LECTURE 5: Degenerate fermions

1° Understanding chemical potential

$$dE = TdS - pdV + \mu dN \Rightarrow \mu = \left(\frac{\partial E}{\partial N}\right)_{S,V}$$

$$F = E - TS \Rightarrow dF = -SdT - pdV + \mu dN \Rightarrow \mu = \left(\frac{\partial F}{\partial N}\right)_{T,V}$$

$$= -T\left(\frac{\partial S}{\partial N}\right)_{E,N}$$

$$G = F + pV = E - TS + pV$$

$$dG = -SdT + Vdp + \mu dN \Rightarrow \mu = \left(\frac{\partial G}{\partial N}\right)_{T,p} = G/N$$

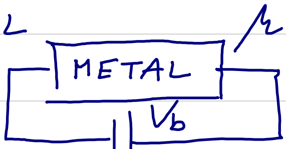
→ assume we apply potential energy V_0 to quantum system ⇒ single particle energy levels then change according to $\varepsilon_n \to \varepsilon_n + V_0$

$$Z_1' = \sum_n e^{-(\varepsilon_n + V_0)/k_BT} = e^{-V_0/k_BT} \sum_n e^{-\varepsilon_n/k_BT} = e^{-V_0/k_BT} Z_1$$

$$F_1' = -k_BT \ln Z' = V_0 - k_BT \ln Z = V_0 + F_1$$

for N particles $\quad F_N' = -N k_BT \ln Z + N V_0$

μ_L $\quad$ μ_R

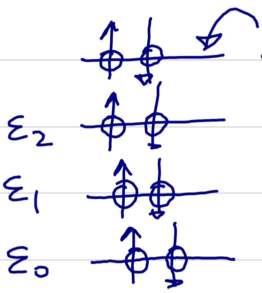


$$\mu_N' = \left(\frac{\partial F'}{\partial N}\right)_{T,V} = \mu + V_0$$

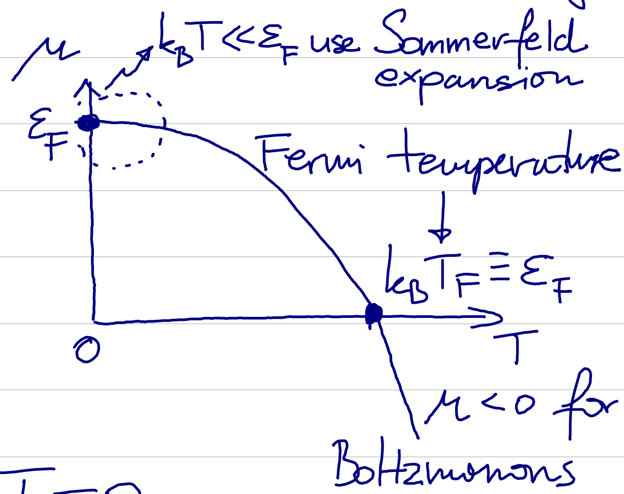
electrochemical potential

$$\left.\begin{aligned} \mu_L &= \mu + eV_b/2 \\ \mu_R &= \mu - eV_b/2 \end{aligned}\right\} \quad \mu_L - \mu_R = eV_b \text{ drives current}$$

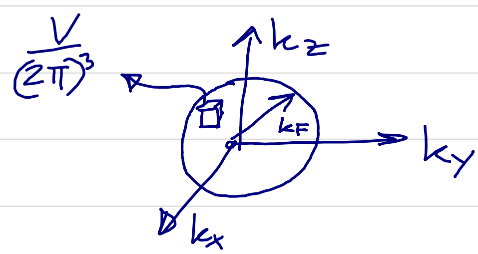
⤳ use $\mu = \left(\frac{\partial E}{\partial N}\right)_{S,V}$ for intuitive understanding



ε_F is Fermi energy as the highest occupied single particle level at $T=0$



2° Degenerate fermions at $T=0$



$$\varepsilon_{\vec{k}} = \hbar^2 k^2/2m \quad , N = g \cdot \sum_{|\vec{k}|\le k_F} 1$$

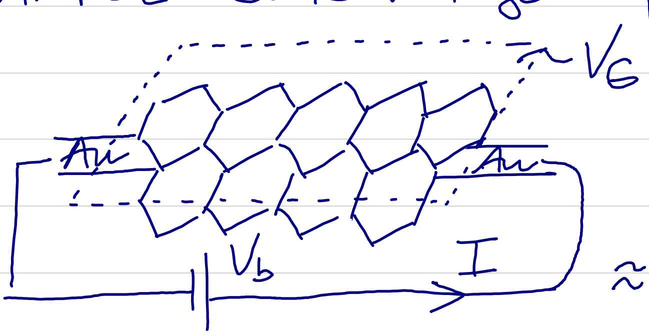
$$= g \cdot \frac{V}{(2\pi)^3} \int_0^{k<k_F} d^3k$$

$g = 2$ for $s=1/2$ of electrons

$$= 2_s \cdot \frac{V}{(2\pi)^3} \cdot \frac{4}{3} k_F^3 \pi = \frac{k_F^3}{3\pi^2} V$$

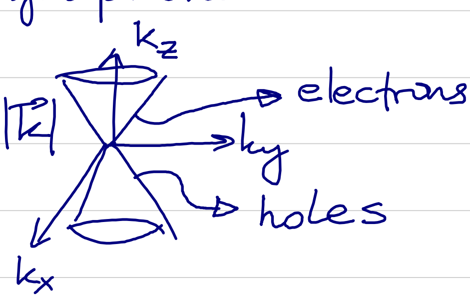
$$k_F = (3\pi^2 n)^{1/3} \Rightarrow \varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

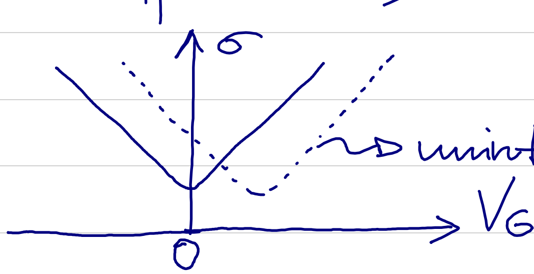
■ EXAMPLE: Gate voltage doping of graphene



$\varepsilon_{\vec{k}} = v_F \hbar |\vec{k}|$

$v_F \approx c/300$



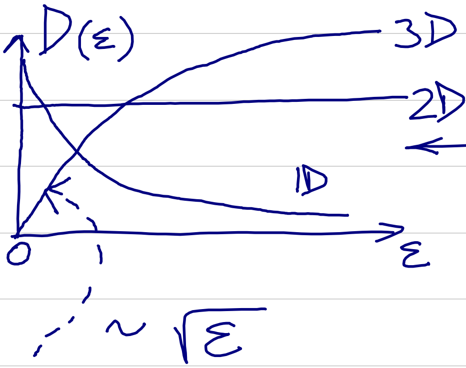


$$G = \frac{I}{V_b} = \sigma \cdot \frac{L_y}{L_x}$$

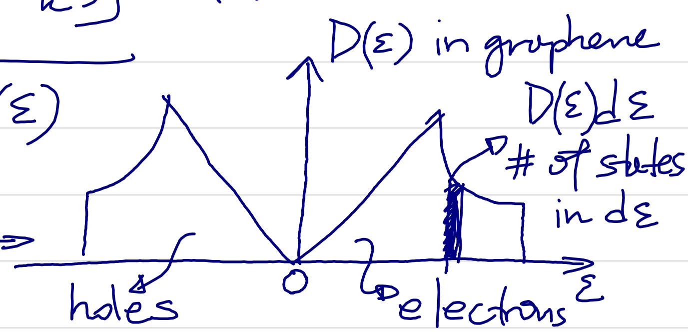
⤳ unintentional doping by impurities

3° Energy integrals via density of states (DOS)

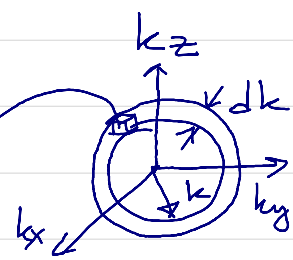
$$\sum_{\vec{k}} A(\varepsilon_{\vec{k}}) = \int_0^\infty d\varepsilon \underbrace{\left[\sum_{\vec{k}} \delta(\varepsilon - \varepsilon_{\vec{k}})\right]}_{D(\varepsilon)} A(\varepsilon)$$



← EXAMPLES →



$$D(\varepsilon)\,d\varepsilon = 2_s\, 4\pi k^2 dk \big/ (2\pi)^3/V$$



if $\varepsilon_{\vec{k}}$ depends on $|\vec{k}|$ only:

use spherical shell — where number of states via two different expressions, along energy axis or in k-space, must be the same

$$D(\varepsilon) = V\frac{k^2}{\pi^2}\left(\frac{d\varepsilon}{dk}\right)^{-1} = V\cdot\frac{k^{\cancel{2}}}{\pi^2}\cdot\frac{m}{\hbar^2 \cancel{k}}$$

$$= V\frac{\sqrt{2}\, m^{3/2}}{\hbar^3 \pi^2}\sqrt{\varepsilon}$$

$\hookrightarrow$ for $\underbrace{\varepsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}}$

$\Rightarrow$ if we change dimensionality of space or energy-momentum dispersion $\varepsilon_{\vec{k}}$, DOS must be recalculated.

$$N = \int_0^{\varepsilon_F} D(\varepsilon)\,d\varepsilon = V\cdot\frac{\sqrt{2}\, m^{3/2}}{\pi^2 \hbar^3}\int_0^{\varepsilon_F}\sqrt{\varepsilon}\,d\varepsilon = V\frac{(2\varepsilon_F m)^{3/2}}{3\pi^2\hbar^3}$$

$$E/N = \frac{\int_0^{\varepsilon_F} \varepsilon D(\varepsilon)\,d\varepsilon}{\int_0^{\varepsilon_F} D(\varepsilon)\,d\varepsilon} = \frac{\int_0^{\varepsilon_F} \varepsilon^{3/2}\,d\varepsilon}{\int_0^{\varepsilon_F} \varepsilon^{1/2}\,d\varepsilon} = \frac{2/5\ \varepsilon_F^{5/2}}{2/3\ \varepsilon_F^{3/2}} = \frac{3}{5}\varepsilon_F$$

4° Landau Fermi liquid justification for treating electrons in metals (or white dwarf stars) as NONINTERACTING quasiparticles

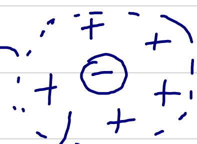
	ε_F (eV)	T_F (10^4 K)
Li	4.7	5.5
Na	3.2	3.8
Al	11.7	13.6
Cu	7	8.2
Ag	5.5	6.4

where is Coulomb interaction ⇒ Landau fermi liquid

a) $D(\varepsilon)\cdot\Delta\varepsilon = n_{\text{quasielectrons}} \ll n$ for $\Delta\varepsilon = k_BT$ or eV_b

so weak short-range interactions

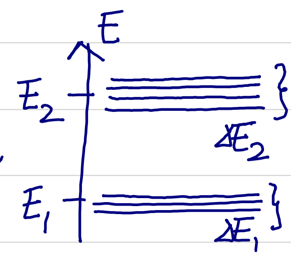
b) Fermi sea screens long-range interactions



Landau quasielectron

exchange-correlation hole surrounding bare electron

complementary explanation



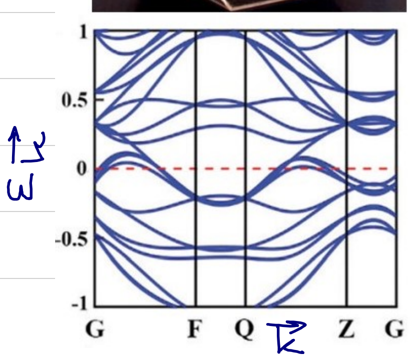
} exact many-body energy levels } of bare electron clusters into quasiparticle levels of finite lifetime

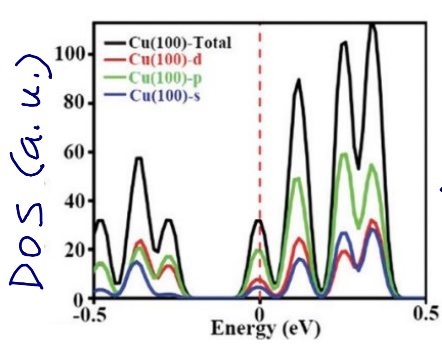
$\tau = \hbar/\Delta E$

Pippard's model of the Fermi surface of copper (P2049)

Colour photograph of Pippard's model of the Fermi surface of copper. Pippard's microwave experiments enabled the three-dimensional Fermi surface of copper to be inferred, the first time this had been done for any material. The Fermi surface lies in momentum space and many of a material's properties are determined by the behaviour of electrons in the vicinity of the surface.

LOCATION: Cavendish Lab at the U. of Cambridge





Phys. Chem. Chem. Phys. **21**, 21341 (2019)

5° Sommerfeld expansion

$$\lim_{z\to\infty} f_m^-(z) = \frac{(\ln z)^m}{m!} \sum_{\alpha=0}^{\text{even}} 2 f_\alpha^-(1) \frac{m!}{(m-\alpha)!} (\ln z)^{-\alpha}$$

Riemann ζ-function

$$= \frac{(\ln z)^m}{m!}\left[1 + \frac{\pi^2}{6}\frac{m(m-1)}{(\ln z)^2} + \frac{7\pi^4}{360}\frac{m(m-1)(m-2)(m-3)}{(\ln z)^4} + \dots\right]$$

modern matematical & physically transparent interpretation

$$f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1} \sim \Theta(\mu-\varepsilon) + \sum_{n=1}^{\infty} \frac{\delta^{[2n-1]}(\mu-\varepsilon)}{2n!}(k_B T)^{2n}(2^{2n}-2) \cdot (-1)^n \pi^{2n} B_{2n}$$

derivatives of δ-function; Bernoulli numbers

$$\sum_{k=0}^{n} B_k \binom{n+1}{k} = 0, \quad \forall n \geq 1, \quad n \in \mathbb{N}$$

$$B_1 = -\frac{1}{2}, \quad B_2 = \frac{1}{6}, \quad B_3 = 0, \quad B_4 = -\frac{1}{30}, \quad B_5 = 0, \quad B_6 = \frac{1}{42}$$

$\Rightarrow$ Sommerfeld expansion is ASYMPTOTIC (divergent) rather than CONVERGENT (Taylor) series

$$f(x) = S_n(x) + R_{n+1}(x), \quad S_N(x) = \sum_{n=0}^{N} a_n x^n$$

C $\to f(x)$, $N \to \infty$, x fixed

A $\to f(x)$, N fixed, $x \to 0$ or ∞

EXAMPLE: error function

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

$$C: \operatorname{erf}(x) \approx \frac{2}{\sqrt{\pi}}\left(x - \frac{1}{3}x^3 + \dots + \frac{(-1)^n}{(2n+1)n!}x^{2n+1} + \dots\right)$$

CONVERGENT for $x \in \mathbb{R}$ but slowly for large x

$$A: \operatorname{erf}(x) \sim 1 - \frac{e^{-x^2}}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^{n+1} \frac{(2n-1)!!}{2^n} \frac{1}{x^{n+1}}$$

$(2n-1)!! = 1 \cdot 3 \cdot \ldots \cdot (2n-1)$; ASYMPTOTIC

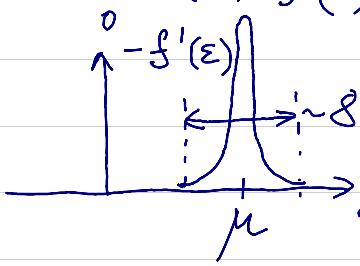
when $x=3$, C needs 31 terms for 10^{-5} accuracy, whereas A needs only 2 terms

$$f_m^-(z) = \frac{1}{(m-1)!}\int_0^\infty \frac{dx\, x^{m-1}}{z^{-1}e^x+1} \xleftarrow{\text{instead of expanding}} \xrightarrow{\text{we can expand DOS}} \int_0^\infty \varphi(\varepsilon)\, f(\varepsilon)\, d\varepsilon$$

based thermal averages

$$f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$$

$$\int_0^\infty \varphi(\varepsilon) f(\varepsilon) d\varepsilon = \overbrace{\Psi(\varepsilon) f(\varepsilon)\Big|_0^\infty}^{\Psi(0)=f(\infty)=0} - \int_0^\infty \Psi(\varepsilon) f'(\varepsilon) d\varepsilon$$



$$\Rightarrow \Psi(\varepsilon) = \int_0^\varepsilon \varphi(\varepsilon')\, d\varepsilon' \quad \text{for smooth } \varphi(\varepsilon')$$

$$\Rightarrow \Psi(\varepsilon) = \underbrace{\sum_{m=0}^\infty \frac{1}{m!}\left(\frac{d^m \Psi}{d\varepsilon^m}\right)_{\varepsilon=\mu} (\varepsilon-\mu)^m}_{\text{Taylor series around } \varepsilon=\mu}$$

$$\int_0^\infty \varphi(\varepsilon) f(\varepsilon) d\varepsilon = -\sum_{m=0}^\infty \frac{1}{m!}\left(\frac{d^m \Psi}{d\varepsilon^m}\right)_{\varepsilon=\mu} \int_0^\infty (\varepsilon-\mu)^m f'(\varepsilon) d\varepsilon$$

$$\int_0^\infty (\varepsilon-\mu)^m f'(\varepsilon) d\varepsilon = -\int_0^\infty (\varepsilon-\mu)^m \frac{\beta e^{\beta(\varepsilon-\mu)}}{[e^{\beta(\varepsilon-\mu)}+1]^2} \qquad x = \beta(\varepsilon-\mu)$$

$$= -\beta^{-m}\int_{-\beta\mu}^\infty dx \frac{e^x}{(e^x+1)^2} x^m$$

$\int_{-\beta\mu}^\infty \mapsto \int_{-\infty}^\infty$ because $\beta\mu \gg 1$ and integrand has sharp peak around $x=0$

$$= -(k_B T)^m I_m$$

$$I_m = \int_{-\infty}^{\infty} \frac{e^x x^m}{(e^x+1)^2}\,dx \qquad \underbrace{\frac{e^x}{(e^x+1)^2} = \frac{1}{(e^x+1)(e^{-x}+1)} \text{ is even under } x \mapsto -x}_{\Leftrightarrow\, I_m \equiv 0 \text{ for } m = 2p+1}$$

$$I_0 = \int_{-\infty}^{\infty} \frac{e^x}{(e^x+1)^2}\,dx = -\frac{1}{e^x+1}\Big|_{-\infty}^{\infty} = 1 \,, \quad I_2 = \pi^2/3$$

$$\boxed{\int_0^{\infty} \varphi(\varepsilon) f(\varepsilon)\,d\varepsilon \approx \int_0^{\mu} \varphi(\varepsilon)\,d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 \left(\frac{d\varphi}{d\varepsilon}\right)_{\varepsilon=\mu} + \dots}$$

■ APPLICATIONS: $\mu(T)$, $E(T)$, $C_V(T)$, $p(T)$ for electrons with $\varepsilon_k = \hbar^2 k^2/2m$

i) $$N = \int_0^{\mu} D(\varepsilon)\,d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 \left(\frac{dD}{d\varepsilon}\right)_{\varepsilon=\mu} + \dots$$

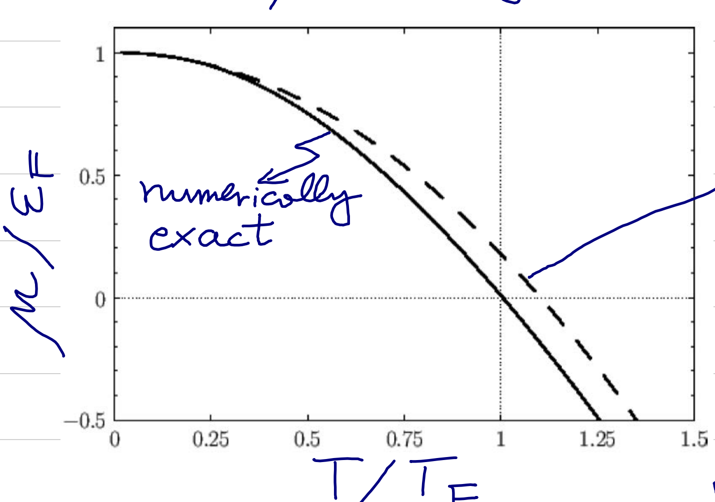
$$\int_0^{\mu} D(\varepsilon)\,d\varepsilon = \frac{V}{3\pi^2}\frac{(2m)^{3/2}}{\hbar^3}\mu^{3/2}$$

$$(dD/d\varepsilon)_{\varepsilon=\mu} = \frac{V}{(4\pi)^2}\frac{(2m)^{3/2}}{\hbar^3}\mu^{-1/2}$$

$$N \approx \frac{V}{3\pi^2}\frac{(2m)^{3/2}}{\hbar^3}\mu^{3/2} + \frac{V}{24}\frac{(2m)^{3/2}}{\hbar^3}(k_B T)^2 \mu^{-1/2}$$

$$\varepsilon_F^{3/2} \approx \mu^{3/2} + \frac{\pi^2}{8}(k_B T)^2 \mu^{-1/2} \Rightarrow \mu \approx \varepsilon_F\left[1 + \frac{\pi^2}{8}\left(\frac{k_B T}{\varepsilon_F}\right)^2\right]^{-2/3}$$

$$\approx \varepsilon_F\left[1 - \frac{\pi^2}{12}\underbrace{\left(\frac{k_B T}{\varepsilon_F}\right)^2}\right]$$



$k_B T/\varepsilon_F$ is natural dimensionless expansion parameter

$T_F = \varepsilon_F/k_B$

ii) $$E(T) = \int_0^{\mu} \varepsilon D(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 \left[\frac{d(\varepsilon D)}{d\varepsilon}\right]_{\varepsilon=\mu} + \dots$$

$$\int_0^{\mu} \varepsilon D(\varepsilon)\, d\varepsilon = \frac{V}{5\pi^2} \frac{(2m)^{3/2}}{\hbar^3} \mu^{5/2}$$

$$\left[\frac{d\varepsilon D}{d\varepsilon}\right]_{\varepsilon=\mu} = \frac{3V}{4\pi^2} \frac{(2m)^{3/2}}{\hbar^3} \mu^{1/2}$$

$$E \approx \frac{V}{5\pi^2} \frac{(2m)^{3/2}}{\hbar^3} \mu^{5/2} + \frac{V}{8} \frac{(2m)^{3/2}}{\hbar^3} (k_B T)^2 \mu^{1/2}$$

$$= \frac{3}{5} N \varepsilon_F \left[\left(\frac{\mu}{\varepsilon_F}\right)^{5/2} + \frac{5\pi^2}{24}\left(\frac{k_B T}{\varepsilon_F}\right)^2 \left(\frac{\mu}{\varepsilon_F}\right)^{1/2}\right]$$

$$= \underbrace{\frac{3}{5} N \varepsilon_F}_{E(T=0)} + \frac{\pi^2}{4} N \varepsilon_F \left(\frac{k_B T}{\varepsilon_F}\right)^2$$

iii) $$C_V(T) = \frac{dE(T)}{dT} = \frac{\pi^2}{2} k_B N \frac{k_B T}{\varepsilon_F} = \frac{\pi^2}{2} k_B N \frac{T}{T_F}$$

$\Delta E \propto k_B T N\, T/T_F \Rightarrow C_V = \frac{d\Delta E}{dt} \propto k_B N\, T/T_F$

INTUITIVE interpretation recovers $\propto T$ linear dependence
so, the role of rigorous theory is just to compute
the prefactor of order 10^0

iv) $$p = \frac{2}{3}\frac{E}{V} = \underbrace{\frac{2}{5} n \varepsilon_F}_{p(T=0)} + \underbrace{\frac{\pi^2}{6} n \varepsilon_F \left(\frac{k_B T}{\varepsilon_F}\right)^2}$$