Hullámcsomag

Szabad elektron

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \varepsilon\psi \qquad \hat{\mathbf{p}} = \frac{\hbar}{i}\nabla \qquad \psi(\mathbf{r}) = \frac{1}{\sqrt{V}}e^{i\mathbf{kr}}$$

energia

$$\boxed{\varepsilon(\mathbf{k}) = \frac{\hbar^2\mathbf{k}^2}{2m}}$$

impulzus

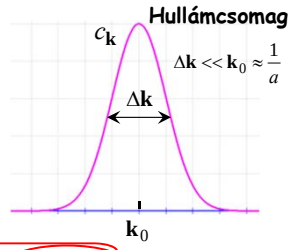
$$\boxed{\mathbf{p} = \hbar\mathbf{k}} \longrightarrow \mathbf{F} = \hbar\dot{\mathbf{k}}$$

közbenső számolás

$$\frac{1}{\hbar}\left(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}_0}\right)t = (\mathbf{k}-\mathbf{k}_0)\frac{1}{\hbar}\frac{\partial\varepsilon_{\mathbf{k}}}{\partial\mathbf{k}}\bigg|_{\mathbf{k}_0} t = (\mathbf{k}-\mathbf{k}_0)\mathbf{v}_{\mathbf{k}_0}t$$

Kváziklasszikus dinamika

$$\psi(\mathbf{r},t) = \mathrm{u}_{\mathbf{k}_0}(\mathbf{r})\sum_{\mathbf{k}} c_{\mathbf{k}}\left(\frac{1}{\sqrt{V}}e^{i\mathbf{kr}}\right)e^{-\frac{i}{\hbar}\varepsilon_{\mathbf{k}}t}$$

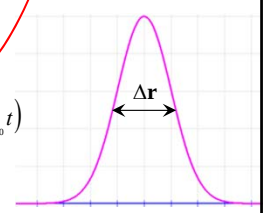


Heisenberg: $\Delta\mathbf{r}\,\Delta\mathbf{p} \approx \hbar^{-1}$

$\Delta\mathbf{r}\,\Delta\mathbf{k} \approx 1 \rightarrow \Delta\mathbf{r} >> a$

$$\psi(\mathbf{r},t) = \frac{1}{\sqrt{V}}e^{i\mathbf{k}_0\mathbf{r}}e^{-\frac{i}{\hbar}\varepsilon_{\mathbf{k}_0}t}\underbrace{\mathrm{u}_{\mathbf{k}_0}\sum_{\mathbf{k}} c_{\mathbf{k}}\; e^{i(\mathbf{k}-\mathbf{k}_0)\mathbf{r}}e^{-\frac{i}{\hbar}\left(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}_0}\right)t}}_{f(\mathbf{r},t)}$$

$$= \frac{1}{\sqrt{V}}e^{i\mathbf{k}_0\mathbf{r}}e^{-\frac{i}{\hbar}\varepsilon_{\mathbf{k}_0}t}\mathrm{u}_{\mathbf{k}_0}\sum_{\mathbf{k}} c_{\mathbf{k}}\; e^{i(\mathbf{k}-\mathbf{k}_0)(\mathbf{r}-\mathbf{v}_{\mathbf{k}_0}t)} = \frac{1}{\sqrt{V}}e^{i\mathbf{k}_0\mathbf{r}}e^{-\frac{i}{\hbar}\varepsilon_{\mathbf{k}_0}t}f\left(\mathbf{r}-\mathbf{v}_{\mathbf{k}_0}t\right)$$



Időbeli szétfolyás: $\boxed{\Delta\mathbf{r}(t) \approx \Delta\mathbf{v}\,t \approx \frac{1}{m}\hbar\Delta\mathbf{k}\,t}$

Szabad elektron

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{V}}e^{i\mathbf{kr}}$$

energia

$$\boxed{\varepsilon(\mathbf{k}) = \frac{\hbar^2\mathbf{k}^2}{2m}}$$

impulzus

$$\boxed{\mathbf{p} = \hbar\mathbf{k}} \longrightarrow \boxed{\mathbf{F} = \hbar\frac{d\mathbf{k}}{dt}}$$

Sáv elektron

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}}u_{n\mathbf{k}}(\mathbf{r})$$

Csoportsebesség: $\boxed{\mathbf{v} = \frac{1}{\hbar}\frac{\partial\varepsilon_{n\mathbf{k}}}{\partial\mathbf{k}}}$

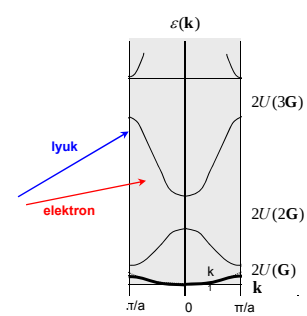
Külső tértől nyert energia:

$$\delta\varepsilon = \mathbf{F}\delta\mathbf{s} = \mathbf{F}\mathbf{v}dt$$

$$\delta\varepsilon = \frac{d\varepsilon}{d\mathbf{k}}\delta\mathbf{k} = \hbar\mathbf{v}\delta\mathbf{k} \longrightarrow \boxed{\mathbf{F} = \hbar\frac{d\mathbf{k}}{dt}}$$

$$\frac{d\mathbf{v}}{dt} = \frac{1}{\hbar}\frac{\partial^2\varepsilon_{n\mathbf{k}}}{\partial\mathbf{k}\partial t} = \frac{1}{\hbar}\frac{\partial^2\varepsilon_{n\mathbf{k}}}{\partial\mathbf{k}^2}\frac{\partial\mathbf{k}}{\partial t} = \frac{1}{\hbar^2}\frac{\partial^2\varepsilon_{n\mathbf{k}}}{\partial\mathbf{k}^2}\mathbf{F} \qquad \boxed{\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial\mathbf{k}^2}}$$

$$m^{-1} = \frac{1}{\hbar^2}\frac{d^2\varepsilon}{dk^2}$$



$$\underline{\underline{\mathbf{m}}}^{-1} = \frac{1}{\hbar^2}\begin{pmatrix} \frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial^2 k_x} & \frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_x\partial k_y} & \frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_x\partial k_z} \\ \frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_y\partial k_x} & \frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial^2 k_y} & \frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_y\partial k_z} \\ \frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_z\partial k_x} & \frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_z\partial k_y} & \frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial^2 k_z} \end{pmatrix}$$

effektív tömeg tenzor

Szabad elektron

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{kr}}$$

energia

$$\varepsilon(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m}$$

impulzus

$$\mathbf{p} = \hbar\mathbf{k} \longrightarrow \mathbf{F} = \hbar\frac{d\mathbf{k}}{dt}$$

Mozgás külső mágneses térben

$$\mathbf{F} = -e\mathbf{v}\times\mathbf{B}$$

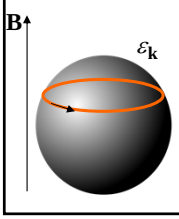
$$\frac{d\mathrm{k}}{dt} = \frac{e\mathrm{B}}{\hbar}\mathrm{v}_\perp$$

$$\frac{d\mathrm{k}}{dt} = \frac{e\mathrm{B}}{m}\mathrm{k}$$

$$e\mathrm{B}\frac{d\mathbf{r}}{dt} = m\frac{d^2\mathbf{r}}{dt^2}$$

$$e\mathrm{B}\,\mathrm{r}\omega = \mathrm{m}\mathrm{r}\omega^2$$

$$\omega = \frac{e\mathrm{B}}{m}$$



A periódusidő független k_z-től

Sáv elektron

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}} u_{n\mathbf{k}}(\mathbf{r})$$

$$\mathbf{v} = \frac{1}{\hbar}\frac{\partial\varepsilon_{n\mathbf{k}}}{\partial\mathbf{k}}$$

$$\mathbf{F} = -e\mathbf{v}_{n\mathbf{k}}\times\mathbf{B}$$

$$\mathbf{F} = \hbar\frac{d\mathbf{k}}{dt}$$

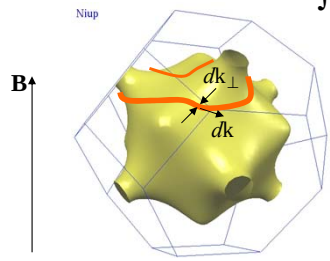
$$\frac{d\varepsilon_{\mathbf{k}}}{dt} = \frac{1}{\hbar}\frac{\partial\varepsilon_{\mathbf{k}}}{\partial\mathbf{k}}\hbar\frac{d\mathbf{k}}{dt} = -e\mathbf{v}_{n\mathbf{k}}(\mathbf{v}_{n\mathbf{k}}\times\mathbf{B}) = 0$$

A mágneses térben a Bloch-elektron is állandó energiájú állapotban marad

A periódusidő

$$dt = \frac{\hbar}{e\mathrm{B}}\frac{d\mathrm{k}}{\mathrm{v}_\perp} \qquad T = \frac{\hbar^2}{e\mathrm{B}}\oint\frac{d\mathrm{k}}{\hbar\mathrm{v}_\perp}$$

$$d\mathrm{A} = \oint d\mathrm{k}\, d\mathrm{k}_\perp = \oint d\mathrm{k}\frac{d\varepsilon}{\hbar\mathrm{v}_\perp}$$



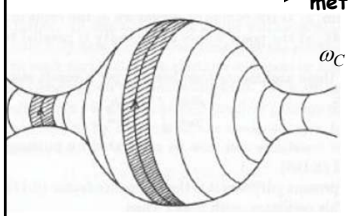
$$T = \frac{\hbar^2}{e\mathrm{B}}\frac{\partial\mathrm{A}}{\partial\varepsilon}$$

$$\omega_C = \frac{e\mathrm{B}}{\hbar^2}2\pi\left(\frac{\partial\mathrm{A}}{\partial\varepsilon}\right)^{-1}$$

$$m_C = \frac{\hbar^2}{2\pi}\frac{\partial\mathrm{A}}{\partial\varepsilon}\bigg|_{\mathrm{k}_z}$$

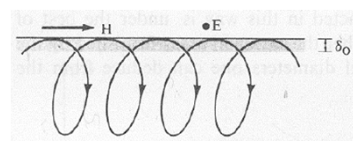
Ciklotronrezonancia

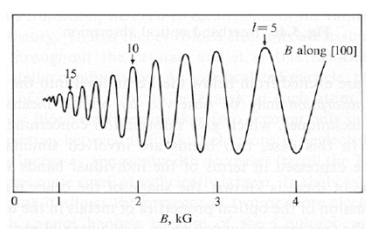
Azbel-Kaner rezonancia (fémek)



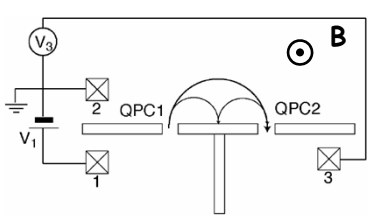
Exrémális Fermi felület metszetek mérése

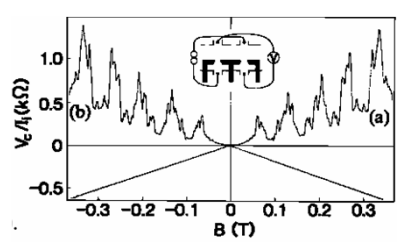
$$\omega_C = \frac{e\mathrm{B}}{\hbar^2}2\pi\left(\frac{\partial\mathrm{A}}{\partial\varepsilon}\right)^{-1}\bigg|_{\mathrm{k}_z}$$





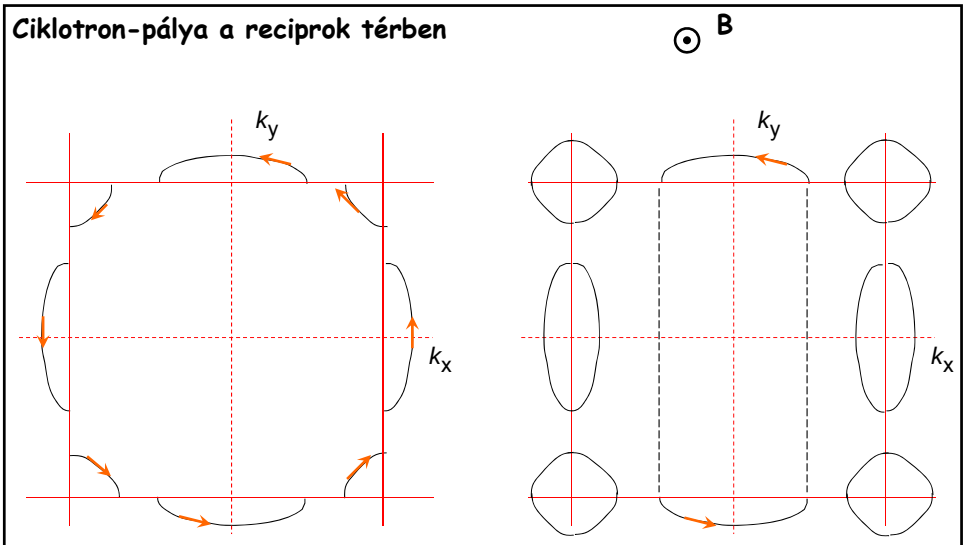
Ciklotronpálya közvetlen kimutatása 2dimenziós elektronrendszerben



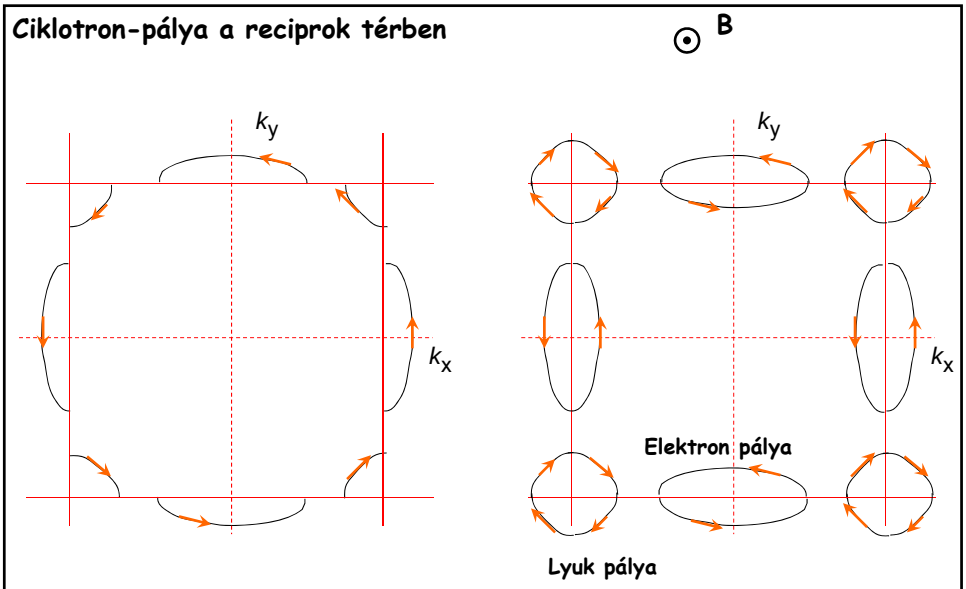


H.Van Houten *et al.*, Phys. Rev. B **39**, 8556 (1989)

Ciklotron-pálya a reciprok térben

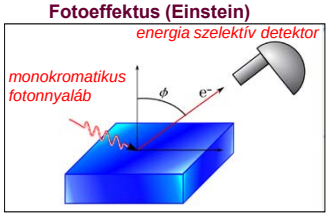


Ciklotron-pálya a reciprok térben



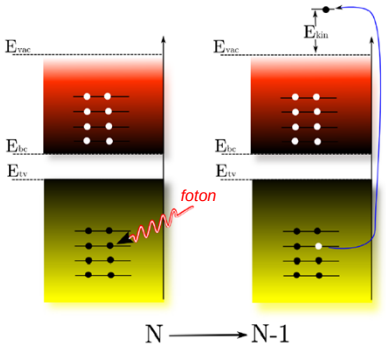
Fotoemissziós spektroszkópia (PES)

Fotoeffektus (Einstein)

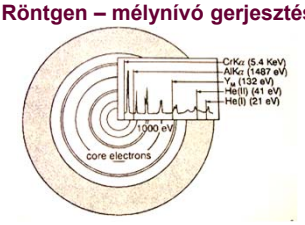


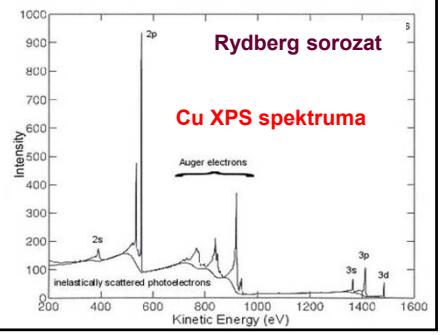
$$h\nu = \varepsilon_{\text{kötési}} + e\Phi_{\text{kilépési}} + \varepsilon_{\text{kinetikus}}$$

$$\varepsilon_{\text{Fermi}} - \varepsilon \qquad \varepsilon_{\text{vákuum}} - \varepsilon_{\text{Fermi}}$$

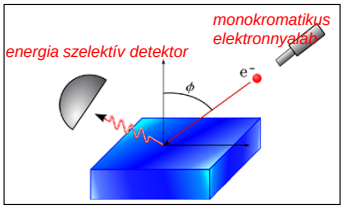


XPS: Röntgen – mélynívó gerjesztések



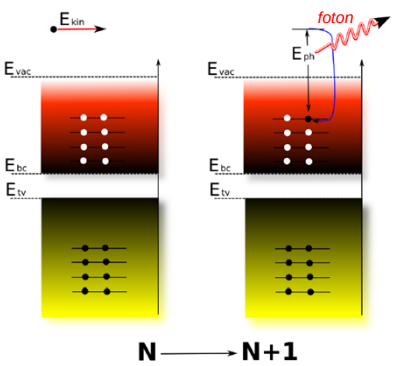


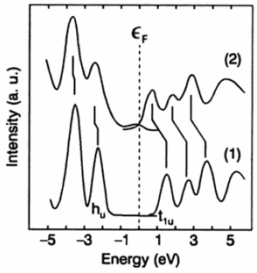
Inverz fotoemissziós spektroszkópia (IPES)



$$h\nu = \varepsilon_{\text{kötési}} + e\Phi_{\text{kilépési}} + \varepsilon_{\text{kinetikus}}$$

$$\varepsilon_{\text{Fermi}} - \varepsilon \qquad \varepsilon_{\text{vákuum}} - \varepsilon_{\text{Fermi}}$$





← K_3C_{60} fémes

(más a rácsállandójuk)

← Fullerén (C_{60}) FCC kristály szigetelő

PES és IPES is felületi állapotokat néz, vizsgálati mélység: - PES: min{ foton behatolási mélység, elektron szökési hossz}
- IPES: min{ elektron behatolási mélység, foton szökési hossz }

UPS : UV foton – valencia sávból (Fermi energia közeli) gerjesztések

Félvezetők valencia sávja

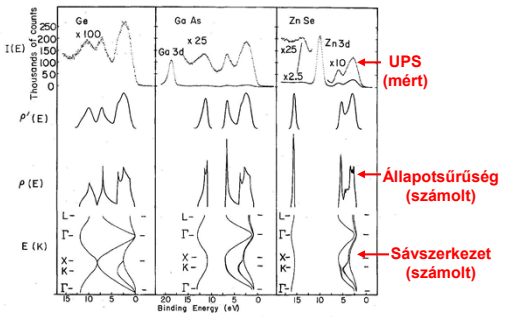


FIG. 1. X-ray photoemission spectra, band structures, and densities of states of Ge, GaAs, and ZnSe. The top row $I(E)$ shows the uncorrected experimental spectra. At the bottom the corresponding band structures $E(k)$ and densities of states $\rho(E)$ as derived from EPM calculations are shown. The broadened theoretical densities of states $\rho'(E)$ in the second row facilitate comparison with experiment.

- Zérus állapotsűrűség a Fermi energiánál ⇔ tiltott sáv

Fémes elektronok egyszerű fémekben

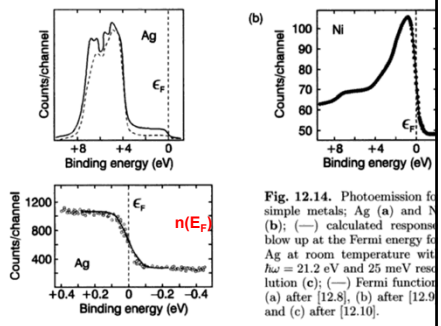


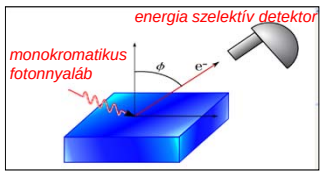
Fig. 12.14. Photoemission fo simple metals; Ag (a) and N (b); (—) calculated response blow up at the Fermi energy fo Ag at room temperature wit $\hbar\omega = 21.2$ eV and 25 meV reso lution (c); (—) Fermi function (a) after [12.8], (b) after [12.9 and (c) after [12.10].

- Véges állapotsűrűség a Fermi energiánál
- T>0 esetén $E>E_F$ állapotok is be lehetnek töltve

UPS : jobb energia felbontás, kisebb behatolási mélység

XPS : gyengébb energia felbontás, nagyobb behatolási mélység

Szögfelbontásos fotoemissziós spektroszkópia (ARPES)



$$\hbar\omega = \varepsilon_{kötési} + e\phi_{kilépési} + \varepsilon_{kin}$$

$$\boldsymbol{k}_i^{\parallel} = \boldsymbol{k}_f^{\parallel} + \boldsymbol{G}^{\parallel}$$

(impulzusmegmaradás a minta síkjában)

$$|\boldsymbol{k}_f^{\parallel}| = \frac{(2m_e\varepsilon_{kin})^{1/2}}{\hbar}\sin\theta$$

2 dimenziós metszetek

⇓

ε = ε(k∥)

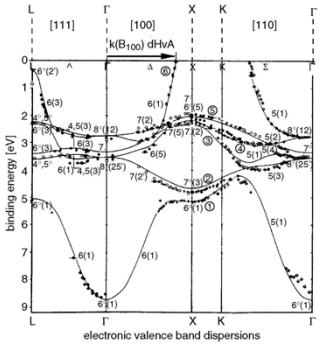
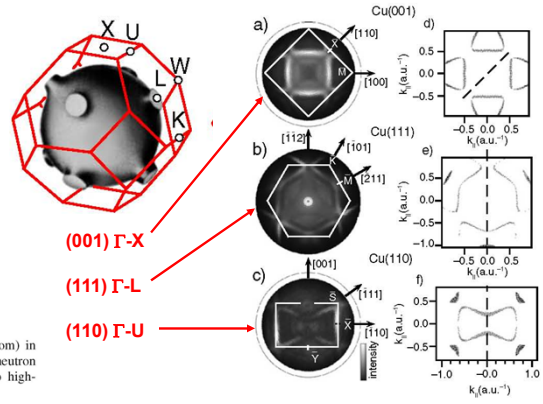



Figure 10. Dispersion relations for phonons (top) and electrons (bottom) in copper [54]–[56]. The phonon dispersion has been determined by neutron scattering, the electronic dispersion by ARUPS. The capitals refer to high-symmetry points in the Brillouin zone (see [2]).