\theta \, d\theta \, dk$$

$$= \frac{2}{(2\pi)^3} \frac{4\pi}{3} k_f^3 = \frac{k_f^3}{3\pi^2}$$

$$k_f = (3\pi^2 n)^{1/3} \Rightarrow E_f = \frac{\hbar^2}{2m} \underbrace{(3\pi^2 n)^{2/3}}_{k_f^2}$$

Bose_Einstein distribution

$$f^{BE}(E) = \frac{1}{e^{\frac{E-\mu}{k_B T}} - 1} \qquad E = \hbar\omega$$