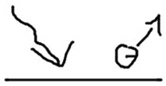
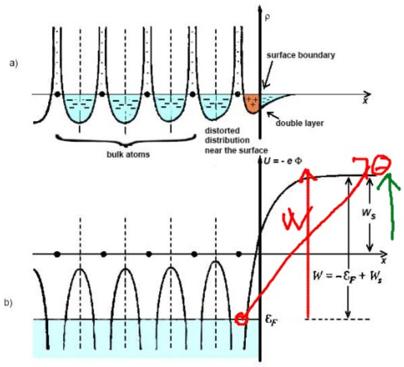
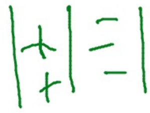
Solid State Physics

Work function



$$h\nu = W + \frac{1}{2} m v^2$$





$$W = W_s - \varepsilon_F = W_s + |\varepsilon_F|$$
$$(\varepsilon_F < 0)$$

Thermionic emission

if T large $k_B T$ is large too

$$\underset{\substack{\uparrow \\ \text{e.g. } \sqrt{\langle v^2 \rangle}}}{j = -e \cdot n \langle \underline{v} \rangle} \qquad v = \frac{\hbar k}{m_e} \rightarrow v = \underline{v}(\underline{k})$$

$$\langle \underline{v}(\underline{k}) \rangle = ?$$

In general:

probability density

$$\langle O(\underline{k}) \rangle = \frac{1}{n} \cdot \frac{1}{V} \sum_{\underline{k}} f(\underline{k}) O(\underline{k})$$

$$\Delta k \ll 1 \Rightarrow \langle O(k) \rangle = \int \dots d^3k$$ – how the integral looks like?

$$d^3k = \lim_{\Delta k \to 0} \Delta^3 k = \lim (\Delta k_x \Delta k_y \Delta k_z)$$

$$\Delta k_x \Delta k_y \Delta k_z = \left(\frac{2\pi}{L}\right) \cdot \left(\frac{2\pi}{L}\right) \cdot \left(\frac{2\pi}{L}\right) = \frac{8\pi^3}{V}$$

so $\underline{\Delta k_x \Delta k_y \Delta k_z \frac{8\pi^3}{V} = 1}$

$$\lim_{\Delta k \to 0} \frac{1}{n} \frac{1}{V} \sum_{\underline{k}} f(\underline{k}) O(\underline{k}) \cdot \underbrace{\Delta^3 k \cdot \frac{V}{8\pi^3}}_{1} = \frac{1}{8\pi^3} \int f(\underline{k}) O(\underline{k}) \, d^3k \cdot \frac{1}{n}$$

Let $O(\underline{k}) := \underline{v}(\underline{k}) \Rightarrow$

$$\langle \underline{v}(\underline{k}) \rangle = \frac{1}{n} \cdot \frac{1}{8\pi^3} \int f(\underline{k}) v(\underline{k}) \, d^3k$$

so $\quad \underline{j} = -e \cdot n \langle \underline{v}(\underline{k}) \rangle = -e \cdot \cancel{n} \frac{1}{\cancel{n}} \frac{1}{8\pi^3} \int f(\underline{k})\, \underline{v}(\underline{k})\, d^3k$

electrons $\quad \uparrow\downarrow \quad \Rightarrow f(k) = 2 \cdot f_{F-D}(k)\,, \quad f_{F-D}(\underline{k}) = \dfrac{1}{e^{(\mathcal{E}(\underline{k}) - \mathcal{E}_F)/k_BT} + 1}$

$$\underline{j} = -\frac{2e}{8\pi^3} \int f_{F-D}(\underline{k})\, \underline{v}(\underline{k})\, d^3\underline{k} = -\frac{1}{4\pi^3} \int \frac{\underline{v}(k)}{e^{(\mathcal{E}(k) - \mathcal{E}_F)/k_BT} + 1} d^3k$$

$$\mathcal{E}(\underline{k}) := \mathcal{E}_{tot} = \mathcal{E}_F + W + \frac{1}{2} m v_x^2(\underline{k}) = \mathcal{E}_F + W + \frac{\hbar^2 k^2}{2 m_e}$$

$$\underline{j} = -\frac{1}{4\pi^3} \int \frac{\underline{v}(k)}{e^{\left(W + \frac{\hbar^2 k^2}{2m_e}\right)/k_BT} + 1} d^3k$$

at $T = 300K \qquad 2m_e \cdot \underbrace{k_BT}_{0.0258\,eV} = 7.5 \cdot 10^{-51}\, kg\, J\,, \quad \dfrac{\hbar^2}{2m_e k_BT} = 1.4 \cdot 10^{-18}\, m^2$

$$k \sim k_F = \frac{2\pi}{\lambda_F} \approx \frac{2\pi}{0.1\,nm} = 6.2 \cdot 10^{10} \frac{1}{m} \Rightarrow \frac{\hbar^2 k^2}{2m_e k_BT} \simeq 5.6 \cdot 10^3 >> 1$$

$$- \qquad e^{\left(W + \frac{\hbar^2 k^2}{2m_e}\right)/k_BT} >> 1 \Rightarrow \frac{1}{e^{(\;)} + 1} \simeq e^{-(\;)}$$

$$\boxed{f(\underline{k}) = e^{-\left(W + \frac{\hbar^2 k^2}{2m_e}\right)/k_BT}}$$

in 1D

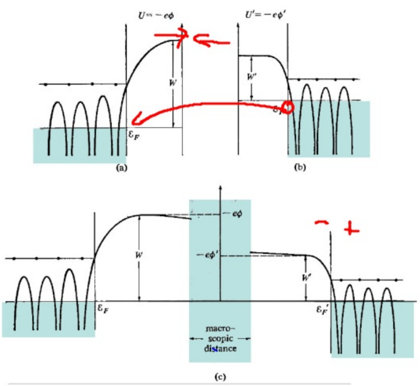
$$j_x = -\frac{4\pi m_e e}{\hbar^3} (k_BT)^2 e^{-W/k_BT}$$

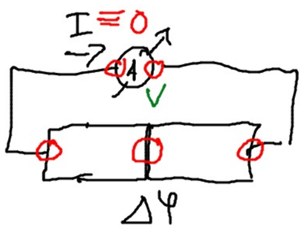
Richardson-Dushman formula

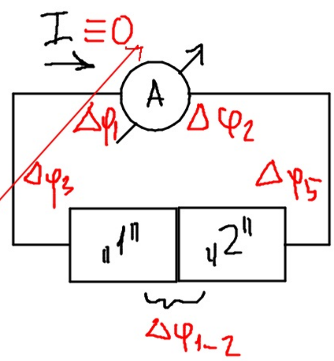
Contact potential

$W - W' = e(\varphi - \varphi') = e\underbrace{\Delta\varphi}_{\text{Voltage}}$

$\uparrow$ potential

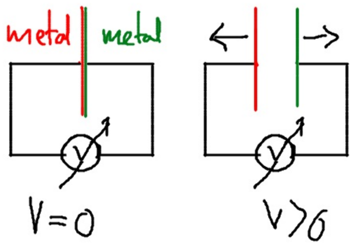


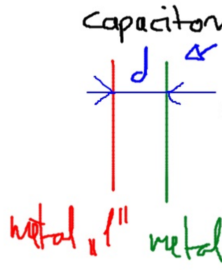




$\Sigma \Delta\varphi = 0$

How to measure





$$C = \frac{\Delta Q}{\Delta U} \Rightarrow \Delta U = \frac{1}{C}\overset{\text{created by } \Delta\varphi}{\Delta Q}$$

$$= \frac{d}{\varepsilon_0 A}\Delta Q$$

$$C = \varepsilon_0 \frac{A}{d} \qquad \frac{\Delta Q}{C} = \Delta U$$

$$V(t) = f(\Delta\varphi)$$

Quantum Mechanics of electrons in a metal

N ion cores + K conduction (Sommerfeld: „free") electrons

$$\hat{H} = \hat{H}_{\text{ion-ion}} + \hat{H}_{\text{ion-electron}} + \hat{H}_{\text{electron-electron}}$$

$$\hat{H}_{\text{ion-ion}} \quad \sum_{j=0}^{N} \frac{P_j^2}{2M_{\text{ion}}} + V_{\text{ion-ion}}(\underline{R}_1, \underline{R}_2, \ldots \underline{R}_N) \qquad \sim 10^{26}$$

$$\hat{H}_{\text{electron}} = \sum_{j=0}^{K} \frac{p_j^2}{2m_e} + V(\underline{r}_1, \underline{r}_2, \ldots, \underline{r}_K) \qquad \sim -\|-$$

$$\hat{H}_{i-e} = V_{i-e}(\underline{R}_1, \underline{R}_2, \ldots, R_N, \underline{r}_1, \underline{r}_2, \ldots \underline{r}_K) \qquad \sim 10^{26}$$

$$V_{\text{ion}}(\underset{\uparrow \text{ equilibrium position}}{\underline{R}_1^{(0)}}, \underline{R}_2^{(0)}, \ldots \underline{R}_N^{(0)}) = 0$$

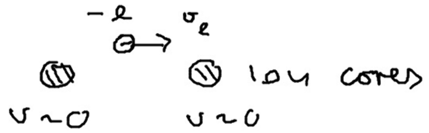
$m_e = 9.1 \cdot 10^{-31}\,\text{kg} \qquad M_{\text{ion}} = (2000 - 20000) \times m_e$

$$\varepsilon_{\text{thermal}} \cong k_B T / \text{particle} \begin{cases} \to \frac{1}{2} m_e v_e^2 \\ \to \frac{1}{2} M_I v_i^2 \end{cases} \Rightarrow v_e \gg v_i$$

Adiabatic principle:

ions: „These young electrons just whizzing around. I can't follow them!"

electrons: „These heavy old ion cores do not move around much."



How to "solve" these 3×10^{26} coupled equations?

$$\hat{H} \approx \hat{H}_e' + \hat{H}_i' \quad \leftarrow \text{adiabatic separation}$$

$\hat{H}_e'$ – electrons in static, periodic potential from ion cores + potential from other electrons

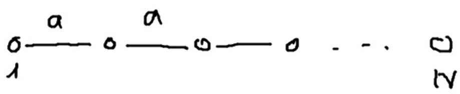
$\hat{H}_i'$ – averaged potential from electrons

$$V_{i-e}(\underline{R}_1, \dots \underline{R}_N, \underline{r}_1 \dots r_K) = \sum_{j=0}^{K} V(\underline{r}_j)$$

Iterative process

a.k.a – Hartree-Fock method or
– self-consistent successive approximation

(1.) 1 electron Schrödinger eq $\quad V_{\text{electron}}$
Ψ $\quad$ ⮤ periodic pot. ~~inside~~ the metal



periodic boundary condition
$$V(R_N + a) = V(R_1)$$
If true: everything is inside

(2) $\rho_e(\underline{r}_1 \dots r_K) \simeq |\Psi|^2 \cdot (-e)$

$\Downarrow$

(3) $V_j(\underline{r})$.

(4) $V_{\text{ion}} + \sum V_j \Rightarrow V_{\text{ion}}'$

(5) 1 electron Schrödinger equation $\Rightarrow \Psi'$

(6) compare Ψ w. Ψ'.
when $\Psi \approx \Psi'$ stop $\Rightarrow$ consistent w. itself

Input

$\overset{e}{\ominus}$ $\overset{e}{\ominus}$ e-e, e-i interactions

$\Psi(\underline{r}_1, \dots, \underline{r}_K)$

interacting electrons

↑

particle ⇒ wave function (state)

„bare" electrons

output

linear combination of one electron wave functions

$\Psi(\underline{r})$

non-interacting electrons

wave function => particle

„clothed"- Bloch - electrons

↑

electron gas

Bloch - electrons : one - electron wave functions in lattice periodic potential

$$\hat{H} = \sum_{j=0}^{K} \hat{H}_0(p_j, \underline{r}_j) \qquad \hat{H}_0 = \frac{\hat{p}^2}{2m_e} + \hat{V}(\underline{r})$$

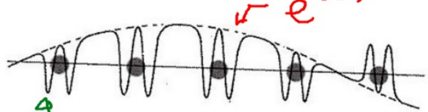
periodicity : $V(\underline{r} + \underline{R}) = V(\underline{r})$

1D

$$\boxed{\psi(x) = u_k(x) e^{ikx}}$$ Bloch function

$u_k(x + n \cdot a) = u_k(x)$

$\int |u(x)|^2 dx = 1$



why can't a Bloch-electron travel to the outside of the crystal?

$k \approx k_F$ $\quad v \sim 10^5 - 10^7 \, m/s$

$\Delta t = \frac{1mm}{10^7 \frac{m}{s}} = 10^{-10} s$!