LECTURE 1 NOTES

Metal as a Free Electron Gas

Electrons in a metal are highly mobile (free), so we represent them using the Hamiltonian

$$H = \frac{\vec{P}^2}{2m} + V(r), \qquad (1)$$

where $V(r)$ confines the electrons to the metal.

We only really consider nuclei for their positive charge in the "Jellium" model; but we later consider their periodic structure.

Density of States

For a particle in a 3D box, the wave function is

$$\psi(\vec{x}) = \frac{1}{(L_1 L_2 L_3)^{\frac{1}{2}}} e^{i k \cdot \vec{x}}. \qquad (2)$$

The periodic boundary conditions imply

$$e^{i k_j (x_j + L_j)} = e^{i k_j x_j}, \qquad (3)$$

which if we expand this using de Moivre's formula gives

$$\cos(k_j(x_j+L_j)) + i\sin(k_j(x_j+L_j)) = \cos(k_j(x_j)) + i\sin(k_j(x_j)). \quad (4)$$

This implies

$$k_j L_j = 2\pi n_j, \qquad (5)$$

so due to (space) translational invariance, our momentum is quantized as

$$\vec{k} = \left(\frac{2\pi n_1}{L_1}, \frac{2\pi n_2}{L_2}, \frac{2\pi n_3}{L_3}\right). \qquad (6)$$

Changing to k-space, the number of states in a volume in k-space is

$$g = \frac{V}{(2\pi)^3} dk_1 dk_2 dk_3. \qquad (7)$$

The <u>Dispersion Relation</u> relates energy and momentum as

$$\epsilon_k = \frac{\hbar^2 k^2}{2m}. \tag{8}$$

To get the number of quantum states, we integrate $D(\epsilon)$ which gives the no. of states in $[\epsilon, \epsilon + d\epsilon]$.

$$\int D(\epsilon)\,d\epsilon = \underset{\substack{\nearrow \\ \text{Spin degeneracy}}}{2}\int g\,\delta(\epsilon - \epsilon_k)\,d\epsilon. \tag{9}$$

Q: Why the δ function? Where did this come from?

We can convert this integral to a spherical integral due to the spherical symmetry of the Dispersion Relation.

$$2\int g\,\delta(\epsilon - \epsilon_k)\,d\epsilon = 2\left(\frac{V}{(2\pi)^3}\right) 4\pi \int k^2\,dk. \tag{10}$$

Q: How do we know that there is spherical symmetry in k-space from the Dispersion Relation?

Q: How do we interpret an angular dependence in k-space? If k is linear momentum, would angular dependence imply angular momentum? How does this manifest physically?

After a change of variables from $k \to \epsilon$, and integrating, we get

$$D(\epsilon) = \left(\frac{V}{2\pi^2}\right)\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \epsilon^{\frac{1}{2}}. \tag{11}$$

The density of states for dimension M is then given by

$$\rho(\epsilon) = \frac{D(\epsilon)}{V} = \underset{\substack{\nearrow \\ \text{degeneracy}}}{S}\,\frac{\Omega_M}{(2\pi)^M} k^{M-1} \frac{d|k|}{d\epsilon}, \tag{12}$$

where Ω_M is the surface area of an M dimensional sphere.

Q: What's so special about the surface area of an M-sphere? Does this come from some physical consideration?

Fermi-Dirac Distribution

This is given by

$$f(\epsilon) = \frac{1}{e^{\frac{(\epsilon-\mu)}{kT}} + 1} . \tag{13}$$

At $T=0$, this goes to

$$f(\epsilon) = \lim_{T\to 0}\left(\frac{1}{e^{\frac{(\epsilon-\mu)}{kT}} + 1}\right) = \begin{cases} 0, & \mu < 0 \\ 1, & 0 < \epsilon < \mu . \\ 0, & 0 < \mu < \epsilon \end{cases} \tag{14}$$

This is like a step function, so only energies $\epsilon \leq \mu$ are filled.
(At $T=0$)

We can then define the Fermi Energy as

$$\epsilon_F = \mu . \tag{15}$$

This gives us

$$N = \int_0^\infty f(\epsilon) D(\epsilon)\, d\epsilon = \int_0^{\epsilon_F} D(\epsilon)\, d\epsilon . \tag{16}$$

Using (11), this gives

$$\epsilon_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}} = \frac{\hbar^2 k_F^2}{2m} . \tag{17}$$

This defines the Fermi surface, where only $k \leq k_F$ are filled.

Q: What's special about $T=0$? Experimentally, we haven't reached absolute zero. Until what temperature range does this approximation hold?

LECTURE 2

Electrical Conductivity

The Lorentz force law for an electron is

$$\vec{F} = -e(\vec{E} + \vec{v} \times \vec{B}) . \quad (1)$$

For $\vec{B} = 0$, and using Fourier transforms to give an ansatz of

$$\vec{p}(t) = \vec{p}(\omega) e^{-i\omega t} \quad (2)$$

$$\vec{E}(t) = \vec{E}(\omega) e^{-i\omega t} , \quad (3)$$

Using the angular frequency ω, we solve for $\vec{v}$ as

$$\vec{v}(\omega) = -\frac{ie}{m\omega} \vec{E}(\omega) . \quad (4)$$

The <u>current density</u>, for $n = \frac{N}{V}$ electrons is then

$$\vec{j}(\omega) = -ne\vec{v}(\omega) = \frac{ie^2 n}{m\omega} \vec{E}(\omega) . \quad (5)$$

We define this coefficient as the <u>electrical/AC conductivity</u>

$$\sigma(\omega) = \frac{ie^2 n}{m\omega} . \quad (6)$$

Q: Why is this automatically AC conductivity? Is it the ω?

Note that as $\omega \to 0$, $\sigma \to \infty$, since resistance was not considered. Superconductors have no resistance, and this divergence in the <u>conductivity's imaginary part</u> is a signature.

Q: How do you measure an imaginary term? How is the imaginary part considered the AC conductivity? Is there a real part?

Drude Model

If we consider damping effects, where electrons scatter on average after time τ, Newton's 2nd Law then gives

$$\frac{d\vec{p}}{dt} = -e\vec{E} - \frac{\vec{p}}{\tau} . \tag{7}$$

Solving this gives

$$\vec{p}(\omega) = \frac{e\tau}{1-i\omega\tau} . \tag{8}$$

Thus, AC conductivity becomes

$$\sigma(\omega) = \frac{ne^2\tau}{m}\frac{1}{1-i\omega\tau} . \tag{9}$$

Q: If I'm not mistaken, taking $\tau\to\infty$, i.e. no damping allows us to recover (6). Is this correct?

Taking a constant electric field

$$E(t) = E_0, \tag{10}$$

we look at the zero-frequency component of the AC conductivity in (9).

$$\sigma(\omega\to 0) = \sigma_0 = \frac{ne^2\tau}{m} . \tag{11}$$

Q: This is a real quantity. Does this mean imaginary: AC, real: DC?

Heat Capacity

We now consider the thermal transport of electrons. Classically, the heat capacity is

$$C_{cl} = \frac{3}{2}Nk_B . \tag{12}$$

However, for low temperatures $T \ll T_F \sim 10^4 - 10^5 K$, only electrons near ϵ_F actually gain the thermal energy k_BT.

The total energy is given by

$$U = \int_0^\infty \epsilon D(\epsilon) f(\epsilon, T)\, d\epsilon \,. \tag{13}$$

The Fermi energy is then given as

$$\epsilon_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}} . \tag{14}$$

We can then get the number of electrons as a function of ϵ_F, and the density as a function of N

$$N = \frac{V}{3\pi^2}\left(\frac{2m\epsilon_F}{\hbar^2}\right)^{\frac{3}{2}} , \tag{15}$$

and

$$D(\epsilon) = \frac{3N}{2\epsilon} \,. \tag{16}$$

We then can get the heat capacity as

$$C_{el} = \frac{\partial U}{\partial T} = \int_0^\infty \epsilon D(\epsilon) \frac{\partial f(\epsilon, T)}{\partial T}\, d\epsilon \,. \tag{17}$$

Since N is not a function of T, $D(\epsilon)$ doesn't really vary at $k_BT \ll \epsilon_F$, and we take $\mu = \epsilon_F$, we get $x = \frac{\epsilon - \epsilon_F}{k_BT}$ $dx = \frac{d\epsilon}{k_BT}$

$$C_{el} = D(\epsilon_F)\int_0^\infty \frac{(\epsilon-\epsilon_F)^2}{k_BT^2}\,\frac{e^{\frac{(\epsilon-\epsilon_F)}{k_BT}}}{\left(e^{\left(\frac{\epsilon-\epsilon_F}{k_BT}\right)}+1\right)^2}\, d\epsilon = \int_{-\frac{\epsilon_F}{k_BT} \to -\infty}^{\infty} \frac{x^2 (k_BT)^2}{k_BT^2}\,\frac{e^x}{(e^x+1)^2}\, dx \,. \tag{18}$$

$\epsilon_F \ll k_BT$

We finally get

$$C_{el} = \left(\frac{\pi^2}{2}\frac{Nk_B}{T_F}\right) T = \gamma_{el} T \,. \tag{19}$$

$$T_F = \frac{\epsilon_F}{k_B} \,. \tag{20}$$

Q: I've never encountered the Riemann zeta function formally before, could you explain this step?

Q: So is the intuition that ϵ_F is the energy at T_F? If yes, then since T_F is so large ~ 10^1-10^5 K doesn't that mean lots of states $\epsilon < \epsilon_F$ are indeed filled at low temperatures? A bit confused about the intuition behind ϵ_F and T_F.

Thermal Conductivity

A thermal gradient leads to an electron's motion in a manner described by the heat current

$$j_H = -K\frac{dT}{dx} = -\frac{1}{3}c_e\bar{v}\ell\frac{dT}{dx}, \tag{21}$$

K: Thermal conductivity

$\bar{v}$: mean velocity

ℓ: mean free path

$c_{el} = \frac{C_{el}}{V}$.

Only electrons near ϵ_F contribute to the thermal excitation, $\bar{v} \approx v_F$, $\ell \approx v_F\tau$, $n = \frac{N}{V}$, $\epsilon_F = k_BT$.

Q: When do you use $\epsilon_F = k_BT_F$ then?

Using (19), we get

$$c_{el} = \frac{\pi^2}{2}nk_B^2\frac{T}{\epsilon_F}. \tag{22}$$

Using $\epsilon_F = \frac{mv_F^2}{2}$, we get a thermal conductivity of

$$K = \frac{\pi^2}{3}nk_B^2T\frac{\tau}{m}. \tag{23}$$

Wiedemann-Franz Law

Considering an electrical conductivity of

$$\sigma_0 = (e^2)\frac{n\tau}{m} \tag{24}$$

and thermal conductivity

$$K = \left(\frac{\pi^2}{3}k_B^2T\right)\frac{n\tau}{m}, \tag{25}$$

We calculate their ratio as

$$\frac{K}{\sigma} = \frac{1}{3}\left(\frac{\pi k_B}{e}\right)^2 T = LT \,. \qquad (26)$$

Equation (26) is the Wiedemann-Franz Law. L is the Lorenz (Ludwig not Edward) number which is a universal proportionality constant.

The Lorenz number is not valid whenever one or both of the assumptions of the free electron model are NOT met:

1) Same kinds of particles (carriers) are responsible for both types of conduction.

2) the carriers (electrons) strongly interact with each other.

Q: I'm a bit confused. I thought the free electron model assumed minimal interaction between electrons. Why is it now saying that strong interactions are an axiom of the model?

LECTURE 3

CLASSICAL HALL EFFECT

We now consider the case where there is a magnetic field and damping

$$m\left(\frac{d}{dt}+\frac{1}{\tau}\right)\vec{v} = -e\left(\vec{E}+\vec{v}\times\vec{B}\right). \qquad (1)$$

Where the vectors have the components

$$\vec{v} = (v,0,0),\ \vec{E}=(E_x,E_y,0),\ \vec{B}=(0,0,B). \qquad (2)$$

E_y comes from charge accumulation due to $\vec{B}$, while E_x was applied directly.

Taking the case of no acceleration, $\frac{d\vec{v}}{dt}\to 0$, the solution is

$$x: \quad \frac{mv}{\tau} = -eE_x \qquad (3)$$

$$y: \quad 0 = -eE_y + evB. \qquad (4)$$

Considering the current density as

$$j = -nev, \qquad (5)$$

we get

$$j_x = \frac{ne^2\tau}{m}E_x = \sigma E_x. \qquad (6)$$

We can then write the steady state velocity as

$$v = \frac{-j_x}{ne}, \qquad (7)$$

so

$$E_y = -\frac{B}{ne}j_x \qquad (8)$$

We can then define the Hall coefficient as

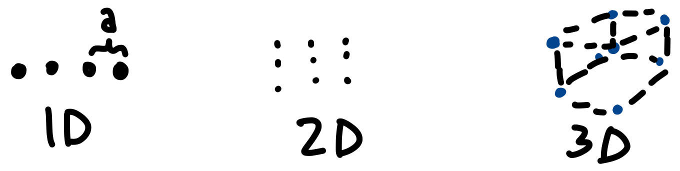
$$R_H = \frac{E_y}{Bj_x} = -\frac{1}{ne}. \qquad (9)$$

This expression for the Hall coefficient breaks down for some metals, such as superconductors. The free electron model thus needs to be improved by taking into account a periodic potential such as in a crystal lattice or atomic lattice.

Q: Intuitively, what does the Hall coefficient measure? Why is that the characteristic measure of the Hall effect? What's a 1-2 sentence description for what the Hall effect is physically?

Crystals

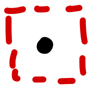
Crystal - material whose components are arranged periodically
Lattice - Repeating pattern of points.



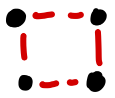
Lattices.

A unit cell is the smallest portion of the lattice that has the same symmetry as the entire crystal structure.

Q: Would a unit cell of a 2D Lattice be



or



?

The position of a point j in the lattice is given by

$$\vec{r}_j = x_j \vec{a}_1 + y_j \vec{a}_2 + z_j \vec{a}_3, \qquad (10)$$

where for a simple cubic lattice, the primitive vectors are

$$\vec{a}_1 = a\hat{x}, \vec{a}_2 = a\hat{y}, \vec{a}_3 = a\hat{z}. \qquad (11)$$

Reciprocal Lattice

A Real lattice

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \qquad (12)$$

has a corresponding lattice in momentum space ("k" space)

$$\vec{G} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3, \qquad (13)$$

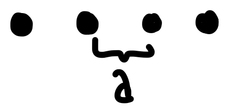
via a Fourier transform.

The Fourier transform gives us the relation for the basis vectors $\vec{b}_i$

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij} \,. \qquad (14)$$

Thus, the primitive vectors in a 1D lattice for example are

$$\vec{a} = a\hat{i} \,,\; \vec{b} = \frac{2\pi}{a}\hat{i} \,. \qquad (15)$$



Real Space

Reciprocal Space.

For an arbitrary crystal structure then, the reciprocal basis vectors are

$$\vec{b}_1 = 2\pi\frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \,,\; \vec{b}_2 = 2\pi\frac{\vec{a}_3\times\vec{a}_1}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \,,\; \vec{b}_3 = 2\pi\frac{\vec{a}_1\times\vec{a}_2}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} \,. \qquad (16)$$

Brillouin Zone

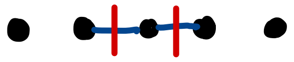
Primitive Cell: Unit cell with one lattice point.

In momentum space,

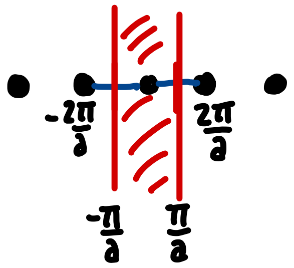
1. Choose a point

2. Draw lines to nearest neighbors

3. Bisect lines.



4. Area enclosed is the first Brillouin zone or just Brillouin zone.



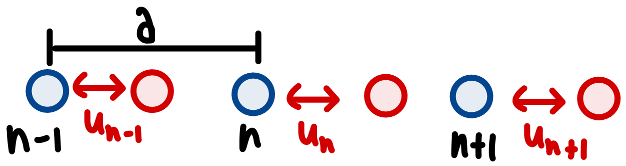
Q: What is the importance of the Brillouin Zone?

By the way, just want to say thank you for your lecture notes. They are some of the easiest to understand readings I've had as a BS Physics student.

LECTURE 4

1D MONATOMIC CHAIN

The harmonic oscillator potential approximates the Lenard-Jones potential. For identical atoms in a lattice, we can think of them as coupled with springs of spring constant c.



Each has mass m.

The motion of one atom is given by

$$m\frac{d^2u_n}{dt^2} = c(u_{n+1}-u_n) + c(u_{n-1}-u_n) . \qquad (1)$$

The periodicity gives the solution ansatz

$$u_{kn}(t) = \mathrm{Re}\left(A_k e^{i(nka-\omega t)}\right) . \qquad (2)$$

Q: Why automatically define a solution in terms of k?

This gives

$$-m\omega^2 = c\left(e^{ika}+e^{-ika}-2\right) = 2c(\cos(ka)-1), \qquad (3)$$

which using the identity

$$2\sin^2\left(\frac{x}{2}\right) = 1-\cos(x), \qquad (4)$$

gives us the frequency as

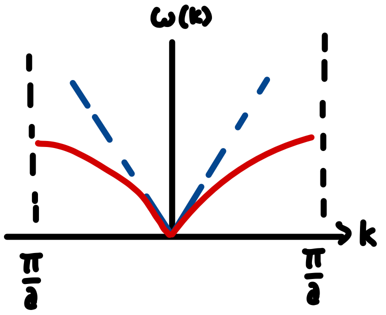
Dispersion Relation:

$$\omega(k) = 2\sqrt{\frac{c}{m}}\left|\sin\left(\frac{k}{a}\right)\right| . \qquad (5)$$

For small k,

$$\omega(k) \approx ka\sqrt{\frac{c}{m}} \qquad (6)$$

Q: How do you solve for this approximation?



We get the group velocity of the wavepacket as

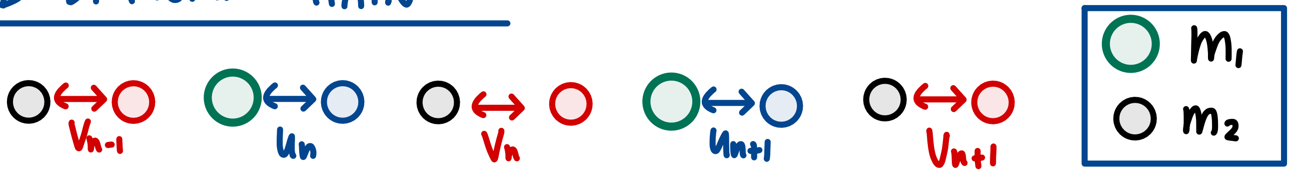
$$V_g = \frac{d\omega}{dk} = a\sqrt{\frac{c}{m}}\cos\left(\frac{ka}{2}\right). \qquad (7)$$

which for small $k \ll \frac{1}{a}$ is approximately constant like the speed of sound

$$V_g \approx a\sqrt{\frac{c}{m}}. \qquad (8)$$

Q: Just to clarify, this is velocity in real space. Right?

1D DIATOMIC CHAIN



We now have equations of motion for m_1 and m_2 as

$$m_1\frac{d^2U_n}{dt^2} = C(V_n - U_n) + (V_{n-1} - U_n) \qquad (9)$$

$$m_2\frac{d^2V_n}{dt^2} = C(U_{n+1} + U_n - 2V_n). \qquad (10)$$

We have the solution ansatz

$$U_n(t) = A_1 e^{i(nka-\omega t)} \qquad V_n(t) = A_2 e^{i(nka-\omega t)}. \qquad (11)$$

We get the matrices

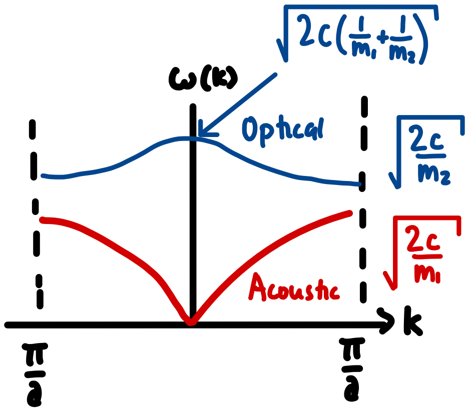
$$-\omega^2\begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix}\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = C\begin{pmatrix} -2 & 1+e^{-ika} \\ 1+e^{ika} & -2 \end{pmatrix}\begin{pmatrix} A_1 \\ A_2 \end{pmatrix}. \qquad (12)$$

This gives the solution for the frequency

Dispersion Relation:

$$\omega^2 = c\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\left(1 \pm \sqrt{1 - \frac{4m_1m_2}{(m_1+m_2)^2}\sin^2\left(\frac{ka}{2}\right)}\right). \qquad (13)$$

For $m_1 > m_2$, we have two branches of excitations.



Acoustic: $A_1 = A_2$ (14)

↳ Two Atoms move in same direction.

$$\omega_{acoustic} = \sqrt{c\left(\frac{1}{m_1}+\frac{1}{m_2}\right)}\left(1 \pm \sqrt{1 - \frac{4m_1m_2}{(m_1+m_2)^2}\sin^2\left(\frac{ka}{2}\right)}\right)^{\frac{1}{2}}. \quad (15)$$

For $ka \ll 1$: $\omega_{acoustic} \approx ka\sqrt{\frac{2c}{m_1+m_2}}$ Linear (16)

↳ V_g Constant like sound wave.

Optical: $m_1A_2 = -m_2A_2$ (17)

↳ Two Atoms move in opposite direction.

↳ May have opposite charges: EM field excitation.

$$\omega_{optical} = \sqrt{c\left(\frac{1}{m_1}+\frac{1}{m_2}\right)}\left(1 + \sqrt{1 - \frac{4m_1m_2}{(m_1+m_2)^2}\sin^2\left(\frac{ka}{2}\right)}\right)^{\frac{1}{2}}. \quad (18)$$

For $ka \ll 1$: $\omega_{optical} \approx \sqrt{\frac{2c(m_1+m_2)}{m_1m_2}}$. Constant (19)

↳ $V_g = 0$.

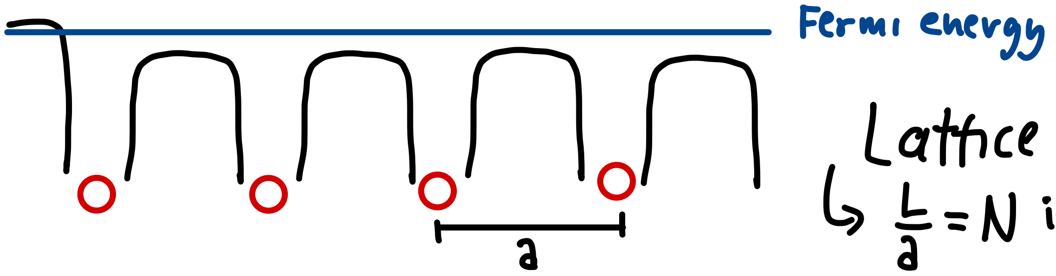
Band Gap: $\Delta E = \sqrt{\frac{2c}{m_2}} - \sqrt{\frac{2c}{m_1}}$. (20)

Therefore, no vibrations for $\sqrt{\frac{2c}{m_2}} > \omega > \sqrt{\frac{2c}{m_1}}$. (21)

LECTURE 5

Electrons in a Lattice

Periodic Potentials



Lattice of ions
↳ $\frac{L}{a} = N$ is an integer.

For the 1D case, we can consider the potential as

$$V(x) = V(x+a), \tag{1}$$

so that the Fourier decomposition is

$$V(x) = \sum_n V_n e^{inkx} . \tag{2}$$

Weak Periodic Potential

The Hamiltonian is

$$\hat{H} = \frac{\hat{P}^2}{2m} + 2\overset{\text{Potential depth}}{\overbrace{V_0}} \cos\left(\frac{2\pi x}{a}\right) . \tag{3}$$

We can treat this as a perturbation of the free particle case

$$\hat{H} = \hat{H}_0 + \hat{V} = \hat{H}_0 + 2V_0 \cos\left(\frac{2\pi x}{a}\right) = \hat{H}_0 + V_0\left(e^{ikx} + e^{-ikx}\right), \tag{4}$$

where

$$k = \frac{2\pi}{a} . \tag{5}$$

Perturbation theory, up to 2nd order, gives

$$\tilde{E}_p = E_p^{(0)} + \langle p^{(0)} | \hat{V} | p^{(0)} \rangle + \sum_{q \neq p} \frac{|\langle q^{(0)} | \hat{V} | p^{(0)} \rangle|^2}{E_p^{(0)} - E_q^{(0)}} . \tag{6}$$

We note that

Free particle momentum: $$|p^{(0)}\rangle = |p\rangle = \frac{1}{\sqrt{L}} e^{ipx} , \tag{7}$$

and

$$\hbar = 1 . \tag{8}$$

1st Order Correction:

Due to periodicity

$$\langle p|\hat{V}|p\rangle = \frac{V_0}{L}\int_0^L e^{-ipx}\left(e^{i\frac{2\pi}{a}x}+e^{-i\frac{2\pi}{a}x}\right)e^{ipx}dx = 0 \,. \qquad (9)$$

2nd Order Correction:

Since $\hat{V}$ only has two Fourier components, as seen in (4), only two terms survive in the sum.

$$\frac{\langle p+\frac{2\pi}{a}|\hat{V}|p\rangle}{E_p^{(0)}-E_{p+\frac{2\pi}{a}}^{(0)}} = \frac{\frac{V_0}{L}\int_0^L e^{-i(p+\frac{2\pi}{a})x}\left(e^{i\frac{2\pi}{a}x}+e^{-i\frac{2\pi}{a}x}\right)e^{ipx}dx}{\frac{p^2}{2m}-\frac{(p+\frac{2\pi}{a})^2}{2m}} \qquad (10)$$

First term:

$$\frac{\langle p+\frac{2\pi}{a}|\hat{V}|p\rangle}{E_p^{(0)}-E_{p+\frac{2\pi}{a}}^{(0)}} = \frac{V_0}{\frac{p^2}{2m}-\frac{(p+\frac{2\pi}{a})^2}{2m}} \,. \qquad (11)$$

$$\frac{\langle p-\frac{2\pi}{a}|\hat{V}|p\rangle}{E_p^{(0)}-E_{p-\frac{2\pi}{a}}^{(0)}} = \frac{\frac{V_0}{L}\int_0^L e^{-i(p-\frac{2\pi}{a})x}\left(e^{i\frac{2\pi}{a}x}+e^{-i\frac{2\pi}{a}x}\right)e^{ipx}dx}{\frac{p^2}{2m}-\frac{(p+\frac{2\pi}{a})^2}{2m}} \qquad (12)$$

Second term:

$$\frac{\langle p-\frac{2\pi}{a}|\hat{V}|p\rangle}{E_p^{(0)}-E_{p-\frac{2\pi}{a}}^{(0)}} = \frac{V_0}{\frac{p^2}{2m}-\frac{(p-\frac{2\pi}{a})^2}{2m}} \qquad (13)$$

Defining

$$\Delta E_+ = E_p^{(0)}-E_{p+\frac{2\pi}{a}}^{(0)} = \frac{p^2}{2m}-\frac{(p+\frac{2\pi}{a})^2}{2m} \qquad (14)$$

$$\Delta E_- = E_p^{(0)}-E_{p-\frac{2\pi}{a}}^{(0)} = \frac{p^2}{2m}-\frac{(p-\frac{2\pi}{a})^2}{2m}, \qquad (15)$$

We find the energy as

$$\tilde{E} = \frac{p^2}{2m} - \frac{V_0^2}{\Delta E_+} - \frac{V_0^2}{\Delta E_-} . \tag{16}$$

We have a problem as ΔE_+ and ΔE_- vanish for $p = \mp \frac{\pi}{a}$.

Q: Is this already a sign that this method is invalid near $p = \mp\frac{\pi}{a}$, or only precisely at these values?

We also note that for $p = \frac{\pi}{a}$, $|p\rangle$ and $|p - \frac{2\pi}{a}\rangle$ have the same $E^{(0)}$. We thus need degenerate perturbation theory.

Degenerate Perturbation Theory

We introduce a small detuning δ, to "lift the degeneracy." We then have the nearly degenerate states

$$|p_1\rangle = |p\rangle = |\tfrac{\pi}{a} + \delta\rangle \tag{17}$$

$$|p_2\rangle = |p - \tfrac{2\pi}{a}\rangle = |-\tfrac{\pi}{a} + \delta\rangle . \tag{18}$$

The matrix equation for such nearly degenerate states is

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = E \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} , \tag{19}$$

where

$$H_{ij} = \langle p_i | \hat{H}_0 + \hat{V} | p_j \rangle . \tag{20}$$

This yields

$$\hat{H} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} = \begin{pmatrix} \frac{(\frac{\pi}{a}+\delta)^2}{2m} & V_0 \\ V_0 & \frac{(-\frac{\pi}{a}+\delta)^2}{2m} \end{pmatrix} . \tag{21}$$

Diagonalizing this matrix, and reinserting $\hbar$, gives the eigenvalues

$$E_\pm(\delta) = \hbar^2 \frac{(\frac{\pi}{a})^2}{2m} \pm \sqrt{\hbar^2 \left(\frac{\pi\delta}{ma}\right)^2 + V_0^2} . \tag{22}$$

Q: What units does δ have?

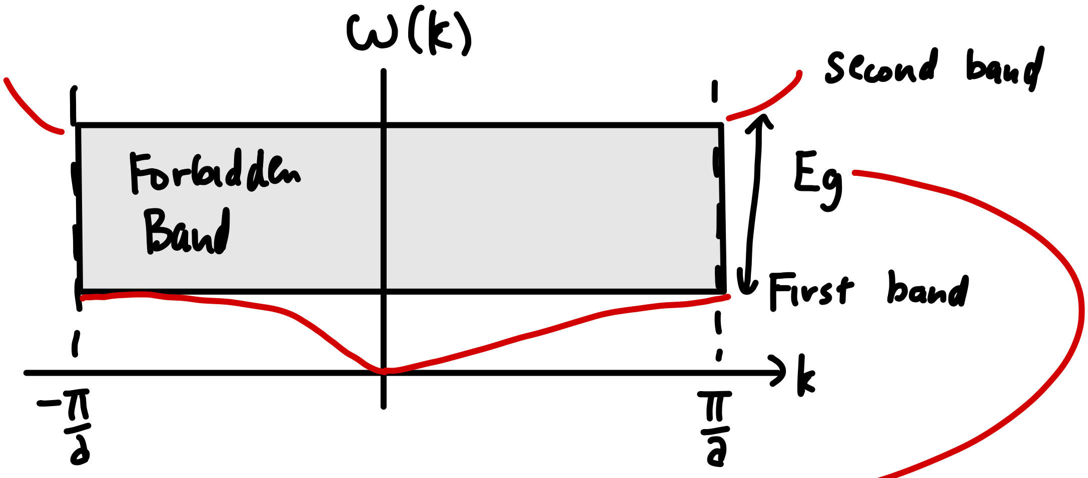
Q: How do you know where to put back $\hbar$?

Removing the detuning

$$\delta \to 0, \tag{23}$$

we find an energy gap

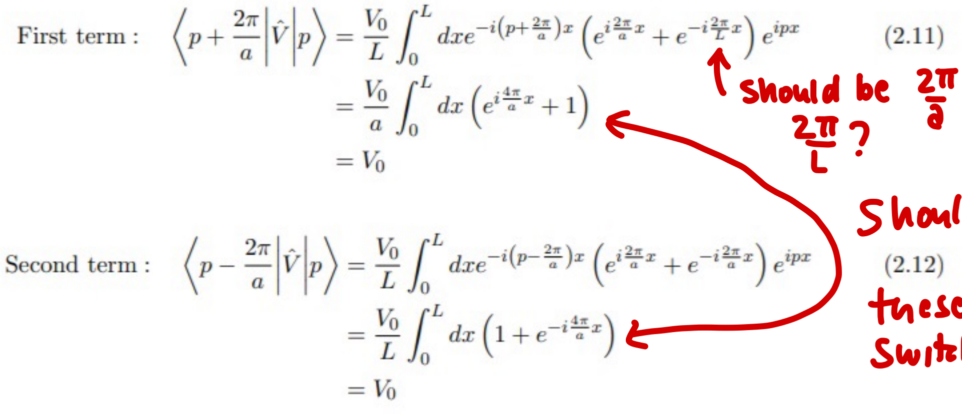
$$E_g = E_+ - E_- = 2V_0 \, . \tag{24}$$



Q: Why do we denote it as E_g in this diagram, if $\omega(k)$ has units of frequency? Is this because $\hbar = 1$?

This band gap separates conductors and insulators.

Extraneous Comments:



First term :
$$\left\langle p+\frac{2\pi}{a}\middle|\hat{V}\middle|p\right\rangle = \frac{V_0}{L}\int_0^L dx e^{-i(p+\frac{2\pi}{a})x}\left(e^{i\frac{2\pi}{a}x}+e^{-i\frac{2\pi}{L}x}\right)e^{ipx} \tag{2.11}$$
$$= \frac{V_0}{a}\int_0^L dx\left(e^{i\frac{4\pi}{a}x}+1\right)$$
$$= V_0$$

Second term :
$$\left\langle p-\frac{2\pi}{a}\middle|\hat{V}\middle|p\right\rangle = \frac{V_0}{L}\int_0^L dx e^{-i(p-\frac{2\pi}{a})x}\left(e^{i\frac{2\pi}{a}x}+e^{-i\frac{2\pi}{a}x}\right)e^{ipx} \tag{2.12}$$
$$= \frac{V_0}{L}\int_0^L dx\left(1+e^{-i\frac{4\pi}{a}x}\right)$$
$$= V_0$$

should be $\frac{2\pi}{a}$ not $\frac{2\pi}{L}$?

Shouldn't these be switched?

LECTURE 6

Electrons in a Lattice II

Bloch Theorem

Consider a 3D crystal with the lattice $\vec{R} = \sum_{i=1}^{3} n_i \vec{a}_i$ and reciprocal lattice $\vec{G} = \sum_{i=1}^{3} m_i \vec{b}_i$, where the basis vectors satisfy $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$. For ideal crystals, the Hamiltonian and wavefunctions are periodic

$$\hat{H}(\vec{r}) = \hat{H}(\vec{r}+\vec{R}), \quad \psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r}+\vec{R}) \,. \qquad (1)$$

The eigenstates $\psi_{\vec{k}}$ are known as Bloch waves/functions.

The Schrödinger equation reads

$$\hat{H}(\vec{r})\psi_{\vec{k}}(\vec{r}) = E(\vec{k})\psi_{\vec{k}}(\vec{r}), \qquad (2)$$

which gives us eigenvalues for a given $\vec{k}$.

1D Case

For periodicity a, $g = \frac{2\pi}{a}$, we can expand (2) in terms of Fourier components

$$E(k)e^{ikx}\sum_{m=-\infty}^{\infty}\psi_m e^{igmx} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \sum_{n=-\infty}^{\infty} V_n e^{ignx}\right) e^{ikx}\sum_{m=-\infty}^{\infty}\psi_m e^{igmx} \,. \qquad (3)$$

Q: Why are there different m and n indices?

This leads to

$$E(k)\sum_{m=-\infty}^{\infty}\psi_m e^{i(k+gm)x} = \frac{\hbar^2(k+gm)^2}{2m_e}\sum_{m=-\infty}^{\infty}\psi_m e^{i(k+gm)x} + \sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} V_n\psi_m e^{i(k+g(n+m))x} \,. \qquad (4)$$

We want to match coefficients of $e^{i(k+gm)x}$, so we take $m \to (m-n)$ in the double sum

$$\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} V_n\psi_m e^{i(k+g(n+m))x} = \sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} V_n\psi_{m-n} e^{i(k+gm)x} \,. \qquad (5)$$

Q: Why does the sum being convergent allow us to do this?

Matching coefficients then gives

$$E(k)\psi_m = \frac{\hbar^2(k+gm)^2}{2m_e}\psi_m + \sum_n V_n\psi_{m-n} \,. \qquad (6)$$

This is an eigenvalue problem which gives the infinite matrix

$$E(k)\begin{pmatrix}\vdots\\ \psi_2\\ \psi_1\\ \psi_0\\ \psi_{-1}\\ \vdots\end{pmatrix} = \begin{pmatrix} \ddots & & & & \\ & \frac{\hbar^2(k+2g)^2}{2m_e} & V_1 & V_2 & \cdots \\ & V_{-1} & \frac{\hbar^2(k+g)^2}{2m_e} & \ddots & \cdots \\ & V_{-2} & V_{-1} & \ddots & \\ & V_{-3} & V_{-2} & & \ddots \\ & \vdots & \vdots & & \end{pmatrix}\begin{pmatrix}\vdots\\ \psi_2\\ \psi_1\\ \psi_0\\ \psi_{-1}\\ \vdots\end{pmatrix}. \tag{7}$$

We can solve this by diagonalizing the matrix for a finite no. of elements, by truncating

$$u_k(x) = \sum_{m=-\infty}^{\infty} \psi_m e^{igmx} \approx \sum_{l=-l_{max}}^{l_{max}} \psi_l e^{iglx}. \tag{8}$$

Q: Does l_{max} have some physical significance?

Considering the simple periodic potential

$$V(x) = 2U_0\cos(gx) = U_0(e^{igx}+e^{-igx}), \tag{9}$$

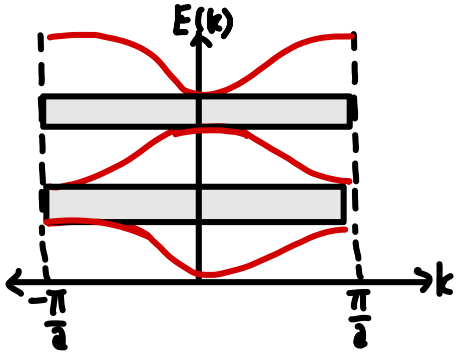
we have for $l_{max}=2$ within the first Brillouin zone

$$E(k)\begin{pmatrix}\psi_2\\ \psi_1\\ \psi_0\\ \psi_{-1}\\ \psi_{-2}\end{pmatrix} = \begin{pmatrix} \frac{\hbar^2(k+2g)^2}{2m_e} & U_0 & 0 & 0 & 0 \\ U_0 & \frac{\hbar^2(k+g)^2}{2m_e} & U_0 & 0 & 0 \\ 0 & U_0 & \frac{\hbar^2k^2}{2m_e} & U_0 & 0 \\ 0 & 0 & U_0 & \frac{\hbar^2(k-g)^2}{2m_e} & U_0 \\ 0 & 0 & 0 & U_0 & \frac{\hbar^2(k-2g)^2}{2m_e}\end{pmatrix}\begin{pmatrix}\psi_2\\ \psi_1\\ \psi_0\\ \psi_{-1}\\ \psi_{-2}\end{pmatrix}. \tag{10}$$

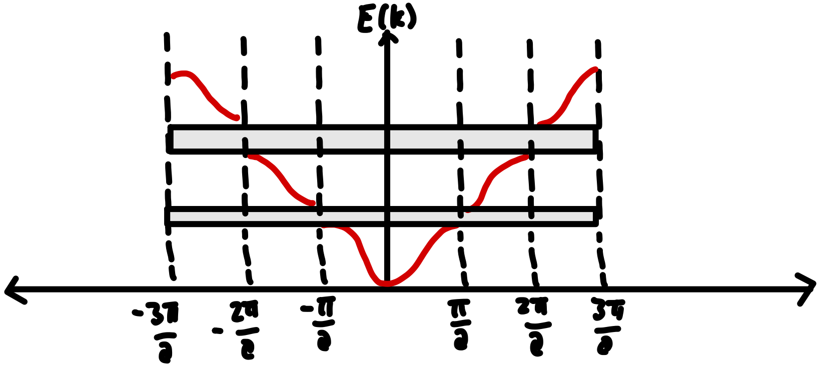
From Bloch Theory, we note that

$$\psi_k(x) = \psi_{k+\frac{2\pi}{a}}(x) = \psi_{k+g}(x). \tag{11}$$

This means that we also have periodicity in k-space.



Bloch Theorem reduced Band diagram for first Brillouin Zone



Extended scheme

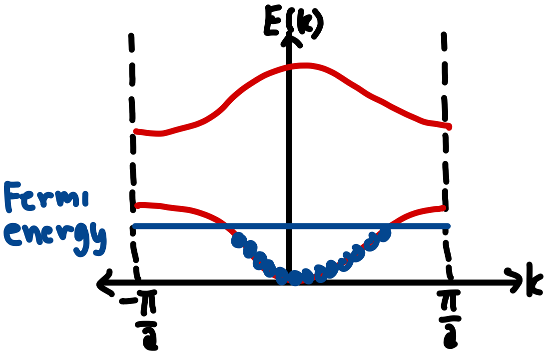
Note that $\vec{k}$ is the crystal momentum/quasimomentum, but this is not the true momentum of the electron as the Bloch state is not an eigenstate of $\hat{p}$.

$\vec{k}$ is the momentum of the combined state $\vec{k} = k + G$, if G is the reciprocal lattice vector.

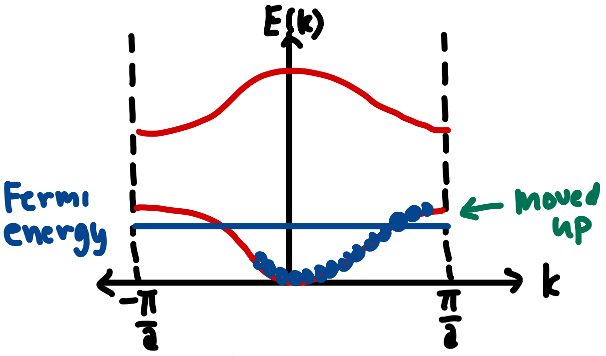
Consequences of Bands

Transport properties

Conductor: Electrons can get excited and surpass E_F.

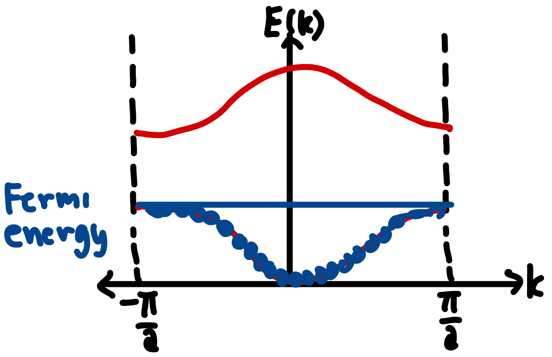


Equilibrium

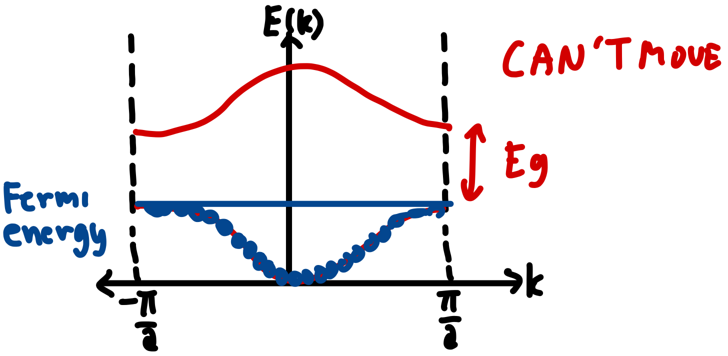


Excited

Insulator: First band is full, and there is an energy gap.



Equilibrium



Excited

Semiconductor: Band gap small enough $E_g \approx k_B T < 3\,eV$, to have e^- thermally excited into empty bands.

Effective Mass

Considering an applied $\vec{E}$ field, the chang in energy is given by

$$\Delta\epsilon = \vec{F}\cdot\Delta\vec{x} = -e\vec{E}\cdot\vec{v}\Delta t. \tag{12}$$

Taking the group velocity as

$$V_g = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{d\epsilon}{dk}, \tag{13}$$

we can get the infinitesimal change as

$$d\epsilon(\vec{k}) = \frac{d\epsilon(\vec{k})}{dk}d\vec{k} = -e\vec{E}\cdot\frac{1}{\hbar}\frac{d\epsilon(\vec{k})}{dk}dt. \tag{14}$$

We then have

$$\frac{d\vec{k}}{dt} = -\frac{e\vec{E}}{\hbar}, \tag{15}$$

So

$$\vec{F} = \frac{d\vec{p}}{dt} = \hbar\frac{d\vec{k}}{dt}. \tag{16}$$

We can then get $\vec{a}$ by considering (13), to get

$$\vec{a} = -\frac{e\vec{E}}{\hbar}\frac{1}{\hbar}\frac{d^2\epsilon(\vec{k})}{dk^2}. \tag{17}$$

Considering the Lorenz force law

$$\vec{F} = -e\vec{E}, \tag{18}$$

we get the effective mass

$$m^* = \left(\frac{1}{\hbar^2}\frac{d^2\epsilon(\vec{k})}{dk^2}\right)^{-1}. \tag{19}$$

This is related to the curvature of the dispersion relation $\epsilon(\vec{k})$.

We can recover $m = m^*$ by considering a free electron.

↳ We also have different signs for m^* depending on the energy band.

Q: Is this curvature interpreted similarly to that in GR? For example, is the difference between m and m^* similar to the difference between the inertial mass and gravitational mass?

LECTURE 7

Ideal Bose Gas

Density of States

For non-interacting bosons, we have the same dispersion relation

$$\epsilon_k = \frac{\hbar^2 \vec{k}^2}{2m}. \qquad (1)$$

Q: What if the boson, like a photon is massless? Wouldn't $m=0$ mess it up?

We recall the number of states occupying the energy levels is

$$\int D(\epsilon)\,d\epsilon = \int g\,\delta(\epsilon-\epsilon_k)\,d\epsilon = \int \frac{V}{(2\pi)^3}\delta(\epsilon-\epsilon_k)\,dk_1 dk_2 dk_3. \qquad (2)$$

There is no factor of 2, since these are bosons not fermions with half integer spin. This becomes for an ideal gas

$$\rho(\epsilon) = \frac{D(\epsilon)}{V} = \frac{1}{\sqrt{2}\,\pi^2}\left(\frac{m}{\hbar^2}\right)^{\frac{3}{2}}\epsilon^{\frac{1}{2}}. \qquad (3)$$

Bose-Einstein Statistics

From a change of sign from the Fermi-Dirac distribution for fermions, we have the Bose-Einstein distribution

$$f_B(\epsilon) = \frac{1}{e^{\frac{\epsilon(k)-\mu}{k_B T}} - 1}. \qquad (4)$$

$\swarrow$ + in Fermi-Dirac

When we consider the ground state

$$\epsilon(k=0) = 0, \qquad (5)$$

the chemical potential is limited as

$$\mu \leq 0, \qquad (6)$$

to get a physical system at

$$T = 0. \qquad (7)$$

This is because a positive μ would give a negative distribution.

The sign of the 1 makes all the difference.

Bose - Einstein Condensation

Unlike fermions, multiple bosons can occupy a single quantum state. This is called **Bose - Einstein Condensation**.

Consider a particle density ρ (not density of states). With fixed T, we increase the no of particles

$$\rho = \frac{1}{V}\int_0^\infty f_B(\epsilon)D(\epsilon)\,d\epsilon = \frac{1}{\sqrt{2}\,\pi^2}\left(\frac{m}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty \frac{\epsilon^{\frac{1}{2}}}{e^{\frac{\epsilon(k)-\mu}{k_BT}}-1}\,d\epsilon. \qquad (8)$$

We can define

$$A = \frac{1}{\sqrt{2}\,\pi^2}\left(\frac{m}{\hbar^2}\right)^{\frac{3}{2}}, \qquad (9)$$

so that we have

$$\rho = A e^{\frac{\mu}{k_BT}}\int_0^\infty \frac{\epsilon^{\frac{1}{2}}}{e^{\frac{\epsilon(k)}{k_BT}}-1}\,d\epsilon. \qquad (10)$$

To increase ρ then, we increase μ, up to a max of zero, to get

$$\rho(\mu=0) = A\int_0^\infty \frac{\epsilon^{\frac{1}{2}}}{e^{\frac{\epsilon(k)}{k_BT}}-1}\,d\epsilon. \qquad (11)$$

Using the Riemann Zeta function $\zeta(x)$ gives

$$\rho_{\overset{\text{critical}}{c}} = \rho(\mu=0) = A(k_BT)^{\frac{3}{2}}\,\Gamma\!\left(\tfrac{3}{2}\right)\zeta\!\left(\tfrac{3}{2}\right). \qquad (12)$$

This is weirdly just a constant, since we've fixed T. So the density of bosons does not change as we increase the number of bosons. The reason for this is that there is a mistake when calculating the mean number of particles using an integral instead of a discrete sum Σ.

This comes from a divergence when $\mu < 0$.

We can fix this by splitting the lowest energy state from other excited states as

$$\rho = \rho_0 + \rho_{ex}, \tag{13}$$

$$\rho = \frac{1}{V}\frac{1}{e^{\frac{-\mu}{k_BT}} - 1} + Ae^{\frac{\mu}{k_BT}} \int_{\vec{k}=0} \frac{\epsilon^{\frac{1}{2}}}{e^{\frac{\epsilon}{k_BT}} - 1} d\epsilon . \tag{14}$$

Approaching $\mu = 0$, the 2nd term is limited by ρ_c, while the first term can be arbitrarily large

$$\rho_0 = \frac{1}{V}\frac{1}{e^{\frac{-\mu}{k_BT}} - 1} \approx -\frac{k_BT}{\mu V} > 0 . \tag{15}$$

since $\mu<0$

Q: So essentially the issue awhile ago was that we only considered the ρ_{ex} term which goes to ρ_c as $\mu \to 0$?

Equation (15) means that past the critical density, the new particles occupy the ground state in Bose-Einstein condensation.

Q: So ρ_0 increases as $\mu \to 0$. So does this mean that increasing the number of bosons is what takes $\mu \to 0$?

Q: Wouldn't increasing T, while $< T_c$, also increase ρ_0? Or no as we've assumed $T =$ constant?

We can get the critical temperature T_c from

$$\rho = \rho_{ex}(\mu=0, T=T_c) = A(k_BT_c)^{\frac{3}{2}}\Gamma(\tfrac{3}{2})\zeta(\tfrac{3}{2}) . \tag{16}$$

Q: So at T_c, all bosons leave ρ_0?

Q: Why is this equal to the total no. of atoms? Where did atoms come in?

The condensate fraction is

$$n_0 = \frac{\rho_0}{\rho} = \frac{N_0}{N} = 1 - \frac{\rho}{\rho_{ex}} = 1 - \left(\frac{T}{T_c}\right)^{\frac{3}{2}} . \tag{17}$$

At $T=0$, they're all in the condensate mode. Above T_c, they're in excited states.

LECTURE 8

Weakly Interacting Condensates

Dilute Interacting Bose Gas

The Hamiltonian for N interacting identical quantum particles interacting via two-particle potentials is

$$\hat{H} = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\nabla_i^2 + \underbrace{V(\vec{r}_i,t)}_{\text{External potential}}\right] + \underbrace{\sum_{i<j}\hat{U}(\vec{r}_i-\vec{r}_j)}_{\text{two-particle potentials}} . \qquad (1)$$

This many-body Hamiltonian neglects other many-particle scattering interactions. The two-body potential is sufficient for the relatively large length scales of ultracold atoms.

For $T \sim 10^{-3}$K, the dominant two-particle interaction is the contact interaction

$$\hat{H} = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\nabla_i^2 + V(\vec{r}_i,t)\right] + \underset{\hookrightarrow\ \text{Strength of contact interaction}}{g}\sum_{i<j}\delta(\vec{r}_i-\vec{r}_j) = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\nabla_i^2 + V(\vec{r}_i,t)\right] + \frac{4\pi\hbar^2 a_s}{m}\sum_{i<j}\delta(\vec{r}_i-\vec{r}_j). \qquad (2)$$

Gross-Pitaeuski Equation

If we don't know a priori if there's a BEC, we use the variational approach known as Hartree-Fock approximation. In finding the ground state, we assume all N-particles are in the same single-particle energy state. The wavefunction is

$$\Psi(\vec{r}_1,\vec{r}_2,\ldots\vec{r}_N,t) = \prod_{j=1}^{N}\phi(\vec{r}_j,t) \quad \Big| \quad |\Psi\rangle = |\phi\rangle\otimes|\phi\rangle\otimes\cdots\otimes|\phi\rangle = (|\phi\rangle)^N . \qquad (3)$$

From normalization, we have both

$$\langle\Psi|\Psi\rangle = \langle\phi|\phi\rangle = 1. \qquad (4)$$

We also assume that the wavefunctions and first derivatives vanish at the boundary.

Q: What is the boundary of the system?

Using Lagrange multipliers, we extremize the energy functional

$$F[\Psi] = \langle\Psi|\hat{H}|\Psi\rangle - \mu\langle\Psi|\Psi\rangle . \qquad (5)$$

Using IBP, we get the Kinetic energy as

$$\langle E_{kin}\rangle = \langle\Psi|-\frac{\hbar^2}{2m}|\Psi\rangle = \sum_{i=1}^{N}\frac{\hbar^2}{2m}\int|\nabla\phi(\vec{r})|^2 d\vec{r} = \frac{-N\hbar^2}{2m}\int\phi^*(\vec{r})\nabla^2\phi(\vec{r})\,d\vec{r}. \qquad (6)$$

The external potential is given by

$$\langle E_{pot} \rangle = N \int \phi^*(\vec{r}) V(\vec{r}) \phi(\vec{r}) d\vec{r} . \qquad (7)$$

The interaction term is

$$\langle E_{int} \rangle = \langle \Psi | g \sum_{i<j}^{N} \delta(\vec{r}_i - \vec{r}_j) | \Psi \rangle = \binom{N}{2} \int g \delta(\vec{r}_i - \vec{r}_j) |\phi(r_i,t)|^2 |\phi(r_j,t)|^2 d\vec{r}_i d\vec{r}_j \qquad (8)$$

$$\langle E_{int} \rangle = \frac{N(N-1)}{2} \int g |\phi(\vec{r})|^4 d\vec{r} . \qquad (9)$$

Q: Where did the time-dependence in ϕ go between (8) and (9)?

We can collect all terms that may be written like

$$\langle \Psi | \hat{H} | \Psi \rangle = \langle E_{kin} \rangle + \langle E_{pot} \rangle + \langle E_{int} \rangle . \qquad (10)$$

We take the first order variation of F as

$$\phi(\vec{r}) \to \phi(\vec{r}) + \delta\phi(\vec{r}) . \qquad (11)$$

To find the minimum configuration (ground state energy and wavefunction) requires

$$\frac{\delta F}{\delta \phi^*(\vec{r})} = 0 . \qquad (12)$$

Q: Why do we need this? Why is the denominator $\delta\phi^*$ instead of $\delta\phi$?

Each term in the functional yields

$$\frac{\delta \langle E_{kin} \rangle}{\delta \phi^*(\vec{r})} = -\frac{N\hbar^2}{2m} \int \nabla^2 \phi(\vec{r}) d\vec{r} \qquad (13)$$

$$\frac{\delta \langle E_{pot} \rangle}{\delta \phi^*(\vec{r})} = N \int V(\vec{r}) \phi(\vec{r}) d\vec{r} \qquad (14)$$

$$\frac{\delta \langle E_{int} \rangle}{\delta \phi^*(\vec{r})} = g N (N-1) \int |\phi(\vec{r})|^2 \phi(\vec{r}) d\vec{r} . \qquad (15)$$

The term with the Lagrange multiplier μ gives

$$\frac{\delta \langle \Psi | \Psi \rangle}{\delta \phi^*(\vec{r})} = N \left(\int |\phi(\vec{r})|^2 d\vec{r} \right)^{N-1} \int \frac{\delta \phi^*(\vec{r})}{\delta \phi^*(\vec{r})} \phi(\vec{r}) d\vec{r} = N \int \phi(\vec{r}) d\vec{r} . \qquad (16)$$

Combining all these terms gives

$$\frac{\delta F}{\delta \phi^*(\vec{r})} = 0 = \int N \left[\frac{-\hbar^2}{2m} \nabla^2 + V(\vec{r}) + (N-1) g |\phi(\vec{r})|^2 - \mu \right] \phi(\vec{r}) d\vec{r} . \qquad (17)$$

This is satisfied when the integrand vanishes, giving the Hartree Equation

$$-\frac{\hbar^2}{2m}\nabla^2\phi(\vec{r}) + V(\vec{r})\phi(\vec{r}) + g(N-1)|\phi(\vec{r})|^2\phi(\vec{r}) = \mu\phi(\vec{r}). \quad (18)$$

For large N, $N \approx N-1$, we get the Gross-Pitaevski Equation

$$-\frac{\hbar^2}{2m}\nabla^2\phi(\vec{r}) + V(\vec{r})\phi(\vec{r}) + gN\,|\phi(\vec{r})|^2\phi(\vec{r}) = \mu\,\phi(\vec{r}). \quad (19)$$

The wavefunction $\phi(\vec{r})$ occupied by N bosons is the condensate wavefunction.

The GPE is also known as the nonlinear Schrödinger Equation since

$$g=0 \quad (20)$$

recovers the original Schrödinger Equation.

The nonlinear interaction term

$$U_{int} = gN|\phi|^2 \quad (21)$$

describes the mean-field potential of the N-1 particles one one particle.

Spontaneous Symmetry Breaking

Symmetry is broken in phase transitions such as a weakly interacting boson gas transitioning into a condensate.

When

$$V(\vec{r}) = 0, \quad (22)$$

the GPE becomes

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + g|\psi(\vec{r})|^2\psi(\vec{r}) = \mu\psi(\vec{r}), \quad (23)$$

where the condensate wavefunction as

$$\psi(\vec{r}) = \sqrt{N}\,\phi(\vec{r}). \quad (24)$$

Energy gets minimized when the wavefunction is flat or uniform.

This means

$$\nabla^2\psi(\vec{r}) = 0, \quad (25)$$

so

$$g|\psi(\vec{r})|^2\psi(\vec{r}) = \mu\psi(\vec{r}) \quad (26)$$

$$g|\psi(\vec{r})|^2 = \mu. \quad (27)$$

The condensate wavefunction is then

$$|\Psi(\vec{r})| = \sqrt{\frac{\mu}{g}} = \underbrace{\sqrt{n_0}}_{\text{uniform density}} . \tag{28}$$

Q: Do we interpret this as the real part of Ψ?

We can introduce the global phase factor

$$\Psi(\vec{r}) = \sqrt{n_0}\, e^{i\theta} . \tag{29}$$

We can always multiply by an arbitrary phase factor

$$\Psi(\vec{r}) \to \Psi(\vec{r}) e^{i\theta} , \tag{30}$$

and the GPE doesn't change

This is a gauge symmetry.

In the transition, the condensate spontaneously picks a phase $\in [0, 2\pi]$. This preference is a spontaneous symmetry breaking.

In this case, U(1) gauge symmetry is broken

LECTURE 9

Introduction to Superfluidity

Time-dependent Gross-Pitaevski Equation

The time-independent GPE for a homogeneous interacting gas of bosons with $V(\vec{r})=0$, breaks $U(1)$ gauge symmetry when the ground state picks a phase θ as

$$\psi_0 = \sqrt{n_0}\, e^{i\theta}. \tag{1}$$

We develop a time-dependent GPE for $V(\vec{r})=0$

$$i\hbar \frac{\partial \psi(\vec{r})}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + g|\psi(\vec{r})|^2\psi(\vec{r}), \tag{2}$$

Q: Shouldn't this have $\psi(\vec{r},t)$ instead of just $\psi(\vec{r})$?

with separation ansatz

$$\psi(\vec{r},t) = \psi_0(\vec{r})\, e^{\frac{-i\mu t}{\hbar}}. \tag{3}$$

Since we can only measure energy differences $\Delta E = E_n - E_m$ instead of the actual value E_n, studying excitations is important.

Low-energy excitations: non-interacting condensate

For a non-interacting BEC,

$$g = 0, \tag{4}$$

so the GPE in (2) becomes

$$i\hbar \frac{\partial \psi(\vec{r})}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}). \tag{5}$$

For this linear equation, we take the ansatz

$$\psi(\vec{r},t) = A_{\vec{k}}\, e^{\frac{-i\mu t}{\hbar}}\, e^{i(\vec{k}\cdot\vec{r}-\omega t)}. \tag{6}$$

Since the non-interacting Bose gas has $\mu \leq 0$, we have the dispersion relation

$$\epsilon_{\vec{k}} = \hbar\omega = \frac{\hbar^2 \vec{k}^2}{2m} + |\mu|. \tag{7}$$

This is the quadratic relation of the free-particle case, but with an energy gap at $\vec{k}=0$ from $|\mu|$.

Low-energy excitations: weakly interacting condensate

We assume a repulsive interaction

$$g > 0, \tag{8}$$

and phase

$$\theta = 0. \tag{9}$$

We include excitations above the ground state by adding plane-wave solutions

$$\Psi(\vec{r},t) = \Psi_0 e^{-\frac{i\mu t}{\hbar}} + \sum_{\vec{k}} u_{\vec{k}} e^{i\left(\vec{k}\cdot\vec{r} - \frac{\mu}{\hbar+\omega}t\right)} + \sum_{\vec{k}} v_{\vec{k}} e^{-i\left(\vec{k}\cdot\vec{r} + \frac{\mu}{\hbar-\omega}t\right)}, \quad (10)$$

where

$$u_{\vec{k}} = \alpha_{\vec{k}} \Psi_0, \; v_{\vec{k}} = \beta_{\vec{k}} \Psi_0 . \quad (11)$$

We only consider low momentum excitations, and thus in linear order of amplitudes that are real

$$u_{\vec{k}} = u_{\vec{k}}^* , \; v_{\vec{k}} = v_{\vec{k}}^* . \quad (12)$$

Thus, we get the LHS of (5) as

$$i\hbar \frac{\partial \Psi(\vec{r})}{\partial t} = \mu \Psi_0 e^{-\frac{i\mu t}{\hbar}} + (\mu + \hbar\omega) \sum_{\vec{k}} u_{\vec{k}} e^{i\left(\vec{k}\cdot\vec{r} - \frac{\mu}{\hbar+\omega}t\right)} + (\mu - \hbar\omega) \sum_{\vec{k}} v_{\vec{k}} e^{-i\left(\vec{k}\cdot\vec{r} + \frac{\mu}{\hbar-\omega}t\right)} . \quad (13)$$

The first term on the RHS gives

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}) = \sum_{\vec{k}} \left(\frac{\hbar^2 \vec{k}^2}{2m}\right) u_{\vec{k}} e^{i\left(\vec{k}\cdot\vec{r} - \frac{\mu}{\hbar+\omega}t\right)} + \sum_{\vec{k}} \left(\frac{\hbar^2 \vec{k}^2}{2m}\right) v_{\vec{k}} e^{-i\left(\vec{k}\cdot\vec{r} + \frac{\mu}{\hbar-\omega}t\right)} . \quad (14)$$

The second term on the RHS, when only considering first-order in amplitudes is

$$g|\Psi(\vec{r})|^2 \Psi(\vec{r}) \approx g|\Psi_0|^2 \left[\Psi_0 e^{-\frac{i\mu t}{\hbar}} + \sum_{\vec{k}} (2u_{\vec{k}} + v_{\vec{k}}) e^{i\left(\vec{k}\cdot\vec{r} - \frac{\mu}{\hbar+\omega}t\right)} + \sum_{\vec{k}} (2v_{\vec{k}} + u_{\vec{k}}) e^{-i\left(\vec{k}\cdot\vec{r} + \frac{\mu}{\hbar-\omega}t\right)} \right] . \quad (15)$$

We can then compare coefficients as

(i) $e^{-\frac{i\mu t}{\hbar}}$:
$$\mu = g|\Psi_0|^2 \quad (16)$$

(ii) $e^{i\left(\vec{k}\cdot\vec{r} - \frac{\mu}{\hbar+\omega}t\right)}$:
$$(\mu + \hbar\omega) u_{\vec{k}} = \left(\frac{\hbar^2 \vec{k}^2}{2m}\right) u_{\vec{k}} + \mu (2u_{\vec{k}} + v_{\vec{k}}) \quad (17)$$

(iii) $e^{-i\left(\vec{k}\cdot\vec{r} + \frac{\mu}{\hbar-\omega}t\right)}$:
$$(\mu - \hbar\omega) v_{\vec{k}} = \left(\frac{\hbar^2 \vec{k}^2}{2m}\right) v_{\vec{k}} + \mu (2v_{\vec{k}} + u_{\vec{k}}) . \quad (18)$$

(ii) and (iii) can be combined to give the matrix equation

$$\hbar\omega \begin{pmatrix} u_{\vec{k}} \\ v_{\vec{k}} \end{pmatrix} = \begin{pmatrix} \frac{\hbar^2 \vec{k}^2}{2m} + \mu & \mu \\ -\mu & -\frac{\hbar^2 \vec{k}^2}{2m} - \mu \end{pmatrix} \begin{pmatrix} u_{\vec{k}} \\ v_{\vec{k}} \end{pmatrix} . \quad (19)$$

This gives the Bogolubov Dispersion

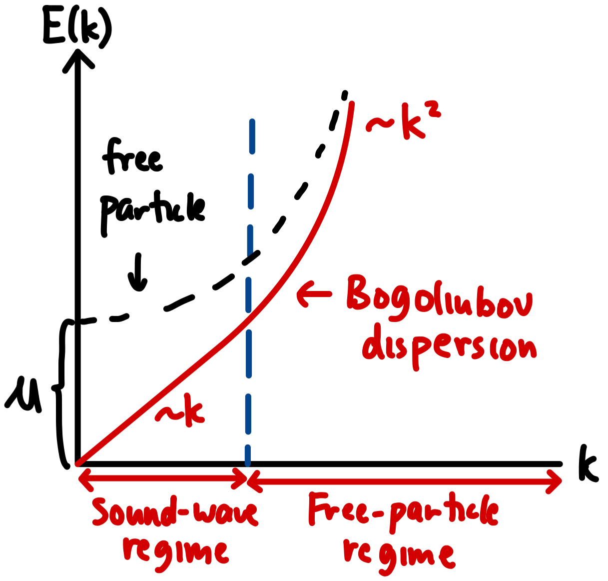
$$\epsilon_{\vec{k}} = \hbar\omega = \sqrt{\left(\frac{\hbar^2\vec{k}^2}{2m}\right)\left(2\mu + \left(\frac{\hbar^2\vec{k}^2}{2m}\right)\right)} \quad . \tag{20}$$

This is linear for small $\vec{k}$

$$\epsilon_{\vec{k}} \approx \sqrt{\frac{\hbar^2\vec{k}^2\mu}{m}}\left(1+\left(\frac{\hbar^2\vec{k}^2}{8\mu m}\right)\right) \approx \hbar|\vec{k}|\sqrt{\frac{\mu}{m}} = \hbar|\vec{k}|\sqrt{\frac{g n_0}{m}} \quad , \tag{21}$$

where $n_0 = |\Psi_0|^2$. Note the non-interacting case is quadratic. However, (20) is actually quadratic for large $\vec{k}$, as kinetic energy dominates

$$\epsilon_{\vec{k}} \to \frac{\hbar^2\vec{k}^2}{2m} \, .$$



Note the Bogolubov dispersion being gapless and linear for small $\vec{k}$. This idea of the Goldstone theorem is what distinguishes a superfluid from a non-interacting condensate.

Q: Are there forms of weakly interacting condensates that are not superfluids?

Q: How does the broken symmetry result in gaplessness?

LECTURE 10

Properties of a Superfluid

Dissipationless Flow

Superfluids don't lose kinetic energy, and thus have zero viscosity, below a critical velocity. This is especially interesting since there is no energy gap.

For a homogeneous gas of particles in a pipe with total mass

$$M = nm \qquad (1)$$

the kinetic energy in the rest frame of the pipe is

$$E_{\text{kin}}(\vec{V}=0) = E_0 = \frac{1}{2}\sum_i m\vec{v}_i^{\,2}. \qquad (2)$$

In the moving frame of a portion of the fluid with velocity $\vec{V}$, we have

$$E_{\text{kin}}(\vec{V}) = \frac{1}{2}\sum_i m\left(\vec{v}_i - \vec{V}\right)^2 = E_0 - \sum_i m\vec{v}_i \cdot \vec{V} + \frac{M\vec{V}^2}{2} = E_0 - \vec{p}\cdot\vec{V} + \frac{M\vec{V}^2}{2}. \qquad (3)$$

The ground state of the condensate is the stationary configuration $\vec{p}=0$

$$E_{\text{kin}}(\vec{V}) = E_0 + \frac{M\vec{V}^2}{2}. \qquad (4)$$

We can expect backscattering or excitation in the opposite direction of the motion due to the walls of the pipe with energy $\epsilon(\vec{p})$ and momentum $\vec{p}$.

In the rest frame: $E_{\text{exc}}(\vec{V}=0) = E_0 + \epsilon(\vec{p}) \qquad (5)$

In the moving frame: $E_{\text{exc}}(\vec{V}) = E_0 + \epsilon(\vec{p}) - \vec{p}\cdot\vec{V} + \frac{M\vec{V}^2}{2}. \qquad (6)$

The change in energy due to the excitation is

$$\Delta E = E_{\text{exc}}(\vec{V}) - E_{\text{kin}}(\vec{V}) = \epsilon(\vec{p}) - \vec{p}\cdot\vec{V}. \qquad (7)$$

An excitation is thus only created if $\Delta E > 0$, or

$$\epsilon(\vec{p}) > \vec{p}\cdot\vec{V}. \qquad (8)$$

Q: How does an excitation in the opposite direction to flow ever increase the energy $\Delta E > 0$? Isn't it like friction?

The Landau Criterion states that no excitations are created when

$$\vec{V} < \vec{V}_c = \min_{\vec{p}}\left(\frac{\epsilon(\vec{p})}{\vec{p}}\right). \qquad (9)$$

Q: If different portions of the fluid move at different velocities $\vec{v}_i$, do they all need to be $< \vec{V}_c$? Or only the average velocity?

For a non-interacting condensate

$$\epsilon(\vec{p}) = \frac{\vec{p}^2}{2m} . \tag{10}$$

Thus,

$$\vec{V}_c = \min_{\vec{p}} \left(\frac{\vec{p}^2}{2m\vec{p}} \right) = \min_{\vec{p}} \left(\frac{\vec{p}}{2m} \right) = 0 . \tag{11}$$

Then even infinitesimal excitations induce dissipation.

For a weakly interacting condensate, for small momenta

$$\epsilon(\vec{k}) \approx \hbar |\vec{k}| \sqrt{\frac{gn_0}{m}} \tag{12}$$

$$\epsilon(\vec{p}) = \vec{p} \sqrt{\frac{gn_0}{m}} . \tag{13}$$

Thus,

$$\vec{V}_c = \min_{\vec{p}} \left(\frac{\vec{p}}{\vec{p}} \sqrt{\frac{gn_0}{m}} \right) = \min_{\vec{p}} \left(\sqrt{\frac{gn_0}{m}} \right) = \sqrt{\frac{gn_0}{m}} \tag{14}$$

Q: It says $\frac{gn_0}{m}$ only in the notes. Shouldn't there by a $\sqrt{\ }$?

The linear dispersion at low momenta allow for this to be a superfluid.

Irrotational Flow

Multiplying $\Psi^*(\vec{r})$ to the time-dependent GPE gives

$$i\hbar \Psi^*(\vec{r}) \frac{\partial \Psi(\vec{r})}{\partial t} = \frac{-\hbar^2}{2m} \Psi^*(\vec{r}) \nabla^2 \Psi(\vec{r}) + V(\vec{r}) |\Psi(\vec{r})|^2 + g |\Psi(\vec{r})|^4 . \tag{15}$$

The complex conjugate is

$$-i\hbar \Psi(\vec{r}) \frac{\partial \Psi^*(\vec{r})}{\partial t} = \frac{-\hbar^2}{2m} \Psi(\vec{r}) \nabla^2 \Psi^*(\vec{r}) + V(\vec{r}) |\Psi(\vec{r})|^2 + g |\Psi(\vec{r})|^4 . \tag{16}$$

Subtracting (16) from (15) and manipulating yields

$$\frac{\partial |\Psi(\vec{r})|^2}{\partial t} = -\frac{\hbar}{2mi} \vec{\nabla} \cdot \left(\Psi^*(\vec{r}) \nabla \Psi(\vec{r}) - \Psi(\vec{r}) \nabla \Psi^*(\vec{r}) \right) . \tag{17}$$

This has the form of the continuity equation

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0 . \tag{18}$$

Therefore the particle density is

$$\rho = |\Psi(\vec{r})|^2 \tag{19}$$

and current density

$$\vec{j} = \frac{\hbar}{2mi} \left(\Psi^*(\vec{r}) \nabla \Psi(\vec{r}) - \Psi(\vec{r}) \nabla \Psi^*(\vec{r}) \right) . \tag{20}$$

We note that

$$\vec{j} = \rho \vec{v} , \tag{21}$$

So it can be shown that we can express $\vec{v}$ in terms of the phase

$$\vec{v} = \frac{\hbar}{m} \vec{\nabla} \phi(\vec{r}) . \tag{22}$$

The line integral of the velocity field is the circulation

$$\Gamma = \oint_c \vec{v} \cdot d\vec{\ell} = \iint (\vec{\nabla} \times \vec{v}) \cdot d\vec{A} . \tag{23}$$

Since the curl of a gradient vanishes,

$$\Gamma = 0 . \tag{24}$$

Thus, a superfluid is irrotational. It tends to stay at rest in a slowly rotating container. For fast rotation, vortices form to retain irrotational flow and conserve angular momentum.

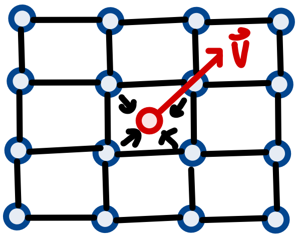
LECTURE II

Introduction to Superconductivity

Basic microscopic concepts

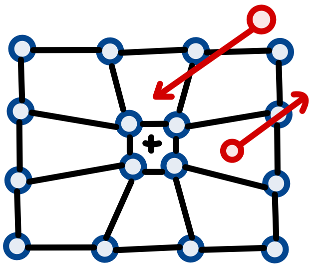
Cooper pairs, made up of two bound electrons, are bosons forming a superfluid below a critical temperature Tc. They have an effective attractive interaction due to electron-phonon interactions.

Cooper pairs carry supercurrents in superconductors.



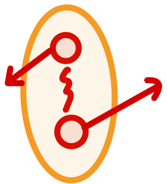
Electron 1 attracts positive ions

$t=0$



Electron 2 is attracted by distortion

$t=t_1$



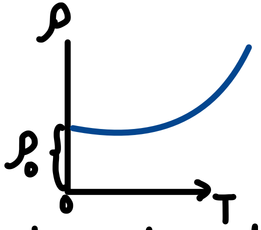
Cooper Pair (Weak bond)

Q: What does it mean when the electron-phonon is retarded in time?

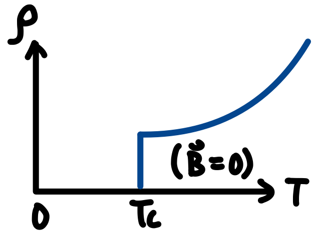
Phenomenology

Properties

1. Zero resistivity: DC resistivity vanishes below Tc.



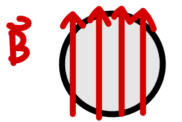
Normal conductor



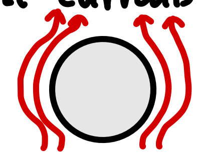
Superconductor

2. Perfect Diamagnetism: Superconductors expel weak $\vec{B}$ fields.

The Meissner effect has screening or surface currents cancelling applied $\vec{B}$ fields.



Normal conductor



Superconductor

3. Superconducting energy gap: Gap between Cooper Pairs and single-particle excitations of electrons. This energy gap is related to the energy needed to break a Cooper pair. This gap is what makes excitations like scattering of electrons impossible.

Conventional superconductors: Tc ~1-10K

High-temperature superconductors: Tc > 30 K.

London Equations

These relate EM fields inside and outside the super-conductor.

Recall from the Drude Model

$$\frac{d\vec{p}}{dt} = -\frac{\vec{p}}{\tau} - e\vec{E}, \qquad (1)$$

with current density

$$\vec{j} = -ne\vec{v}. \qquad (2)$$

Since in superconductors there is no dissipation/damping

$$\tau \to \infty , \qquad (3)$$

so we have the

First London Equation: $$\frac{\partial \vec{j}}{\partial t} = \frac{n_s e^2}{m}\vec{E}. \qquad (4)$$

This leads to the conductivity

$$\sigma(\omega) = \frac{\vec{j}(\omega)}{\vec{E}(\omega)} = \frac{i e^2 n_s}{m}\frac{1}{\omega}. \qquad (5)$$

This $\frac{1}{\omega}$ dependence is a signature of superconductivity. We expect a diverging imaginary part as $\omega \to 0$.

Faraday's Equation is

$$\nabla \times \vec{E} = -\frac{1}{c}\partial_t \vec{B}. \qquad (6)$$

Substituting (4) into this and manipulating yields

$$\frac{\partial}{\partial t}\left(\vec{\nabla} \times \vec{j} + \frac{n_s e^2}{mc}\vec{B}\right) = 0. \qquad (7)$$

However, the Meissner effect requires the inside to vanish

$$\vec{\nabla} \times \vec{j} = -\frac{n_s e^2}{mc}\vec{B}. \qquad (8)$$

We show this requirement by first considering the Maxwell equation

$$\vec{\nabla} \times \vec{B} = \frac{4\pi}{c}\vec{j} + \frac{1}{c}\partial_t \vec{E}. \qquad (9)$$

For the static case

$$\partial_t \vec{E} = 0. \qquad (10)$$

Q: So does superconductivity require a non-time varying $\vec{E}$?

This gives

$$\vec{\nabla}\times\vec{B} = \frac{4\pi}{c}\vec{j}\,. \tag{11}$$

We take the curl of this

$$\vec{\nabla}\times(\vec{\nabla}\times\vec{B}) = \frac{4\pi}{c}(\vec{\nabla}\times\vec{j}). \tag{12}$$

Expanding this and considering Gauss' Law for magnetism

$$\vec{\nabla}\cdot\vec{B} = 0, \tag{13}$$

we get

$$\nabla^2\vec{B} = \frac{4\pi n_s e^2}{mc^2}\vec{B}\,. \tag{14}$$

The solution to this takes the form

$$\vec{B}(\vec{x}) \propto e^{-\frac{\vec{x}}{\lambda}}\,. \tag{15}$$

The length scale is the Londou penetration depth

$$\lambda = \sqrt{\frac{mc^2}{4\pi n_s e^2}}\,. \tag{16}$$

This exponential decay describes surface currents which screen the applied $\vec{B}$ field.