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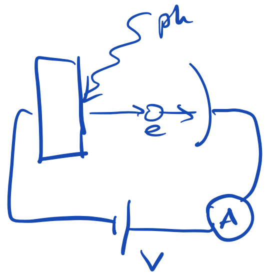
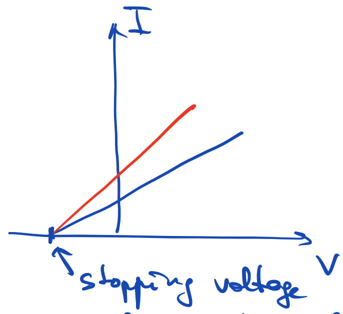
4.3. Elementary theory of photoelectric effect and the fermion spectral function.

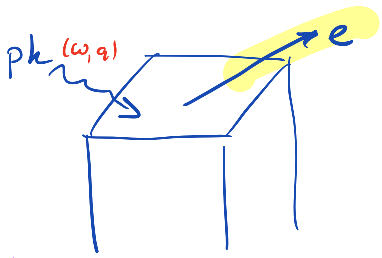


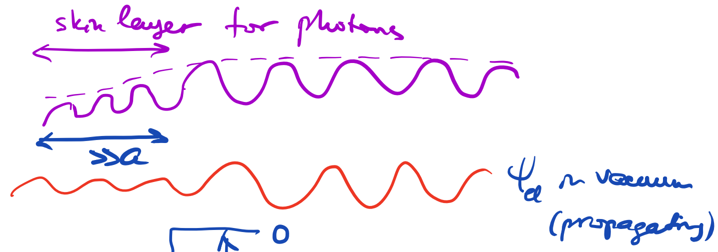


indep. of the light intensity, but depends on $\hbar\omega$

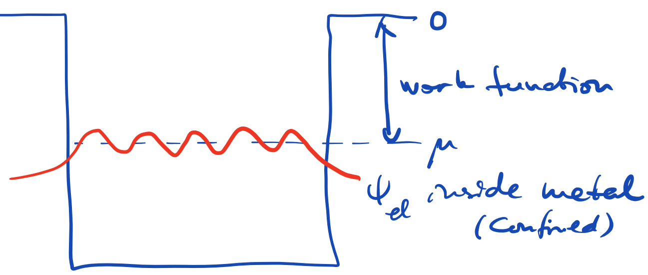
Lenard 1902

ARPES – is a descendant of Lenard's 1902 experiments. Allows to gain info about electron states inside a metal.





We will develop a grossly simplified description, which roughly corresponds to step 1 of so-called 3-step ARPES theory



$$\hat{\Psi}^{+}(\vec{r}) = \underbrace{\sum \psi_i^* a_i^+}_{\substack{\text{confined} \\ \hat{\psi}^+(r)}} + \underbrace{\sum \varphi_k^* a_k^+}_{\substack{\text{propagating} \\ \hat{\varphi}^+(r)}} \equiv \hat{\psi}^+(r) + \hat{\varphi}^+(r)$$

Photon with momentum $\hbar\vec{q}$ creation operator : $\hat{d}^+_{\vec{q}}$

Model Hamiltonian:

$$\mathcal{H} = \underbrace{\mathcal{H}_e}_{\substack{\text{confined} \\ \text{electrons}}} + \underbrace{\sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} \hat{a}^+_{\vec{k}} \hat{a}_{\vec{k}}}_{\text{propagating electrons}} + \sum_{\vec{q}} \hbar\omega_{\vec{q}} \hat{d}^+_{\vec{q}} \hat{d}_{\vec{q}}$$

(may interact with each other!)

$$+ \left(\lambda \sum_{\vec{q}} \int d\vec{r}\, \hat{\varphi}^+(\vec{r})\, \hat{\psi}(\vec{r})\, e^{i\vec{q}\vec{r}} \hat{d}_{\vec{q}} + \text{h.c.} \right)$$

comes from interaction of electrons with light

Motivation:

Electrons in a time-periodic potential: $\mathcal{H} = \int d\vec{r}\, U(\vec{r},t)\,\hat{n}(\vec{r})$

$$\hat{n}(\vec{r}) = \hat{\Psi}^+(\vec{r})\hat{\Psi}(\vec{r}) = \underbrace{\hat{\varphi}^+(\vec{r})\hat{\varphi}(\vec{r}) + \hat{\varphi}^+(\vec{r})\hat{\psi}(\vec{r})} + \hat{\psi}^+(\vec{r})\hat{\psi}(\vec{r}) + \hat{\psi}^+(\vec{r})\hat{\varphi}(\vec{r})$$

$U(\vec{r},t) \to$ Quantized EM field; $\hat{U}(\vec{r},t) \sim \sum_q e^{i\vec{q}\vec{r}}\hat{d}_{\vec{q}} + h.c.$

The initial state $\qquad |\vec{q}\rangle = d^+_{\vec{q}}|0\rangle$

$$\underbrace{\hat{\rho}}_{\text{total density matrix}} = \underbrace{\hat{\rho}_0}_{\text{Gibbs distr. for confined el-ns}} \otimes \underbrace{|0\rangle\langle 0|}_{\text{density matrix of el-ns propagating in vacuum}} \otimes \underbrace{|\vec{q}\rangle\langle\vec{q}|}_{\text{one photon in pure state } \vec{q}}$$

$$\hat{\rho}_0 = \frac{1}{Z}\sum_n \rho_{nn} e^{-\beta E_n}$$

$\rho_{nn} = |n\rangle\langle n|$

Many-body eigenstates of N electrons in metal (electrons may interact with each other and with other degrees of freedom)

The rate of scattering events $(n, 0, \vec{q}) \to (\ell, \vec{k}, 0)$

photon momentum

initial many-body state of N electrons

final many-body state of N-1 electrons

momentum of el-n propagating in vacuum

Fermi's Golden Rule:

$$w_{n,0,\vec{q}\to\ell,\vec{k},0} = \frac{2\pi}{\hbar}|\lambda|^2 \left|\langle \ell,\vec{k},0|\sum_{\vec{q}_1}\int d\vec{r}\,\varphi^+(\vec{r})\psi(\vec{r})e^{i\vec{q}_1\vec{r}}\hat{d}_{\vec{q}_1}|n,0,\vec{q}\rangle\right|^2$$

$$\delta\Big(\underbrace{E_n + \hbar\omega_{\vec{q}}}_{\text{init state}} - \underbrace{E_\ell - \frac{\hbar^2 k^2}{2m}}_{\text{final state}}\Big)$$

(of the entire system)

$\langle 0|\hat{d}_{\vec{q}_1}|\vec{q}\rangle = \delta_{\vec{q},\vec{q}_1}$

removes $\sum_{\vec{q}_1}\ldots$

The **total** transition rate at **given** $\vec{q}$ and $\vec{k}$: sum over **all** outcomes for the el-n states in metal (ℓ) and average over the initial states $|n\rangle$ with the weight given by $\hat{\rho}_0$

$$w_{\vec{q},\vec{k}} = \sum_n \frac{1}{Z}e^{-\beta E_n}\sum_\ell w_{n,0,\vec{q}\to\ell,\vec{k},0}$$

$$= \frac{2\pi}{\hbar}|\lambda|^2\frac{1}{Z}\sum_n e^{-\beta E_n}\sum_\ell \left|\langle \ell,\vec{k}|\int d\vec{r}\,e^{i\vec{q}\vec{r}}\,\hat{\varphi}^+(\vec{r})\psi(\vec{r})|n,0\rangle\right|^2$$

$$\times\,\delta\Big(E_n - E_\ell - \frac{\hbar^2k^2}{2m} + \hbar\omega_{\vec{q}}\Big)$$

Note that: $\delta(\omega) = \frac{1}{\pi} \mathrm{Re} \int_{-\infty}^{0} dt\, e^{-i\omega t + 0\cdot t}$; $\delta(\hbar\omega) = \frac{1}{\hbar}\delta(\omega)$

$$w_{\vec{q},\vec{k}} = \frac{2\pi}{\hbar^2} |\lambda|^2 \frac{1}{Z} \sum_n e^{-\beta E_n}$$

$$\times \sum_{\ell} \langle n,0| \int d\vec{r}_1\, e^{-i\vec{q}\vec{r}_1} \hat{\varphi}^+(r_1)\, \hat{\varphi}(r_1) |\ell,\vec{k}\rangle \langle \ell,\vec{k}| \int d\vec{r}_2\, e^{i\vec{q}\vec{r}_2} \hat{\varphi}^+(\vec{r}_2)\, \hat{\psi}(\vec{r}_2) |n,0\rangle$$

$$\times \frac{1}{\pi} \mathrm{Re} \int_{-\infty}^{0} dt\; e^{+0\cdot t} \exp\left\{-i\left(E_n - E_\ell - \frac{\hbar^2 k^2}{2m} + \hbar\omega_{\vec{q}}\right)\frac{t}{\hbar}\right\}$$

$$= \frac{2\pi}{\hbar^2} |\lambda|^2 \frac{1}{Z} \sum_{n\ell} e^{-\beta E_n} \int d\vec{r}_1 d\vec{r}_2\; e^{-i\vec{q}(\vec{r}_1 - \vec{r}_2)} \underbrace{\langle n|\psi^+(\vec{r}_1)|\ell\rangle\langle 0|\varphi(\vec{r}_1)|\vec{k}\rangle}$$

(used that $|\ell,\vec{k}\rangle = |\ell\rangle \otimes |\vec{k}\rangle$, $|n,0\rangle = |n\rangle \otimes |0\rangle$)

$$\times \langle \vec{k}|\, \hat{\varphi}^+(r_2)\, |0\rangle \langle \ell|\, \hat{\psi}(r_2)\, |n\rangle$$

$$\times \frac{1}{\pi} \mathrm{Re} \int_{-\infty}^{0} dt\; e^{+0\cdot t} \exp\left\{-i\left(E_n - E_\ell - \frac{\hbar^2 k^2}{2m} + \hbar\omega_{\vec{q}}\right)\frac{t}{\hbar}\right\}$$

02.23.23

$$w_{\vec{q},\vec{k}} =$$

$$= \frac{2\pi}{\hbar^2} |\lambda|^2 \frac{1}{\pi} \mathrm{Re} \int_{-\infty}^{0} dt\, e^{+0t} \int d\vec{r}_1 \int d\vec{r}_2\; e^{-i\vec{q}(\vec{r}_1 - \vec{r}_2)}\; e^{-i\omega_{\vec{q}} t} \cdot \frac{1}{L^3} \cdot \underbrace{e^{i\vec{k}(\vec{r}_1 - \vec{r}_2)}}_{\text{comes from } \langle \vec{k}|\hat{\varphi}^+(r_2)|0\rangle \ldots} \cdot e^{\frac{i}{\hbar}\frac{\hbar^2 k^2}{2m} t}$$

normalizing volume

$$\times \frac{1}{Z} \sum_{n,\ell} e^{-\beta E_n} \langle n|\psi^+(r_1)|\ell\rangle \langle \ell|\, e^{i\frac{\mathcal{H}_e}{\hbar} t}\, \psi(\vec{r}_2)\, e^{-i\frac{\mathcal{H}_e}{\hbar} t} |n\rangle$$

(we used:

$$e^{-i\frac{\hat{\mathcal{H}}_e}{\hbar} t} |n\rangle = e^{-i\frac{E_n}{\hbar} t} |n\rangle \;;\; \langle \ell|\, e^{i\frac{\hat{\mathcal{H}}_e}{\hbar} t} = \langle \ell|\, e^{i\frac{E_\ell}{\hbar} t}$$)

Note that:

$$\langle \ell|\, e^{i\frac{\hat{\mathcal{H}}_e}{\hbar} t}\, \hat{\psi}(\vec{r}_2)\, e^{-i\frac{\hat{\mathcal{H}}_e}{\hbar} t} |n\rangle = \langle \ell|\, \hat{\psi}(\vec{r}_2, t)\, |n\rangle \quad \text{(Heisenberg rep.)}$$

$$\frac{1}{Z}\sum_{n,\ell} e^{-\beta E_n} \langle n|\hat{\Psi}^+(r_1)|\ell\rangle\langle\ell| e^{i\frac{\hat{\mathcal{H}}_e}{\hbar}t}\, \hat{\Psi}(\vec{r}_2)\, e^{-i\frac{\hat{\mathcal{H}}_e}{\hbar}t}|n\rangle$$

$$= \frac{1}{Z}\sum_n e^{-\beta E_n}\sum_\ell \langle n|\hat{\Psi}^+(\vec{r}_1,0)|\ell\rangle\langle\ell|\hat{\Psi}(\vec{r}_2,t)|n\rangle$$

$$= \frac{1}{Z}\sum_n e^{-\beta E_n} \langle n|\hat{\Psi}^+(\vec{r}_1,0)\hat{\Psi}(\vec{r}_2,t)|n\rangle = \mathrm{Tr}\{\hat{\rho}_0\hat{\Psi}^+(\vec{r}_1,0)\hat{\Psi}(\vec{r}_2,t)\}$$

$$= \langle\Psi^+(\vec{r}_1,0)\Psi(\vec{r}_2,t)\rangle \quad \text{(at temperature } T)$$

Use it in $w_{\vec{q},\vec{k}}$:

$$w_{\vec{q},\vec{k}} = \frac{2\pi}{\hbar^2}|\lambda|^2\frac{1}{\pi}\mathrm{Re}\int_{-\infty}^{0}dt\, e^{-\frac{i}{\hbar}\left(\hbar\omega_{\vec{q}}-\frac{\hbar^2k^2}{2m}\right)t+0\cdot t}\cdot\frac{1}{L^3}\int dr_1\, e^{-i(\vec{q}-\vec{k})\vec{r}_1}$$

$$\times\int dr_2\, e^{i(\vec{q}-\vec{k})\vec{r}_2}\langle\Psi^+(r_1,0)\Psi(r_2,t)\rangle$$

Assume the system is transl.-invariant (this is a simplification!)

$$\langle\Psi^+(r_1,0)\Psi(r_2,t)\rangle = \langle\Psi^+(0,0)\Psi(\vec{r}_2-\vec{r}_1,t)\rangle$$

$$w_{\vec{q},\vec{k}} = \frac{2\pi}{\hbar^2}|\lambda|^2\frac{1}{\pi}\mathrm{Re}\int_{-\infty}^{0}dt\, e^{-\frac{i}{\hbar}\left(\hbar\omega_q-\frac{\hbar^2k^2}{2m}\right)t+0\cdot t}\int d\vec{r}\, e^{i(\vec{q}-\vec{k})\vec{r}}$$

$$\times\langle\Psi^+(0,0)\Psi(\vec{r},t)\rangle\ ; \qquad \vec{r}\equiv\vec{r}_2-\vec{r}_1$$

(used $\int dr_1\int dr_2\ldots = \int dr_1\int d(r_2-r_1)\ldots = L^3\int dr\ldots$)

One more re-writing to introduce $\delta(\omega+\ldots)$ and $\delta(\vec{p}+\ldots)$:

$$w_{\vec{q},\vec{k}} = \frac{2\pi}{\hbar^2}|\lambda|^2\int d\omega\,\delta\left(\omega+\left(\omega_q-\frac{\hbar^2k^2}{2m}\right)\right)\int dp\,\delta(\vec{p}+(\vec{q}-\vec{k}))$$

$$\times\frac{1}{\pi}\mathrm{Re}\int_{-\infty}^{0}dt\, e^{i\omega t+0\cdot t}\int d\vec{r}\, e^{-i\vec{p}\vec{r}}\langle\Psi^+(0,0)\Psi(\vec{r},t)\rangle$$

We introduced Fourier transform:

$$\langle \psi^+(0,0)\psi(\vec r,t)\rangle_{p\omega} =$$

$$= \frac{1}{\pi} \mathrm{Re} \int_{-\infty}^{0} dt\, e^{i\omega t + 0\cdot t} \int d\vec r\, e^{-i\vec p \vec r} \langle \psi^+(0,0)\psi(\vec r,t)\rangle$$

(any T)

At $T=0$, $Tr(\hat\rho_0 \ldots) = \langle G| \ldots |G\rangle$ ($|G\rangle$ is the ground state)

Introduce the hole spectral function:

$$A_h(\vec p,\omega) = \frac{1}{\pi} \mathrm{Re} \int_{-\infty}^{0} dt\, e^{i\omega t + 0\cdot t} \int d\vec r\, e^{-i\vec p \vec r} \langle G| \psi^+(0,0)\psi(\vec r,t)|G\rangle$$

Probability amplitude for a hole to propagate from point $\vec r$ at t ($t<0$) to point $\vec r = 0$ at time $t=0$

At $T=0$:

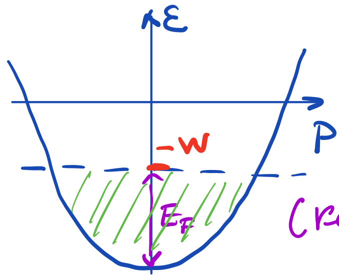
$$\boxed{w_{\vec q,\vec k} = \frac{2\pi}{\hbar^2}|\lambda|^2 \int d\omega\, \delta\left(\omega + \left(\omega_q - \frac{\hbar k^2}{2m}\right)\right) \int d\vec p \left(\vec p + (\vec q - \vec k)\right) A_h(\vec p,\omega)}$$

Note that derivation <u>did not</u> assume absence of interaction in the electron system! (We only used transl. invariance and time independence of $\mathcal{H}_e$.)

It appears from the derived relation that one may extract a full dependence of $A_h(\vec p,\omega)$ on a 3D-vector $\vec p$ and energy $\hbar\omega$ from a measurement of $w_{\vec q,\vec k}$. In reality, this is not the case. The fundamental limitation is that only the in-plane momentum $\vec p_{\parallel}$ may be conserved in the process of electron emission. The normal-to-surface component is not conserved, as the surface presence breaks the transl. invariance in that direction.

Further limitation of the resolution in ω comes from the photo-electron interaction with the rest of the system, before it leaves the material (we disregarded that effect in declaring the Hamiltonian of photoelectrons to be that of free particles, $\sum_{k} \frac{\hbar^2 k^2}{2m} a_k^+ a_k$)

Now let us look at $A_h(\bar{p}, \omega)$ for non-interacting fermions



$$\varepsilon(\vec{p}) = \frac{p^2}{2m^*} - (E_F + W) \; ; \quad E_F \equiv \frac{p_F^2}{2m^*} \; ; \; \varepsilon(p_F) = -W$$

(ref. point for energy is set by $k^2/2m$ for free electron)

$\hbar = 1$

$$\langle G | \psi^+(0,0)\, \psi(\vec{r}, t) | G \rangle = \frac{1}{L^3} \sum_{\vec{p}_1, \vec{p}_2} \langle G | a^+_{\vec{p}_1} e^{i \mathcal{H}_0 t} a_{\vec{p}_2} e^{-i \mathcal{H}_0 t} | G \rangle e^{i \bar{p}_2 \bar{r}}$$

$$= \frac{1}{L^3} \sum_{\bar{p}_1, \bar{p}_2} e^{i \bar{p}_2 \bar{r}} \langle G | a^+_{p_1} \exp\left\{ i \sum_{\bar{p}_3} \varepsilon_{\bar{p}_3} a^+_{\bar{p}_3} a_{\bar{p}_3} t \right\} a_{\bar{p}_2} \exp\left\{ -i \sum_{\bar{p}_4} \varepsilon_{\bar{p}_4} a^+_{\bar{p}_4} a_{\bar{p}_4} t \right\} | G \rangle$$

$$|G\rangle = \prod_{|k| < p_F} a_k^+ |0\rangle$$