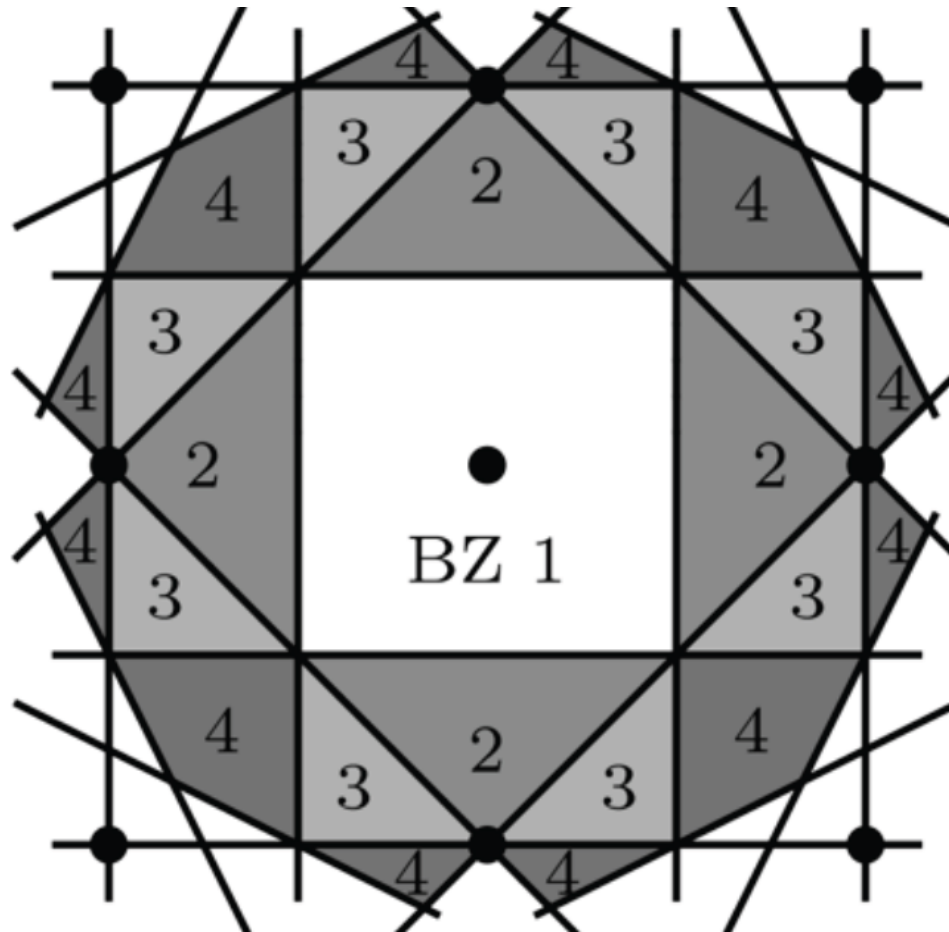
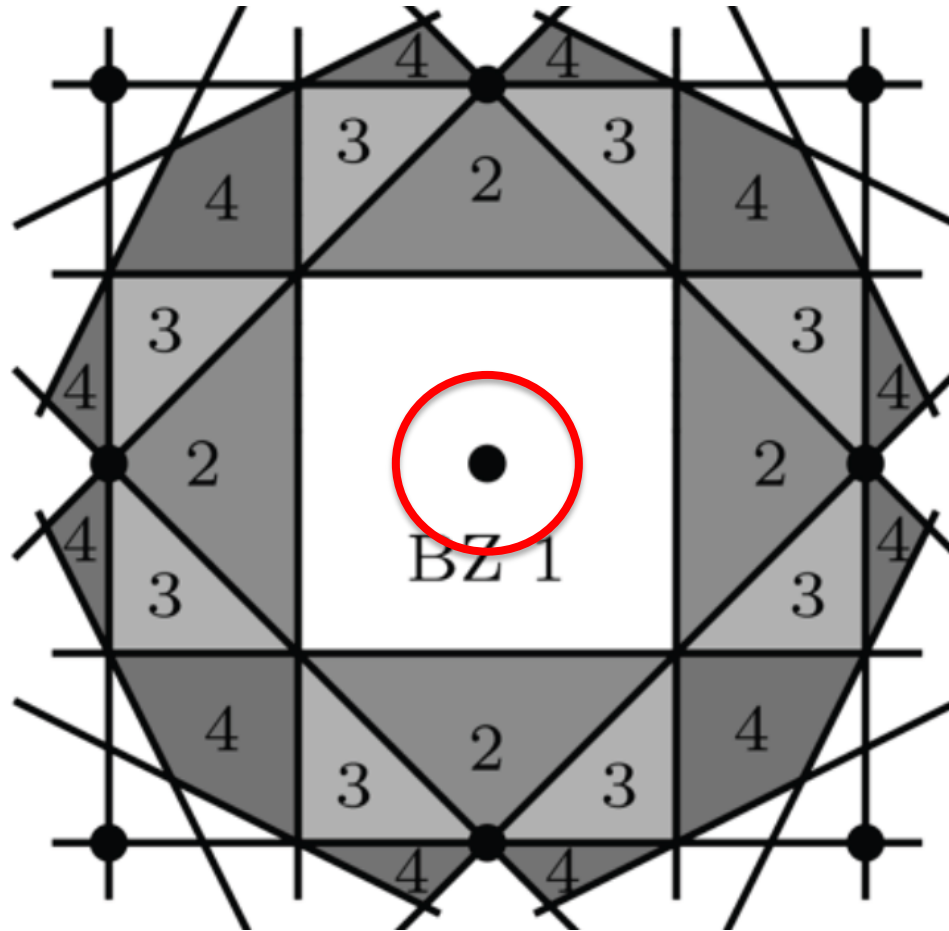


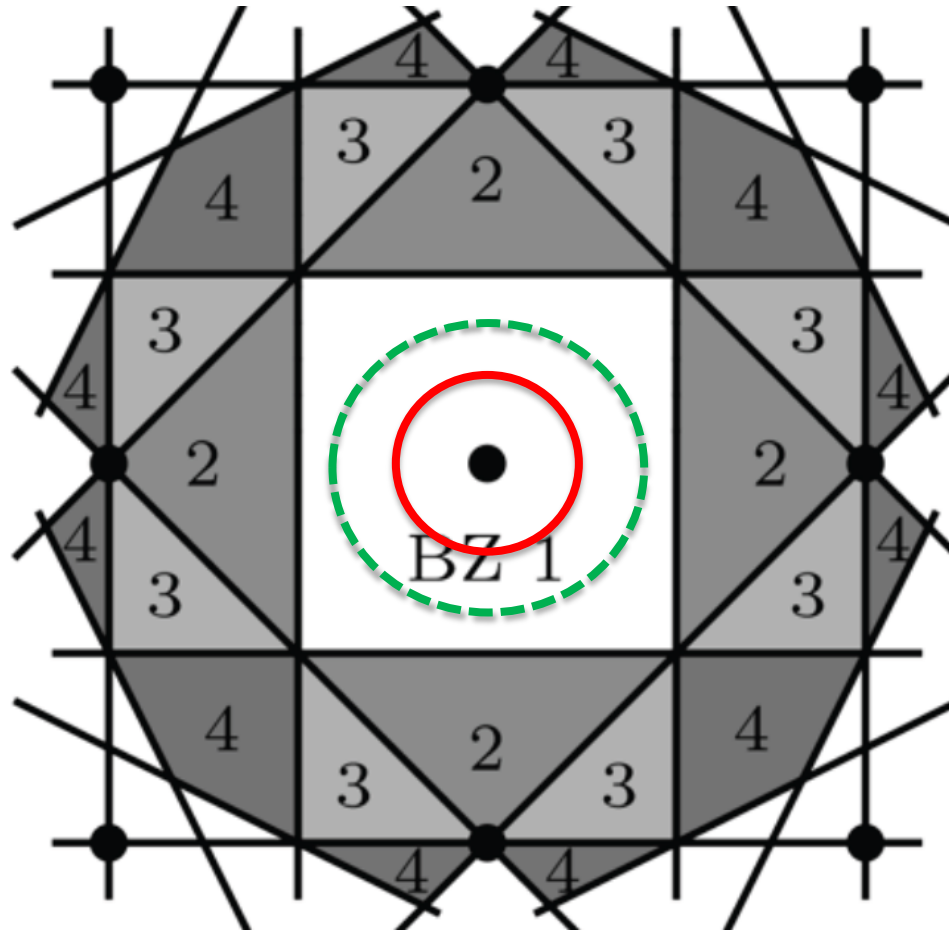
Zonas de Brillouin e sup. de Fermi



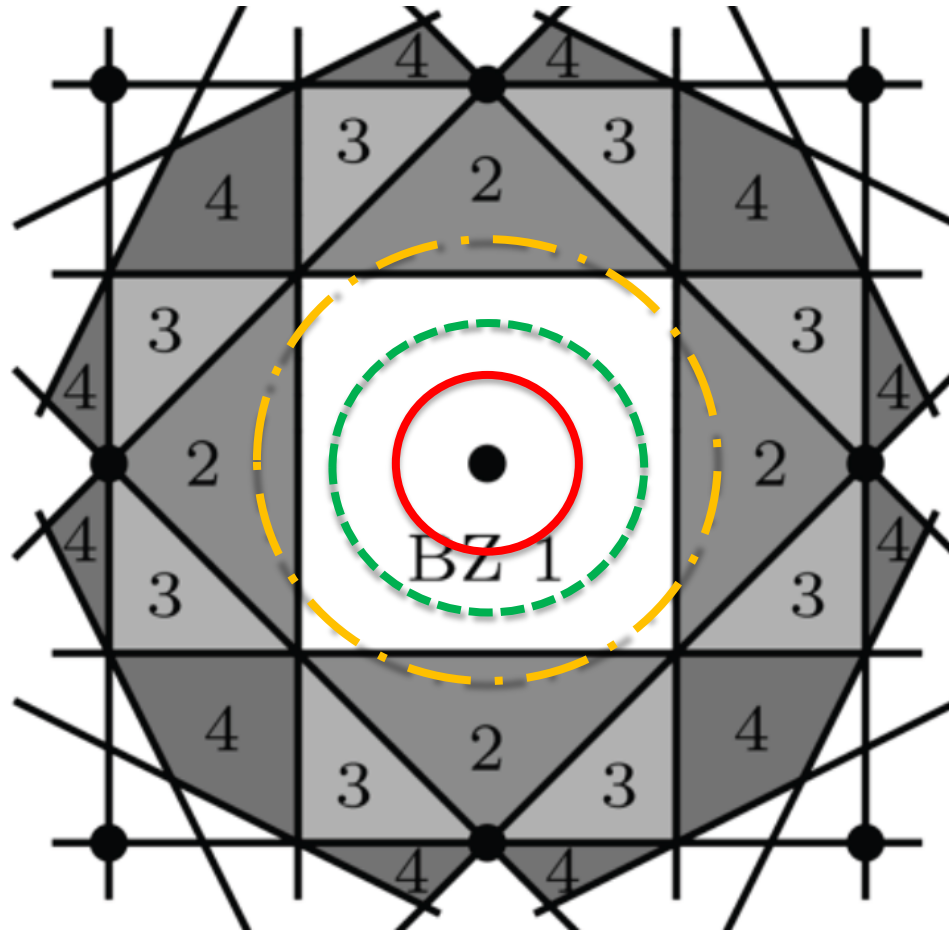
Zonas de Brillouin e sup. de Fermi



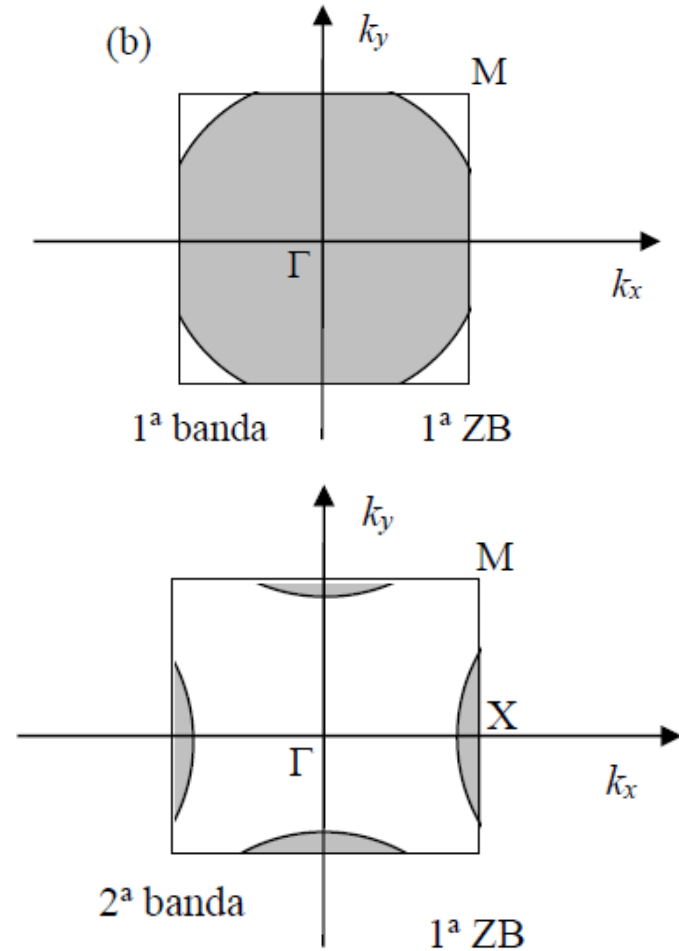
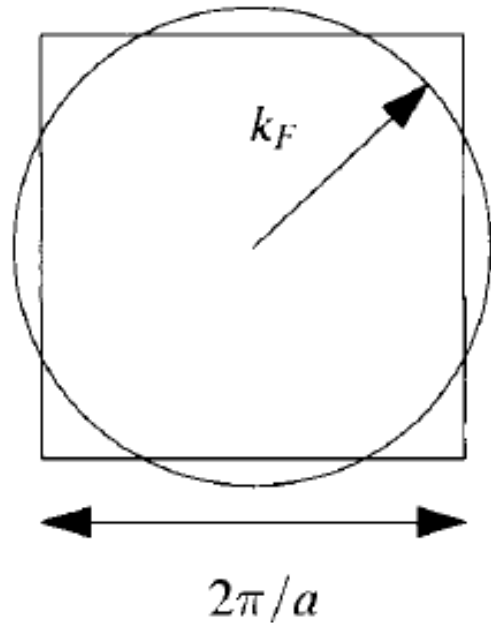
Zonas de Brillouin e sup. de Fermi



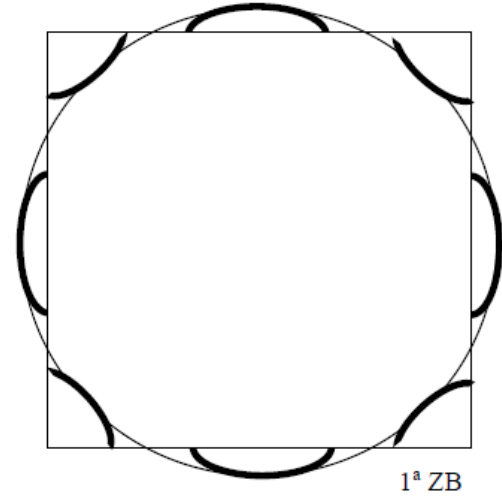
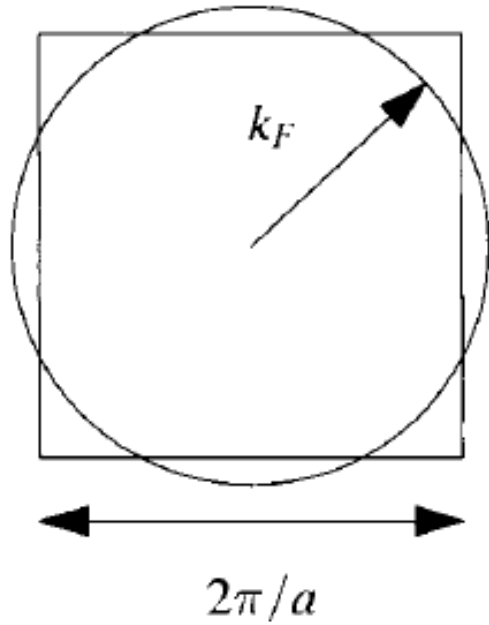
Zonas de Brillouin e sup. de Fermi



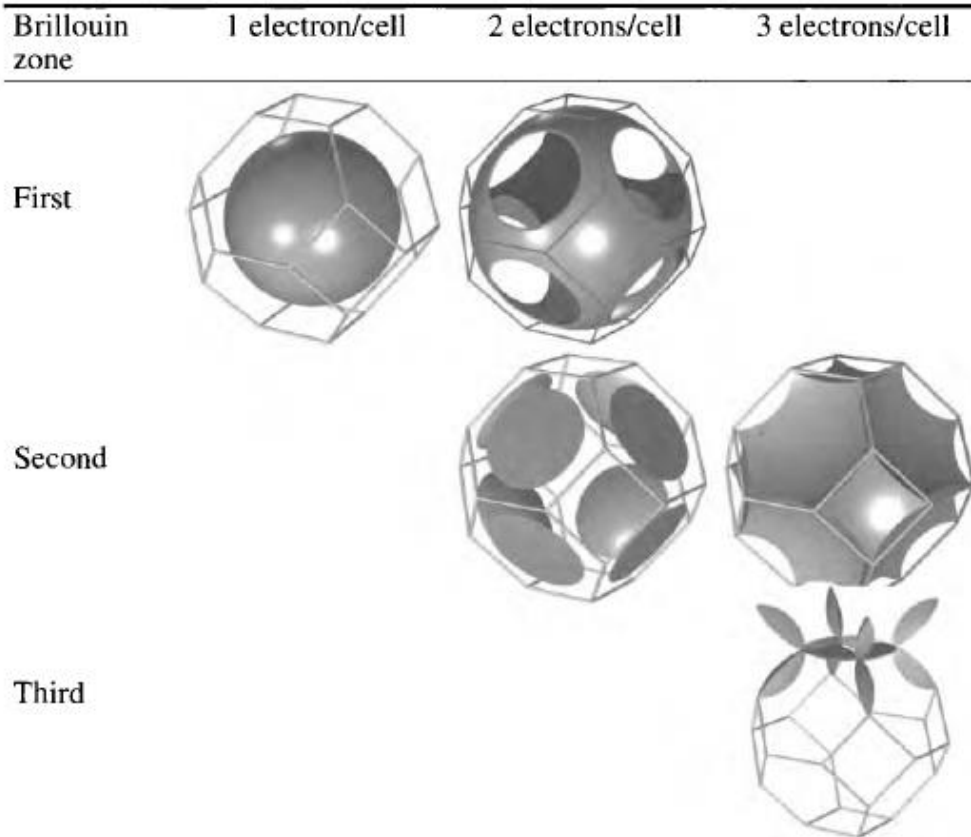
Zonas de Brillouin e sup. de Fermi



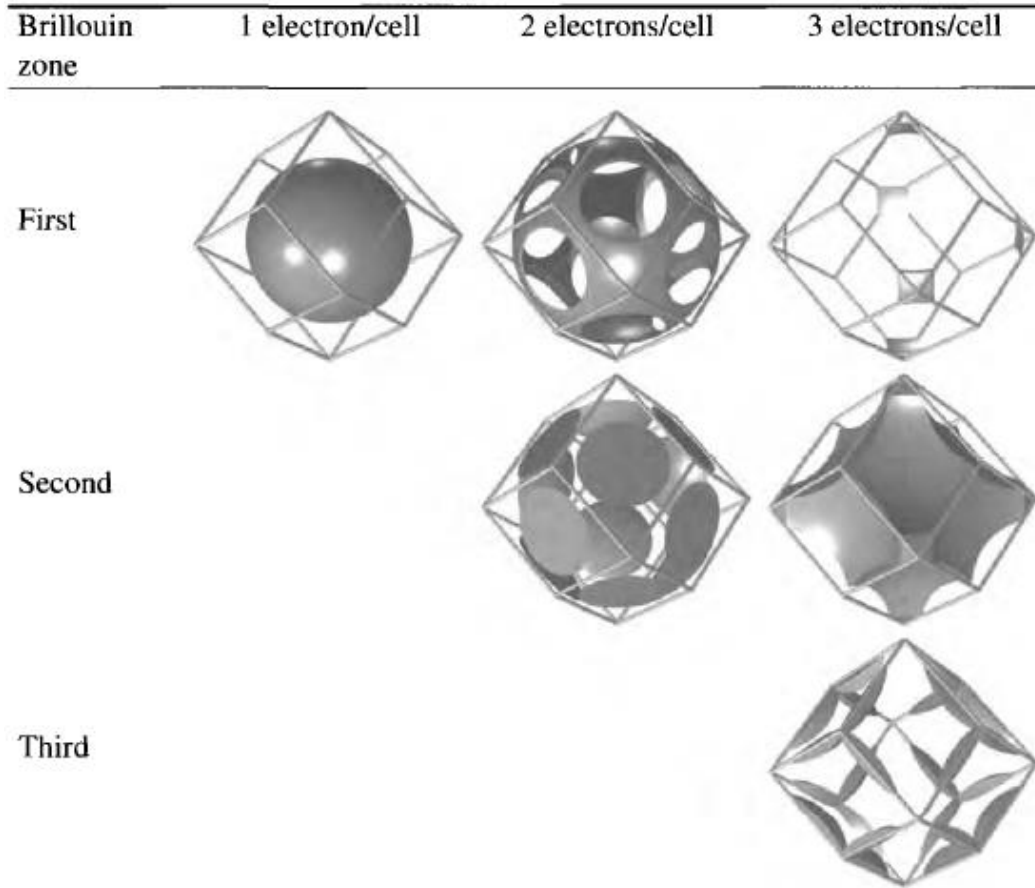
Zonas de Brillouin e sup. de Fermi



Superfícies de Fermi para um cristal FCC



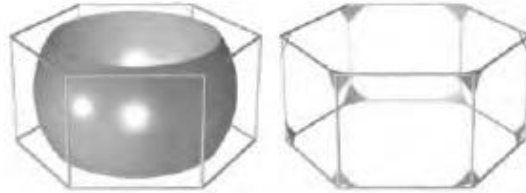
Superfícies de Fermi para um cristal BCC



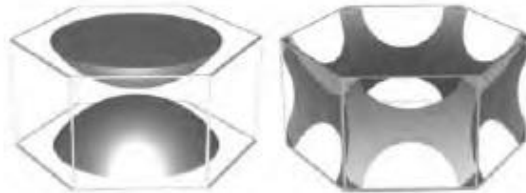
Superfícies de Fermi para um cristal HEX

Brillouin zone	2 electrons/cell	4 electrons/cell
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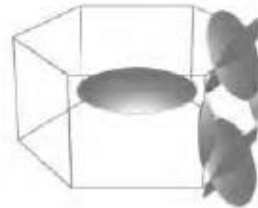
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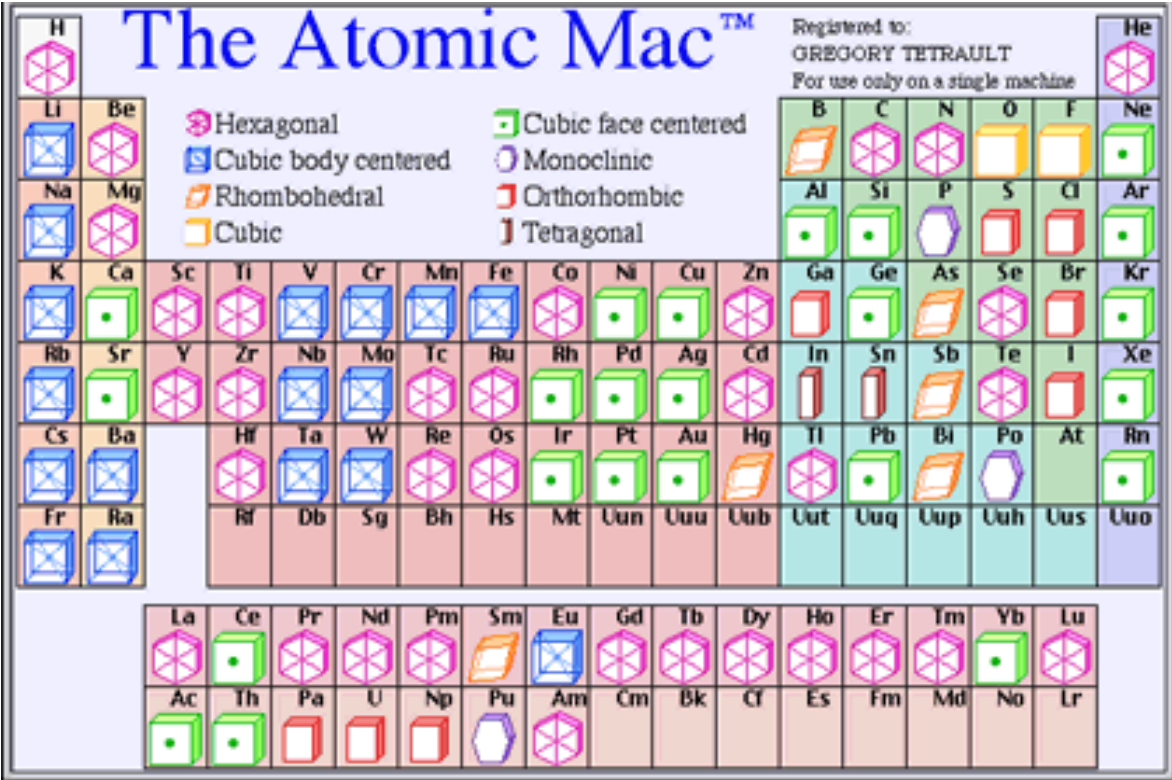
Second



Third

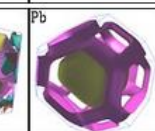
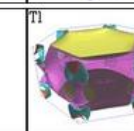
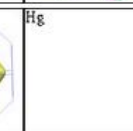
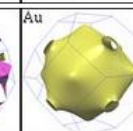
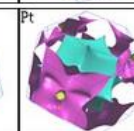
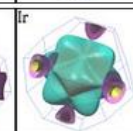
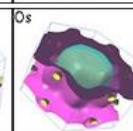
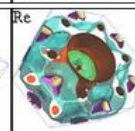
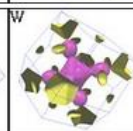
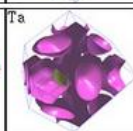
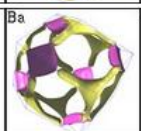
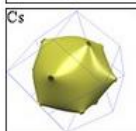
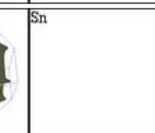
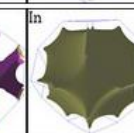
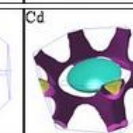
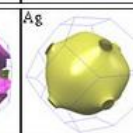
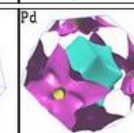
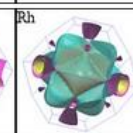
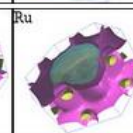
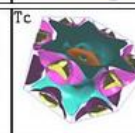
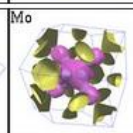
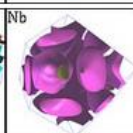
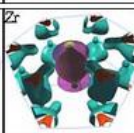
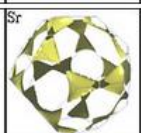
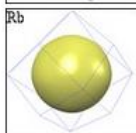
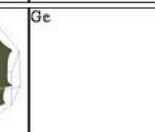
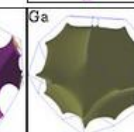
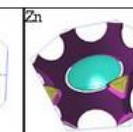
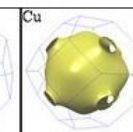
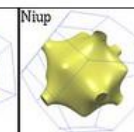
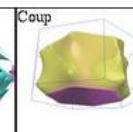
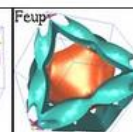
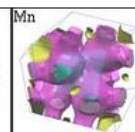
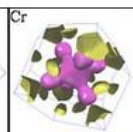
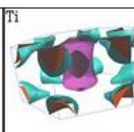
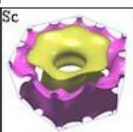
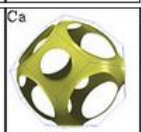
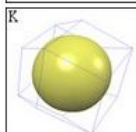
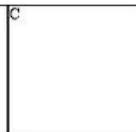
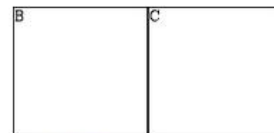
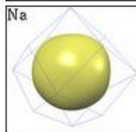
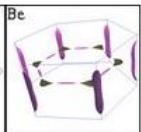
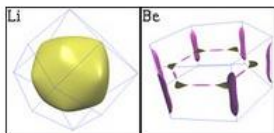


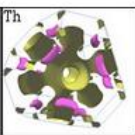
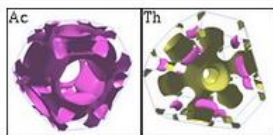
Zonas de Brillouin e sup. de Fermi

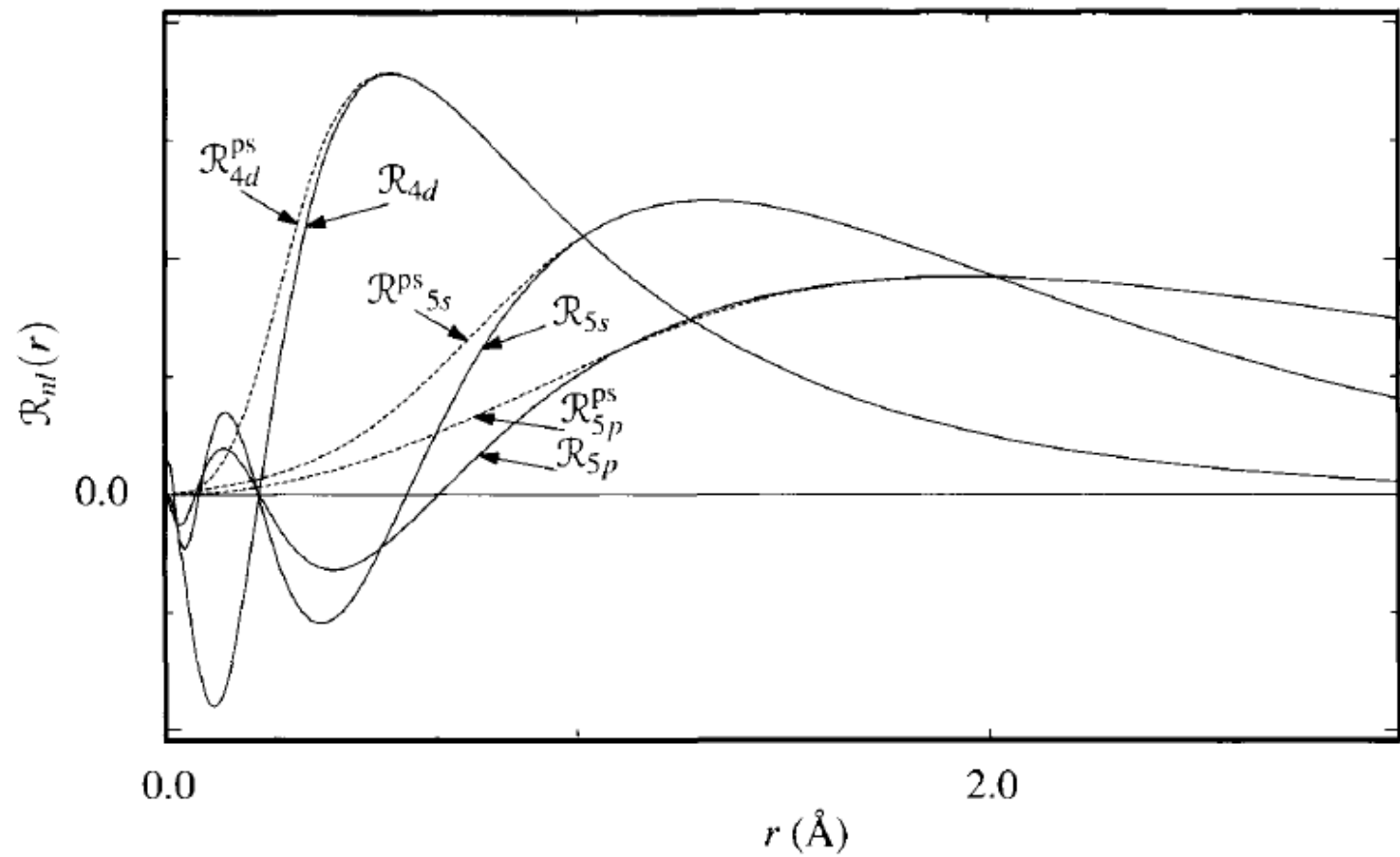


The Fermi Surface Database

(click icons)





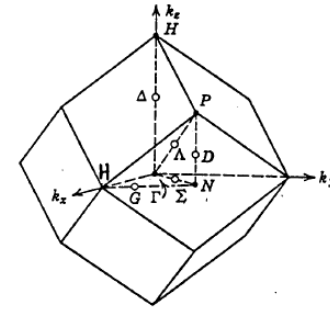


Metais Monovalentes

Element	Electronic structure	Crystalline structure	Element	Electronic structure	Crystalline structure
Li	$1s^2 2s^1$	bcc			
Na	$[\text{Ne}] 3s^1$	bcc			
K	$[\text{Ar}] 4s^1$	bcc	Cu	$[\text{Ar}] 3d^{10} 4s^1$	fcc
Rb	$[\text{Kr}] 5s^1$	bcc	Ag	$[\text{Kr}] 4d^{10} 5s^1$	fcc
Cs	$[\text{Xe}] 6s^1$	bcc	Au	$[\text{Xe}] 4f^{14} 5d^{10} 6s^1$	fcc

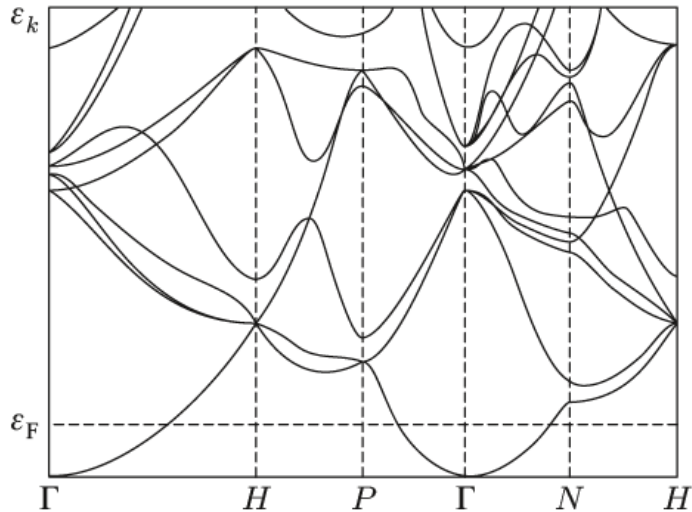
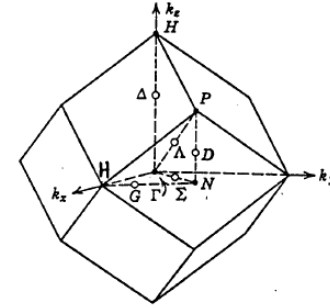
Metais Monovalentes

Element	Electronic structure	Crystalline structure	Element	Electronic structure	Crystalline structure
Li	$1s^2 2s^1$	bcc			
Na	$[\text{Ne}] 3s^1$	bcc			
K	$[\text{Ar}] 4s^1$	bcc	Cu	$[\text{Ar}] 3d^{10} 4s^1$	fcc
Rb	$[\text{Kr}] 5s^1$	bcc	Ag	$[\text{Kr}] 4d^{10} 5s^1$	fcc
Cs	$[\text{Xe}] 6s^1$	bcc	Au	$[\text{Xe}] 4f^{14} 5d^{10} 6s^1$	fcc



Metais Monovalentes

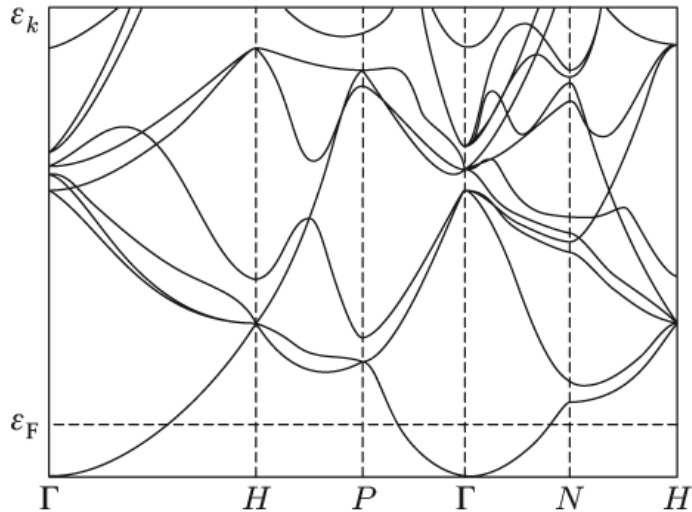
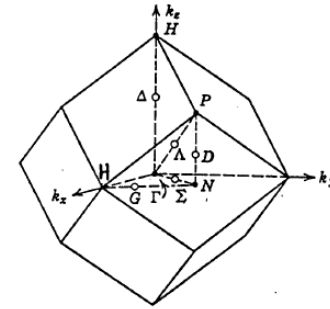
Element	Electronic structure	Crystalline structure	Element	Electronic structure	Crystalline structure
Li	$1s^2 2s^1$	bcc			
Na	$[\text{Ne}] 3s^1$	bcc			
K	$[\text{Ar}] 4s^1$	bcc	Cu	$[\text{Ar}] 3d^{10} 4s^1$	fcc
Rb	$[\text{Kr}] 5s^1$	bcc	Ag	$[\text{Kr}] 4d^{10} 5s^1$	fcc
Cs	$[\text{Xe}] 6s^1$	bcc	Au	$[\text{Xe}] 4f^{14} 5d^{10} 6s^1$	fcc



→ $k_F = 0.620(2\pi/a)$

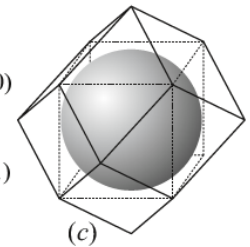
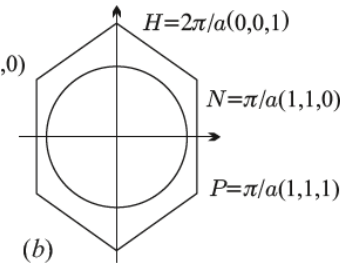
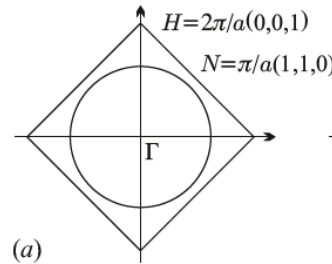
Metais Monovalentes

Element	Electronic structure	Crystalline structure	Element	Electronic structure	Crystalline structure
Li	$1s^2 2s^1$	bcc			
Na	$[\text{Ne}] 3s^1$	bcc			
K	$[\text{Ar}] 4s^1$	bcc	Cu	$[\text{Ar}] 3d^{10} 4s^1$	fcc
Rb	$[\text{Kr}] 5s^1$	bcc	Ag	$[\text{Kr}] 4d^{10} 5s^1$	fcc
Cs	$[\text{Xe}] 6s^1$	bcc	Au	$[\text{Xe}] 4f^{14} 5d^{10} 6s^1$	fcc



$$\longrightarrow k_F = 0.620(2\pi/a)$$

$$\longrightarrow \overline{\Gamma N} = (2\pi/a)\sqrt{\left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2} = 0.707(2\pi/a)$$

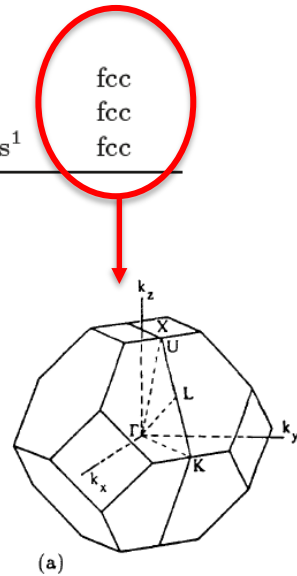
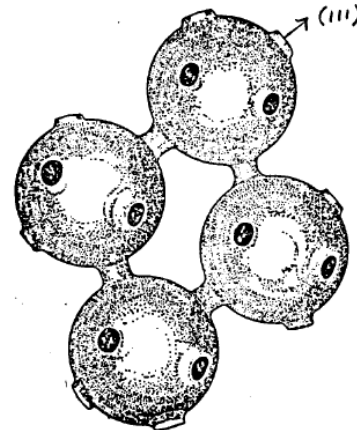
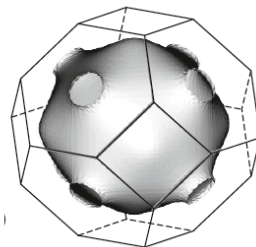
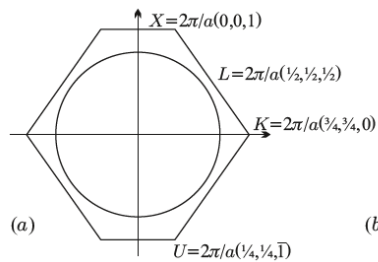
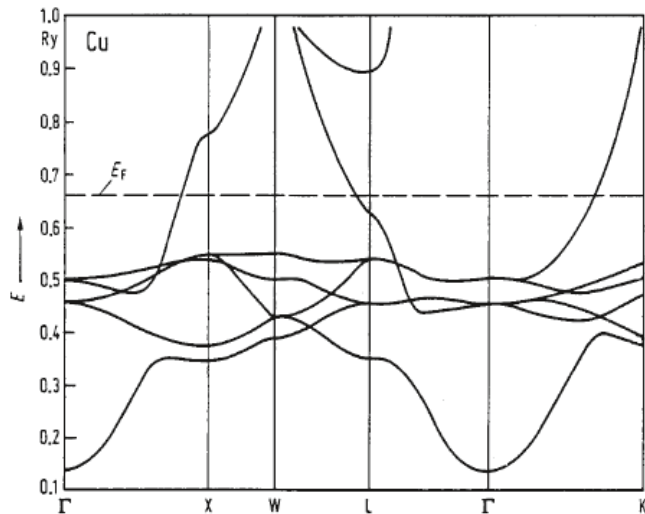


Element	m_{ds}^*/m_e	m_c/m_e	m_{calc}^*/m_e
Li	2.168	1.8	1.66
Na	1.210	1.24	1.00
K	1.234	1.22	1.09
Rb	1.226	1.20	1.21
Cs	1.355	1.44	1.76

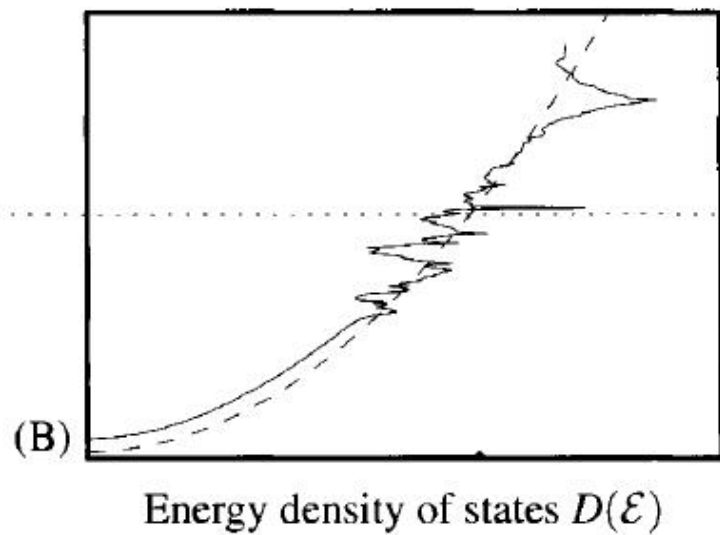
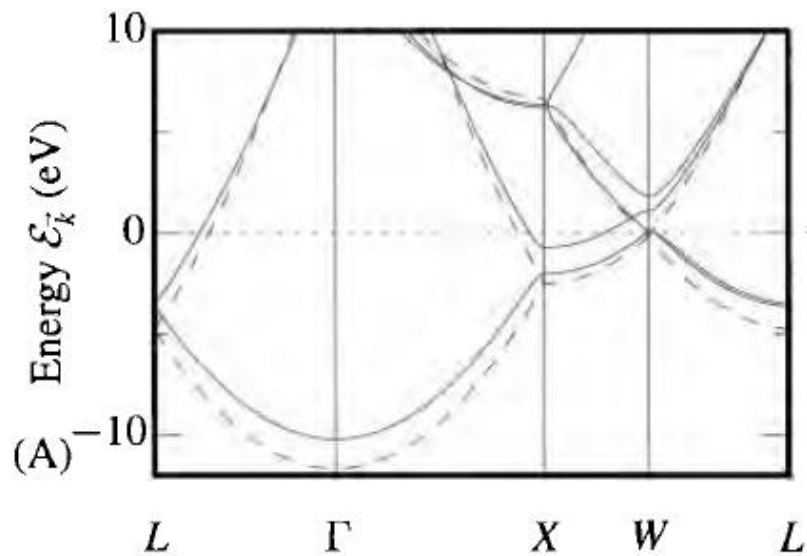
Element	Electronic structure	Crystalline structure	Element	Electronic structure	Crystalline structure
Li	$1s^2 2s^1$	bcc	Cu	$[Ar] 3d^{10} 4s^1$	fcc
Na	$[Ne] 3s^1$	bcc	Ag	$[Kr] 4d^{10} 5s^1$	fcc
K	$[Ar] 4s^1$	bcc	Au	$[Xe] 4f^{14} 5d^{10} 6s^1$	fcc
Rb	$[Kr] 5s^1$	bcc			
Cs	$[Xe] 6s^1$	bcc			

→ $k_F = 0.782(2\pi/a)$

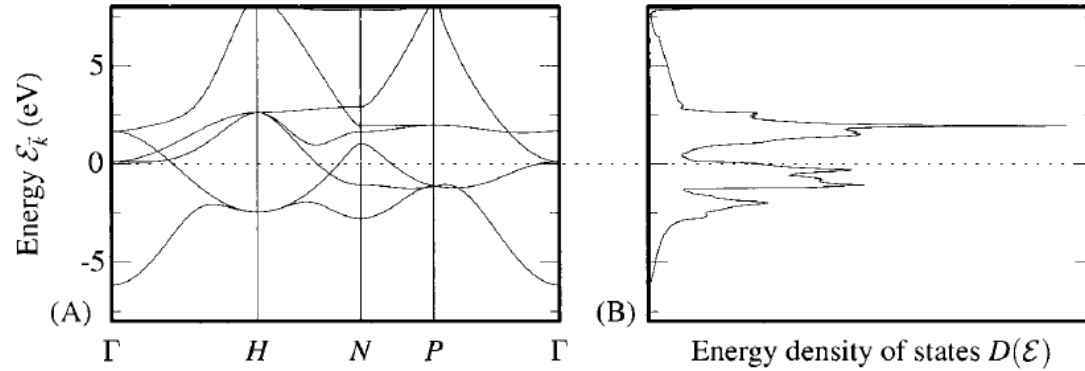
$\overline{\Gamma L} = 0.866(2\pi/a)$

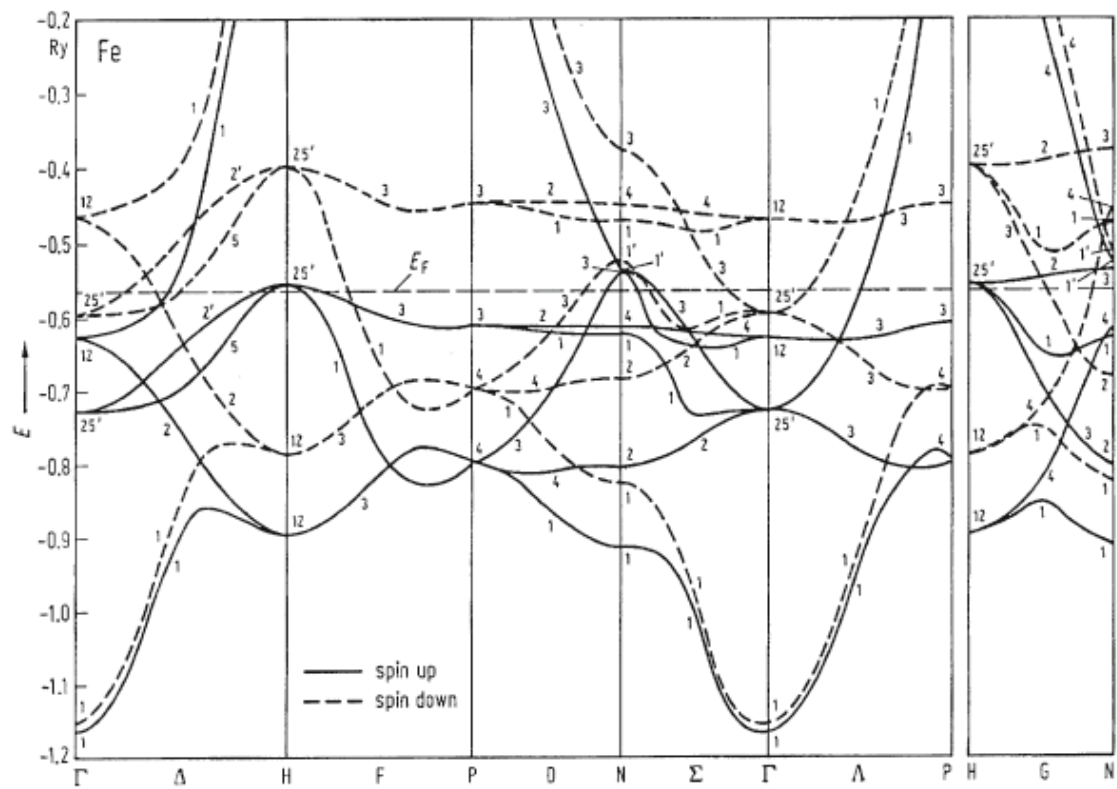


Metais trivalentes (alumínio)

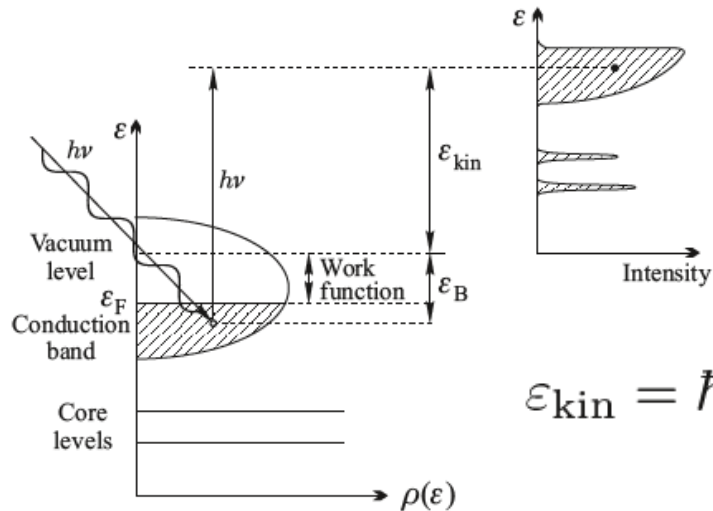


Metais de transição e terras raras



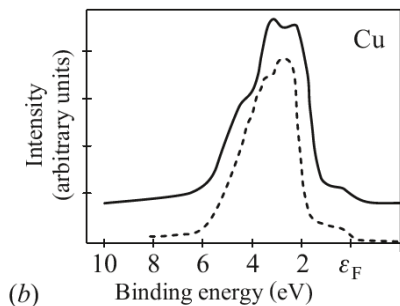
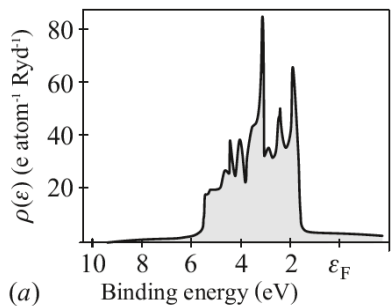
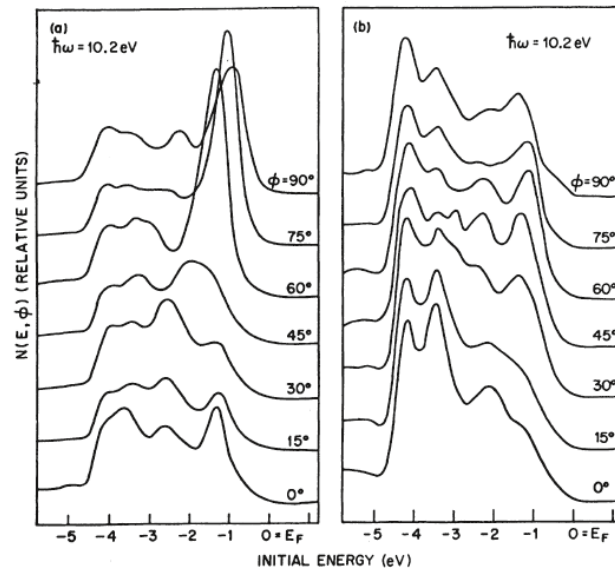


Photoemission spectroscopy



$$\epsilon_{kin} = \hbar\omega - \Phi - |\epsilon_i|$$

ARPES



Dinâmica de elétrons

Dinâmica de elétrons

Para entendermos a dinâmica dos elétrons nas bandas, o primeiro passo é encontrar a “velocidade” associada a eles.

$$\begin{aligned} \mathbf{v} &= \frac{1}{m} \int \psi^* \mathbf{p} \psi \, d\mathbf{r} \\ &= -\frac{i\hbar}{m} \int \psi^* \nabla \psi \, d\mathbf{r}. \end{aligned}$$

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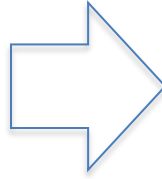
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Logo $\mathcal{H}_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r}) = \mathcal{E}_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r})$ com $\mathcal{H}_{\mathbf{k}} \equiv -\frac{\hbar^2}{2m} (\nabla + i\mathbf{k})^2 + V(\mathbf{r})$

Dinâmica de elétrons

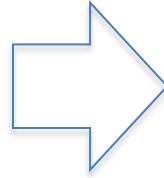
$$\begin{aligned}(\mathcal{H}_{\mathbf{k}} - \mathcal{E}_{\mathbf{k}}) \frac{\partial}{\partial \mathbf{k}} u_{\mathbf{k}}(\mathbf{r}) &= - \left[\frac{\partial}{\partial \mathbf{k}} (\mathcal{H}_{\mathbf{k}} - \mathcal{E}_{\mathbf{k}}) \right] u_{\mathbf{k}}(\mathbf{r}) \\ &= \left[\frac{i\hbar}{m} (\nabla + i\mathbf{k}) + \frac{\partial \mathcal{E}_{\mathbf{k}}}{\partial \mathbf{k}} \right] u_{\mathbf{k}}(\mathbf{r}).\end{aligned}$$



$$\hbar \mathbf{v}_{\mathbf{k}} = \frac{\partial \mathcal{E}_{\mathbf{k}}}{\partial \mathbf{k}} - \int u_{\mathbf{k}}^*(\mathbf{r}) (\mathcal{H}_{\mathbf{k}} - \mathcal{E}_{\mathbf{k}}) \frac{\partial}{\partial \mathbf{k}} u_{\mathbf{k}}(\mathbf{r}) \mathbf{d}\mathbf{r}.$$

Dinâmica de elétrons

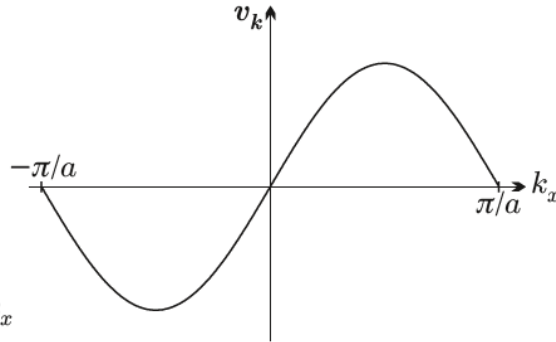
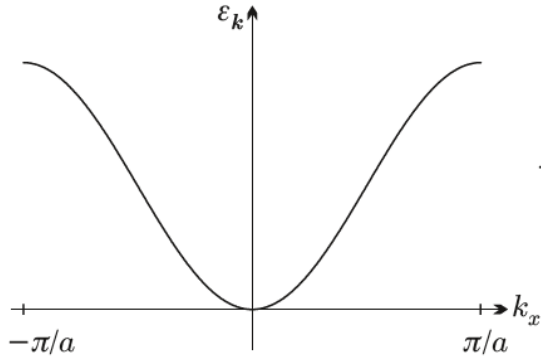
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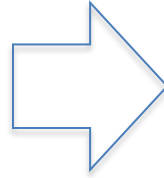
$$\mathbf{v}_{\mathbf{k}} = \frac{1}{\hbar} \frac{\partial \mathcal{E}_{\mathbf{k}}}{\partial \mathbf{k}}.$$

Velocidade de grupo!!



Dinâmica de elétrons

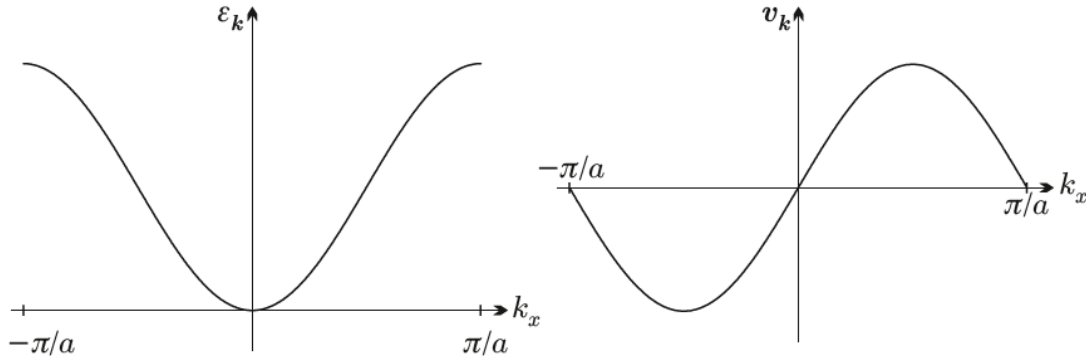
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Velocidade de grupo!!



$$\mathbf{j} = \sum_{\mathbf{k}} n_{\mathbf{k}} e \mathbf{v}_{\mathbf{k}}.$$

Resultado idêntico ao caso clássico, de elétrons como partículas

Aproximação Semiclássica

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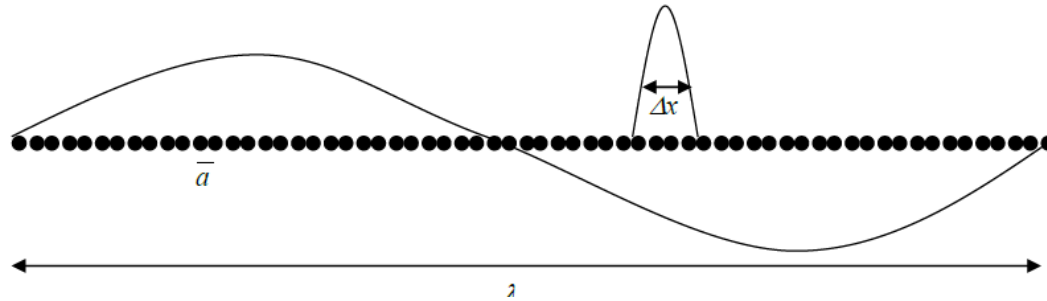
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3. O elétron é descrito por um pacote de ondas cujos momentos cristalinos relevantes estão limitados a um pequeno intervalo $\Delta\mathbf{k} = \mathbf{k}' - \mathbf{k}$, com $|\Delta\mathbf{k}| \ll |\mathbf{k}|$

$$\phi_{n\mathbf{k}}(\mathbf{r}, t) = \sum_{\mathbf{k}'} g(\mathbf{k}') \psi_{n\mathbf{k}'}(\mathbf{r}) e^{-i\varepsilon_{n\mathbf{k}'} t / \hbar}$$

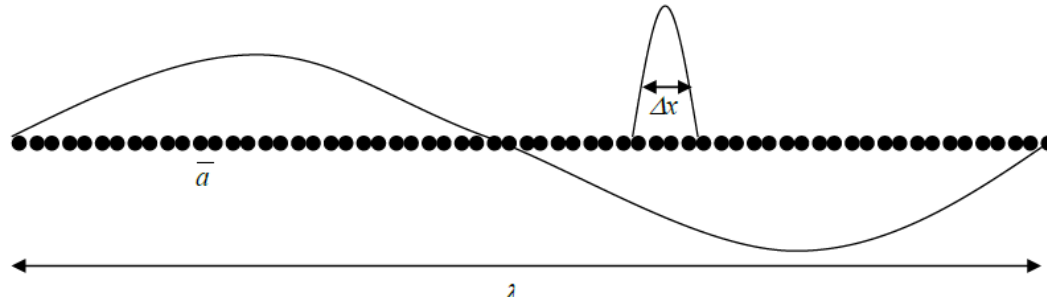
Aproximação Semiclássica

4. Sendo $|\Delta k| \cdot |\Delta r| \sim 1$, logo $|\Delta r| \gg a$, no entanto ainda deve ser muito menor que o comprimento de onda dos campos envolvidos.



Aproximação Semiclássica

4. Sendo $|\Delta \mathbf{k}| \cdot |\Delta \mathbf{r}| \sim 1$, logo $|\Delta \mathbf{r}| \gg a$, no entanto ainda deve ser muito menor que o comprimento de onda dos campos envolvidos.



5. A velocidade do elétron é dada pela velocidade de grupo do pacote de onda.

$$\mathbf{v}_{\mathbf{k}} = \frac{1}{\hbar} \frac{\partial \mathcal{E}_{\mathbf{k}}}{\partial \mathbf{k}}.$$

Equação de movimento

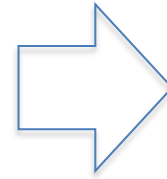
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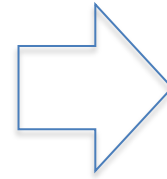


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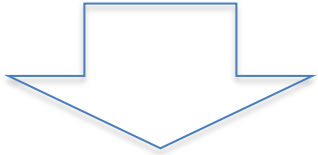
De uma forma mais geral, podemos escrever a equação de movimento como incluindo ambos campos elétrico e magnético

$$\hbar \dot{\mathbf{k}} = -e[\mathbf{E}(\mathbf{r}, t) + \mathbf{v}_{n\mathbf{k}} \times \mathbf{B}(\mathbf{r}, t)]$$

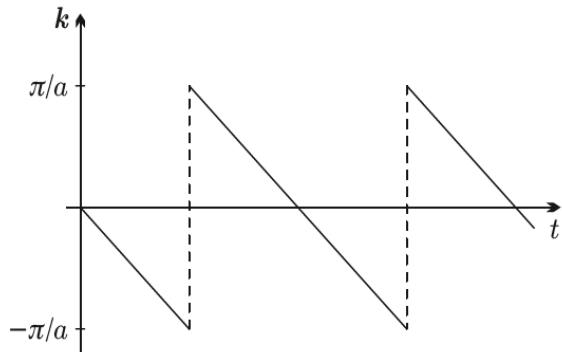
Elétrons sob ação de um
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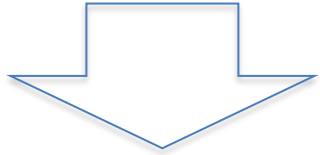


$$\hbar \mathbf{k}(t) = \hbar \mathbf{k}(0) - e\mathbf{E}t$$

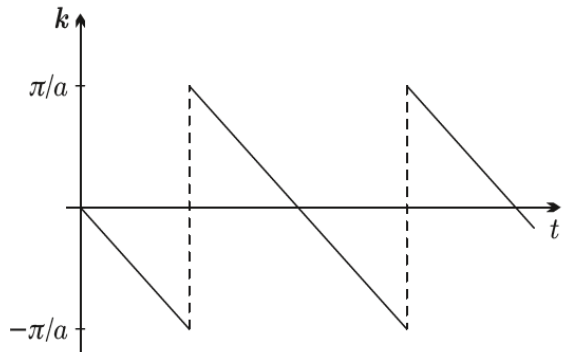


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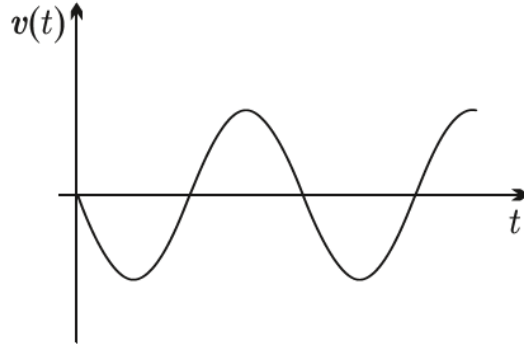
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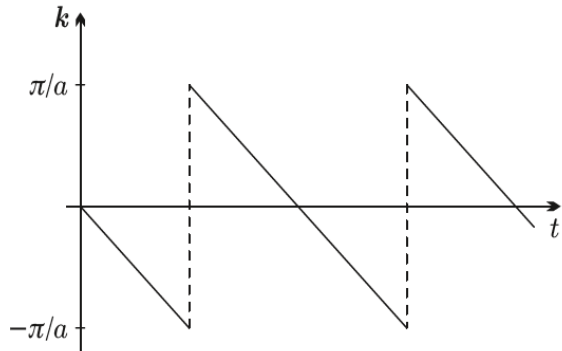


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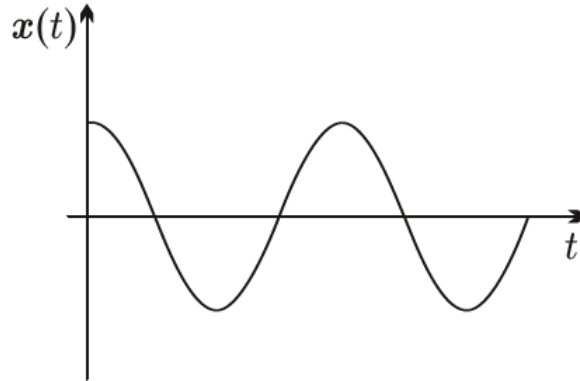
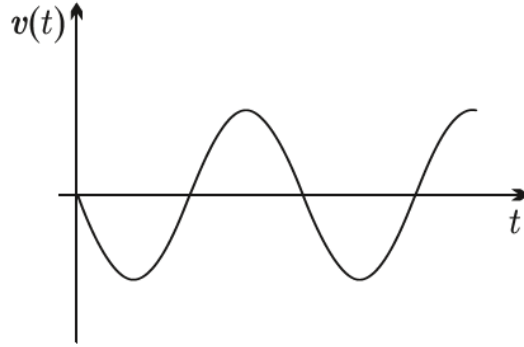
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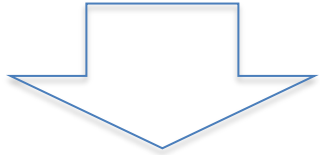


$$T = \hbar(2\pi/a)/eE$$

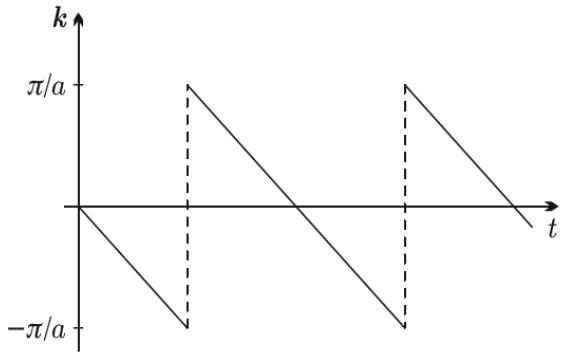
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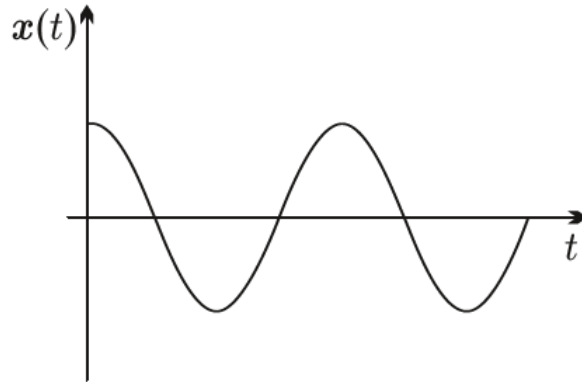
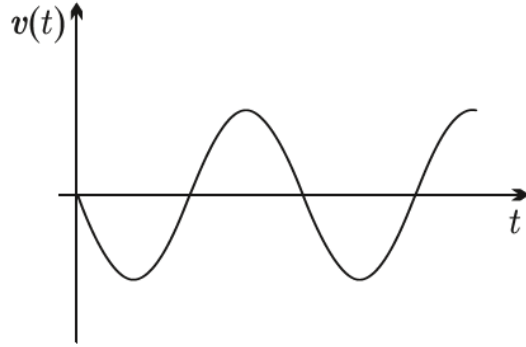
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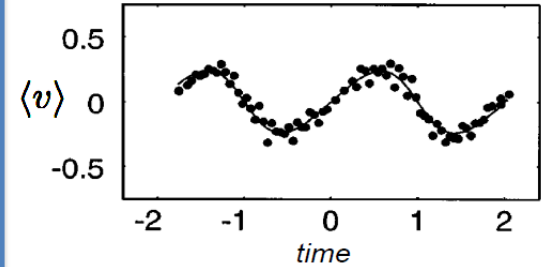


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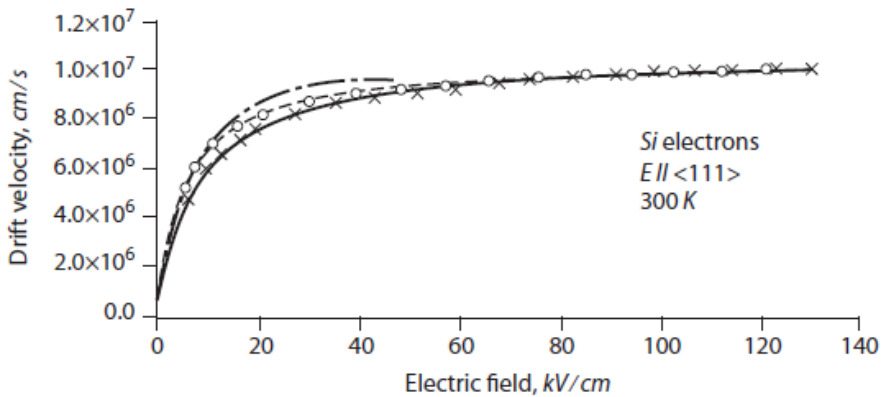
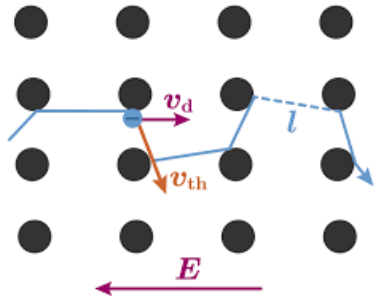


M.B. Dahan et al,

Phys. Rev. Lett. 76, 4508 (1996)

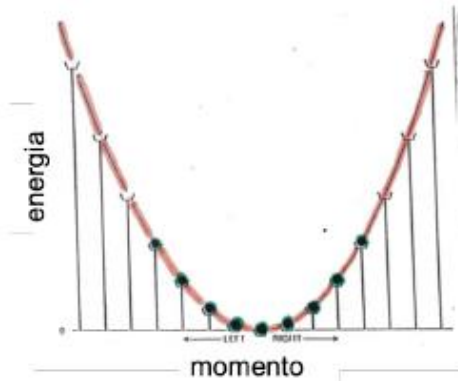
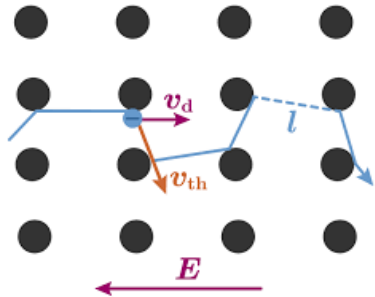
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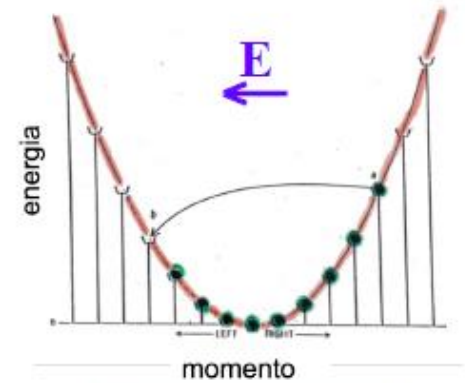


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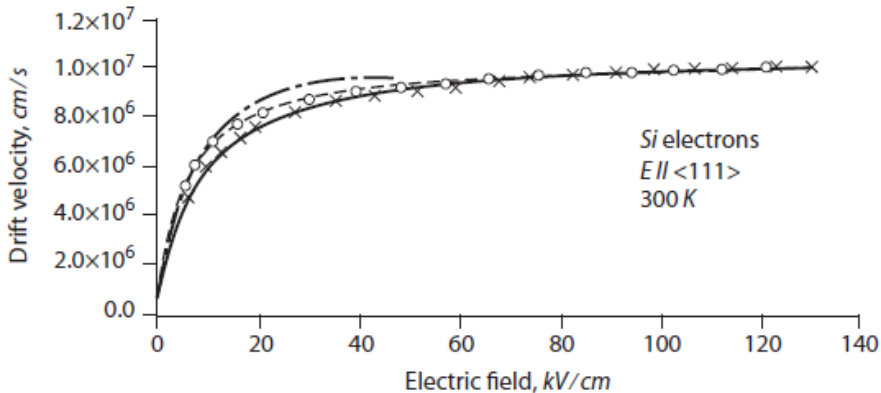
$$\sum_i \mathbf{k}_i = 0 \Rightarrow \mathbf{j} = 0$$



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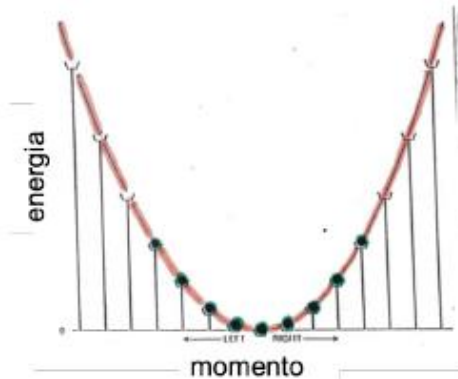
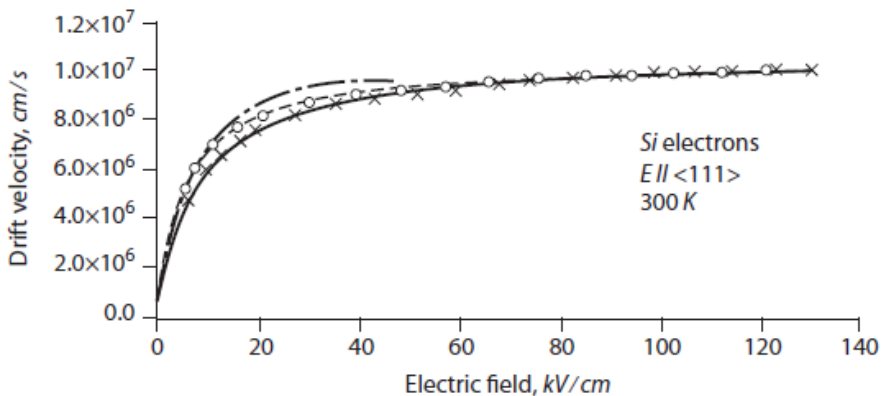
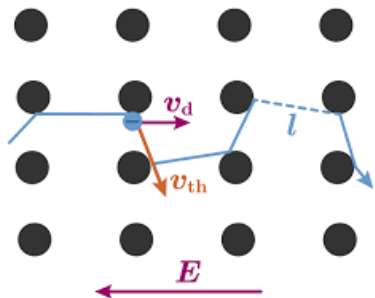
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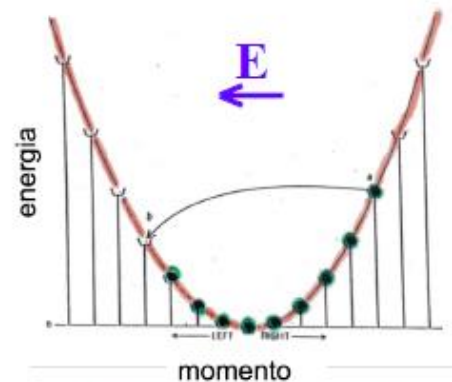


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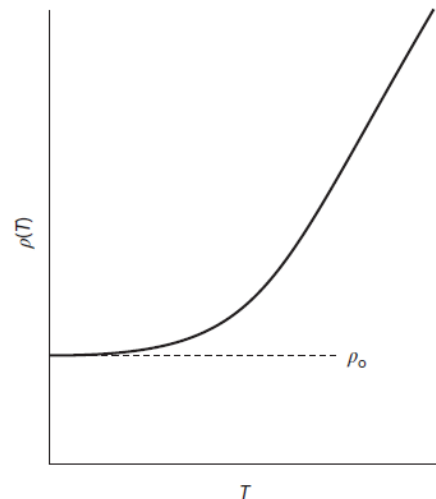


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$$\rho(T) = \frac{m}{ne^2\tau_t} = \frac{2\pi m\lambda_t}{ne^2\hbar} k_B T$$



1. Existência de buracos

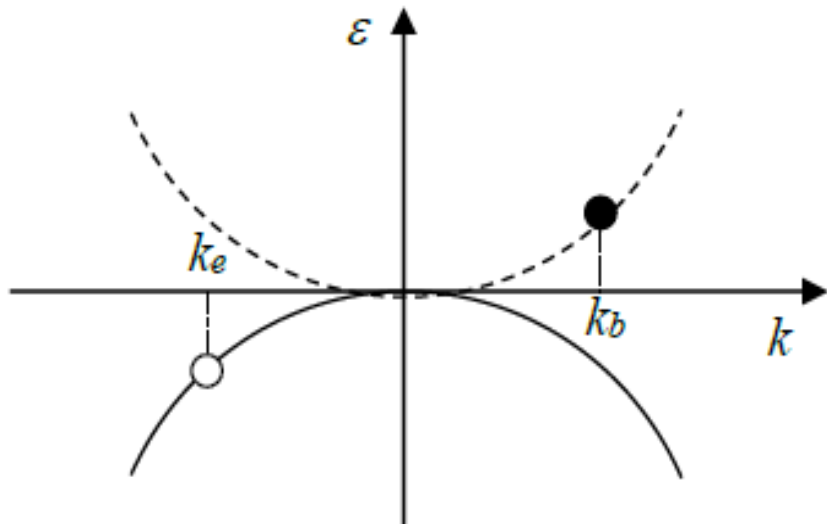
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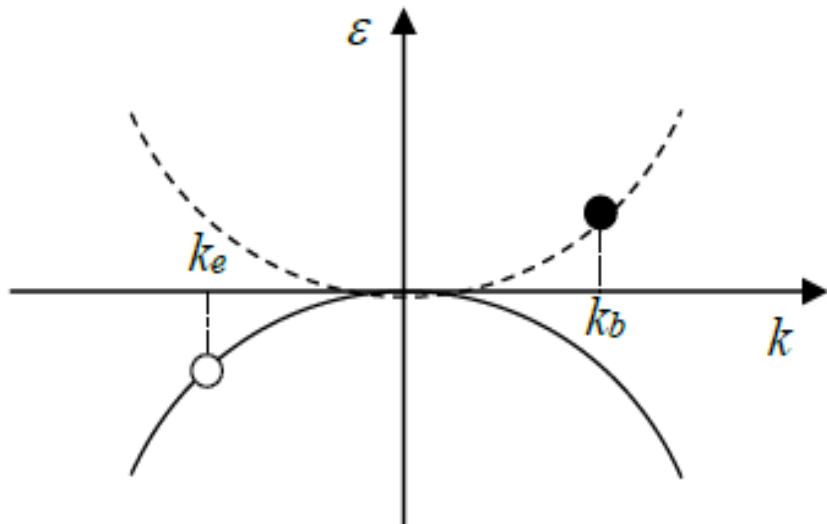
Na ausência de um elétron de momento k_e : $\mathbf{k}_{total} = \sum_{\mathbf{k}} \mathbf{k} = -\mathbf{k}_e$



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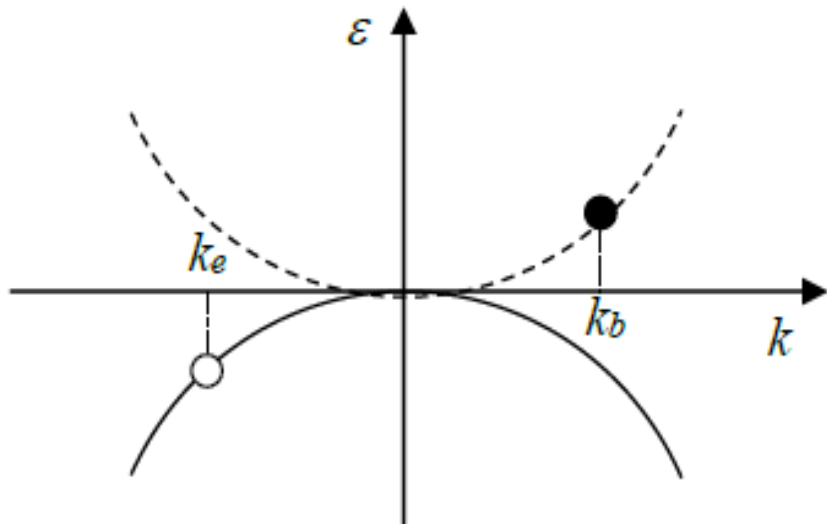
Definindo $\mathbf{k}_b = -\mathbf{k}_e$,

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Por sua vez

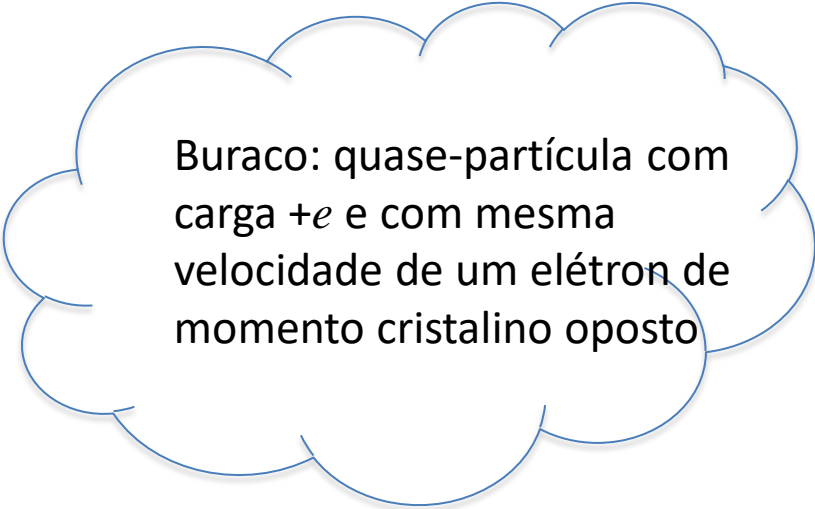
$$\mathbf{v}_{hn}(\mathbf{k}_h) = \frac{1}{\hbar} \frac{\partial \varepsilon_{hn}(\mathbf{k}_h)}{\partial \mathbf{k}_h}$$

$$\hbar \dot{\mathbf{k}}_h = +e [\mathbf{E}(\mathbf{r}, t) + \mathbf{v}_{hn}(\mathbf{k}_h) \times \mathbf{B}(\mathbf{r}, t)]$$

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Buraco: quase-partícula com carga $+e$ e com mesma velocidade de um elétron de momento cristalino oposto

Definindo $\mathbf{k}_b = -\mathbf{k}_e$,

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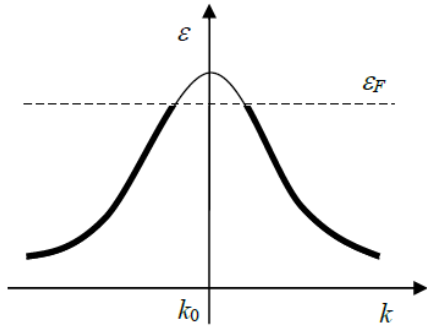
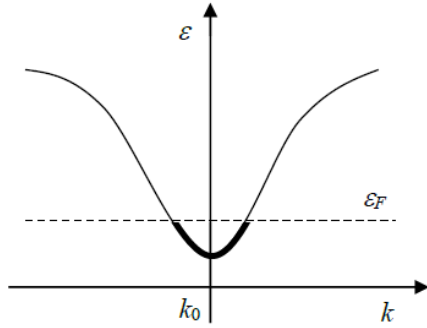
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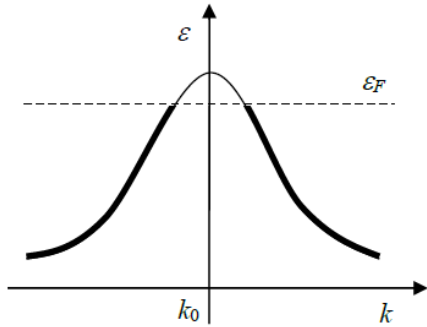
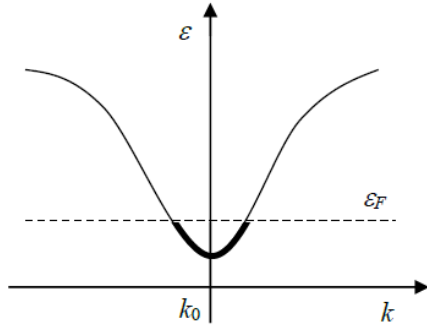
2. Massa efetiva

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$$\varepsilon(k) = \varepsilon_0 \pm \frac{\hbar^2}{2m^*} (k - k_0)^2$$

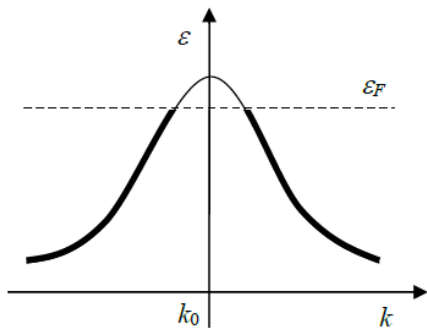
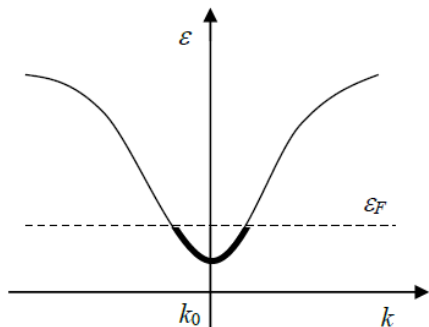
2. Massa efetiva



$$\varepsilon(k) = \varepsilon_0 \pm \frac{\hbar^2}{2m^*} (k - k_0)^2$$

Do ponto de vista clássico $\dot{\mathbf{v}} = \frac{1}{m^*} \mathbf{F}$

2. Massa efetiva



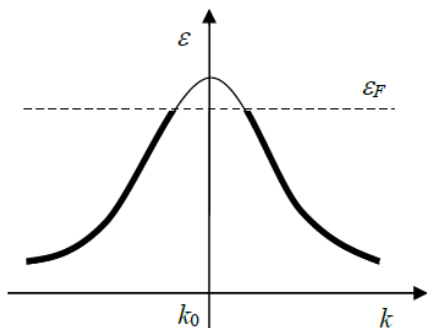
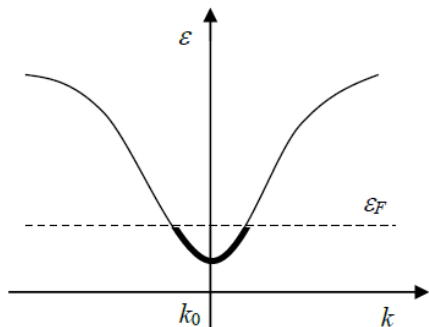
$$\epsilon(k) = \epsilon_0 \pm \frac{\hbar^2}{2m^*} (k - k_0)^2$$

Do ponto de vista clássico $\dot{\mathbf{v}} = \frac{1}{m^*} \mathbf{F}$

Sendo $\dot{v}_{nk} = \frac{d}{dt} \left(\frac{1}{\hbar} \frac{\partial \epsilon_{nk}}{\partial k} \right)$, logo

$$\dot{v}_{\mathbf{k}} = \frac{\partial}{\partial k} \left(\frac{1}{\hbar} \frac{\partial \epsilon_{\mathbf{k}}}{\partial k} \right) \frac{dk}{dt} = \frac{1}{\hbar^2} \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k^2} \hbar \dot{k}$$

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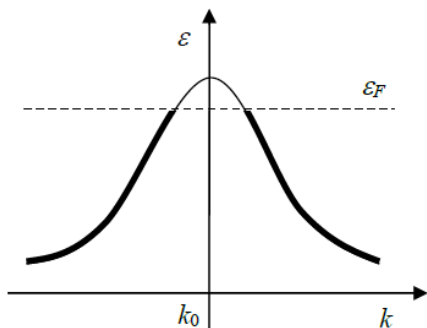
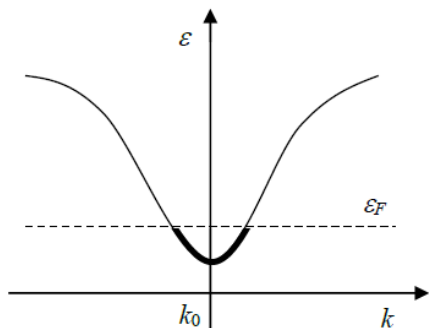
Sendo $\dot{v}_{nk} = \frac{d}{dt} \left(\frac{1}{\hbar} \frac{\partial \varepsilon_{nk}}{\partial k} \right)$, logo

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$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k^2}$$

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$$\varepsilon(k) = \varepsilon_0 \pm \frac{\hbar^2}{2m^*} (k - k_0)^2$$

Do ponto de vista clássico $\dot{\mathbf{v}} = \frac{1}{m^*} \mathbf{F}$

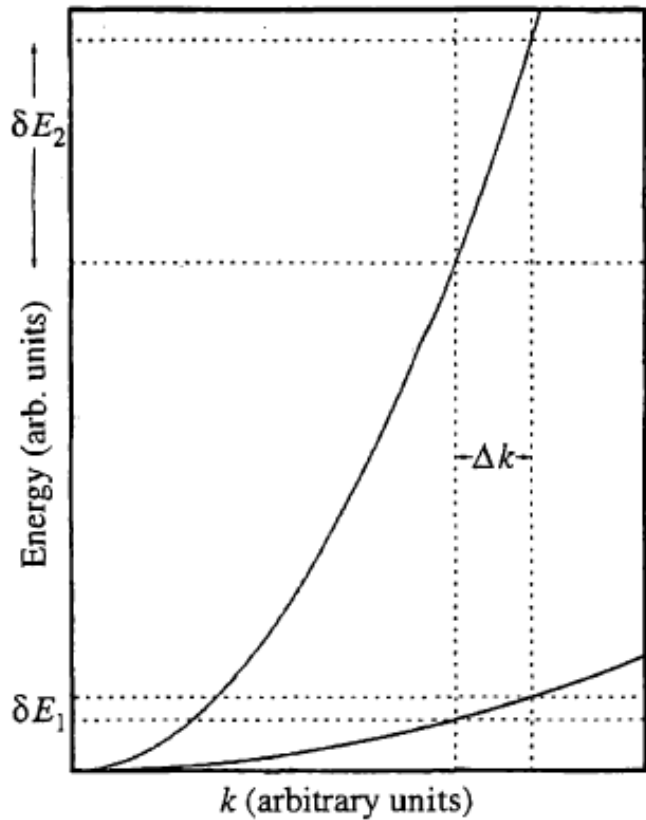
Sendo $\dot{\mathbf{v}}_{n\mathbf{k}} = \frac{d}{dt} \left(\frac{1}{\hbar} \frac{\partial \varepsilon_{n\mathbf{k}}}{\partial \mathbf{k}} \right)$, logo

$$\dot{\mathbf{v}}_{\mathbf{k}} = \frac{\partial}{\partial \mathbf{k}} \left(\frac{1}{\hbar} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} \right) \frac{d\mathbf{k}}{dt} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}^2} \hbar \dot{\mathbf{k}}$$



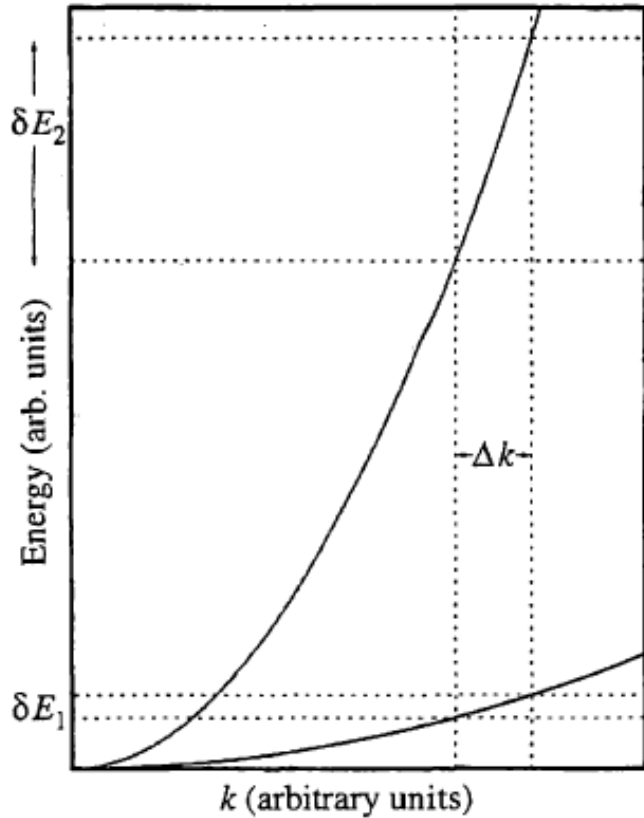
$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}^2}$$

$$\left(\frac{1}{M^*} \right)_{\alpha\beta} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k_\alpha \partial k_\beta}, \quad \alpha, \beta = x, y, z$$



Notem que a massa efetiva pode ser observada pela densidade de estados

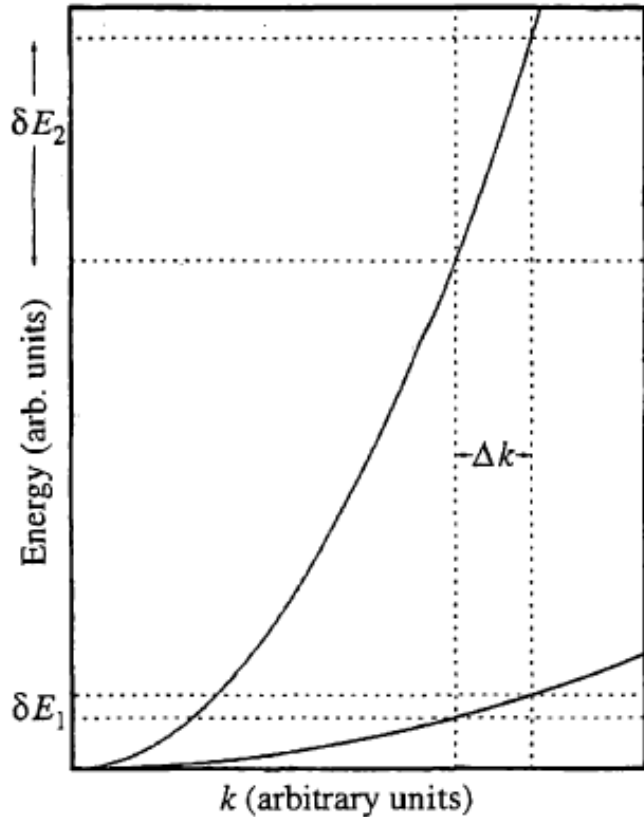
$$g(E) \equiv \frac{dn}{dE}$$



Notem que a massa efetiva pode ser observada pela densidade de estados

$$g(E) \equiv \frac{dn}{dE}$$

$$g(E) \equiv \frac{dn}{dE} = \frac{dn}{dk} \frac{dk}{dE}$$



Notem que a massa efetiva pode ser observada pela densidade de estados

$$g(E) \equiv \frac{dn}{dE}$$

$$g(E) \equiv \frac{dn}{dE} = \frac{dn}{dk} \frac{dk}{dE}$$

$$g(E) \equiv \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{\frac{3}{2}} (E - E_0)^{\frac{1}{2}}.$$

3. Elétrons sob ação de um campo magnético constante

$$\hbar \dot{\mathbf{k}} = -e [\mathbf{E}(\mathbf{r}, t) + \mathbf{v}_{n\mathbf{k}} \times \mathbf{B}(\mathbf{r}, t)]$$

3. Elétrons sob ação de um campo magnético constante

$$\frac{d\mathbf{k}}{dt} = -\frac{e}{\hbar} \mathbf{v}_{\mathbf{k}} \times \mathbf{B},$$

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$$\frac{d\varepsilon_{\mathbf{k}}}{dt} = -e \mathbf{v}_{\mathbf{k}} \cdot (\mathbf{v}_{\mathbf{k}} \times \mathbf{B}) = 0.$$

Trajatórias em superfícies equipotenciais

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Trajatórias em superfícies equipotenciais (Superfície de Fermi)

3. Elétrons sob ação de um campo magnético constante

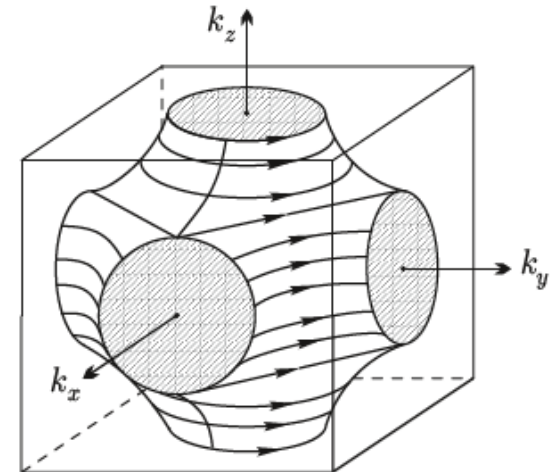
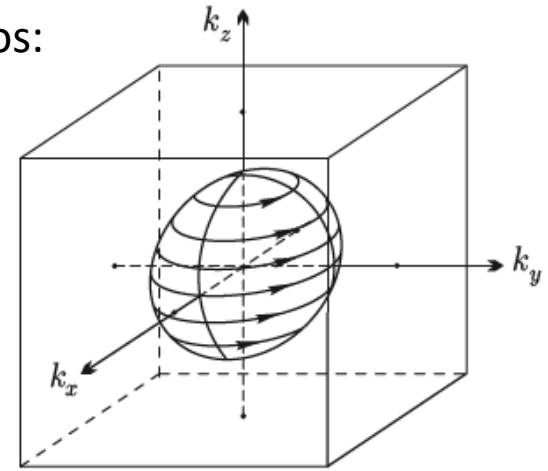
$$\frac{d\mathbf{k}}{dt} = -\frac{e}{\hbar} \mathbf{v}_{\mathbf{k}} \times \mathbf{B},$$

$$\frac{d\varepsilon_{\mathbf{k}}}{dt} = \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} \cdot \frac{d\mathbf{k}}{dt}$$

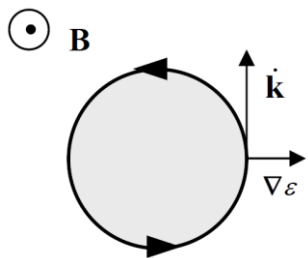
$$\frac{d\varepsilon_{\mathbf{k}}}{dt} = -e \mathbf{v}_{\mathbf{k}} \cdot (\mathbf{v}_{\mathbf{k}} \times \mathbf{B}) = 0$$

Trajatórias em superfícies equipotenciais (Superfície de Fermi)

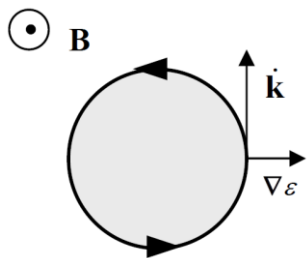
Exemplos:



Órbitas fechadas



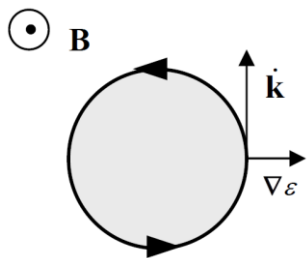
Órbitas fechadas



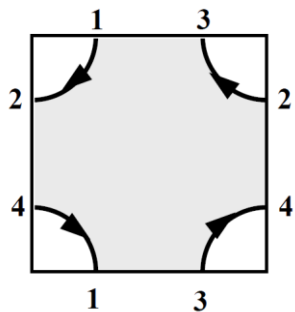
Órbita de elétron



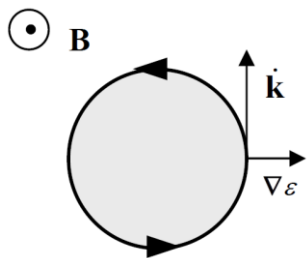
Órbitas fechadas



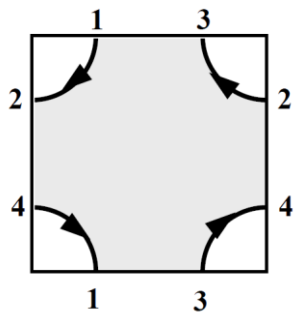
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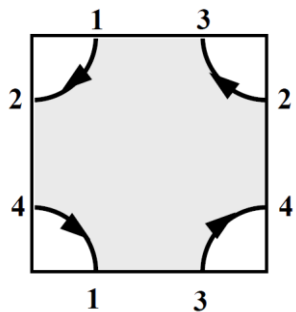
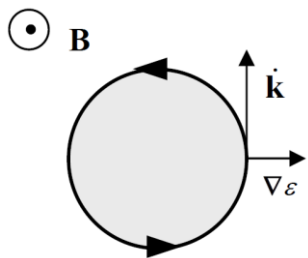
Órbitas fechadas



Órbita de elétron



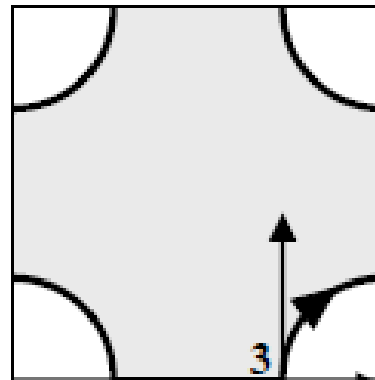
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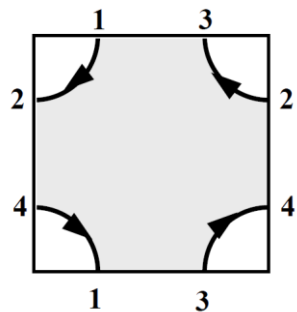
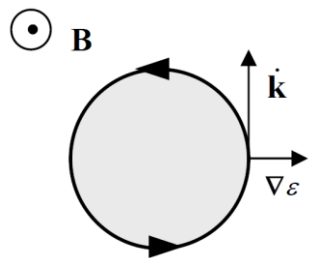
Órbita de elétron



B



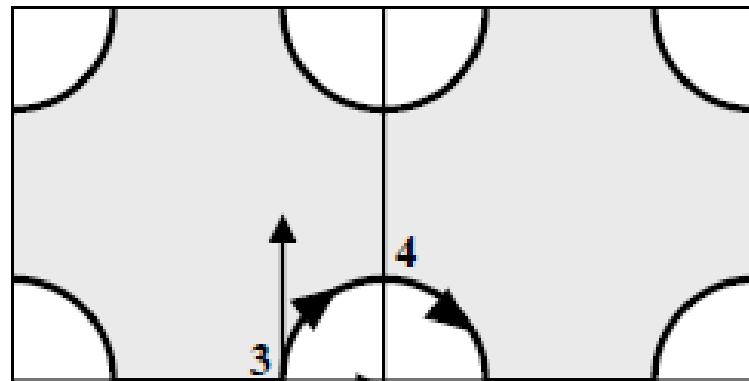
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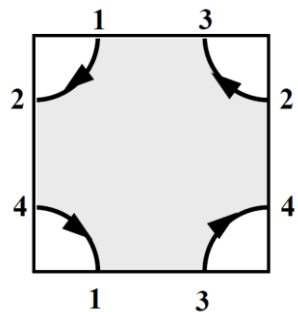
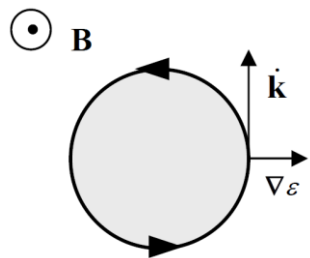
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B



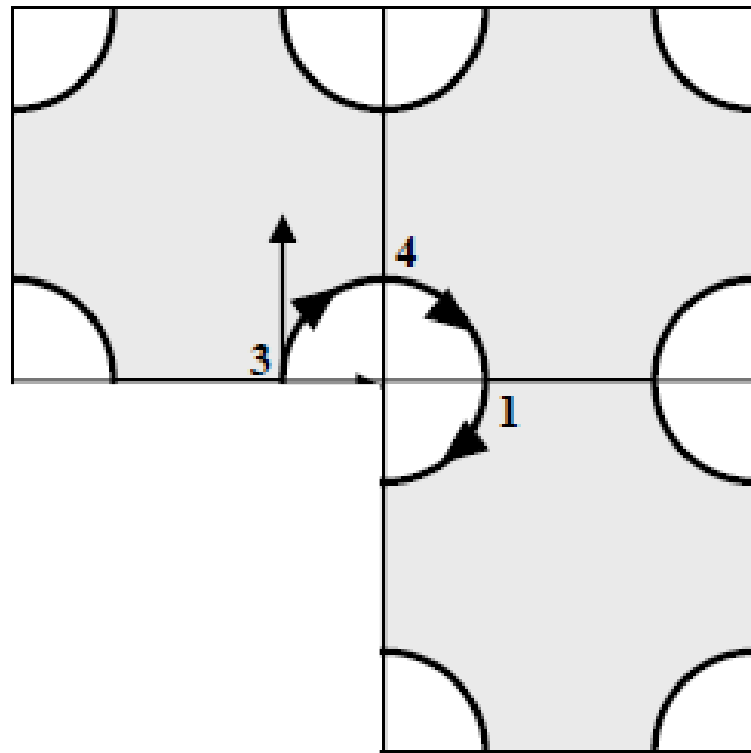
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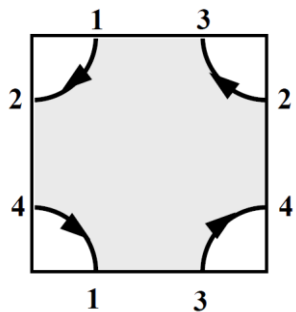
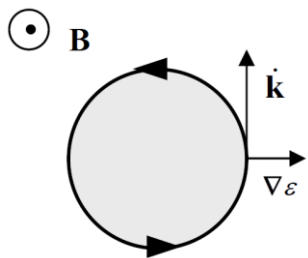
Órbita de elétron



B



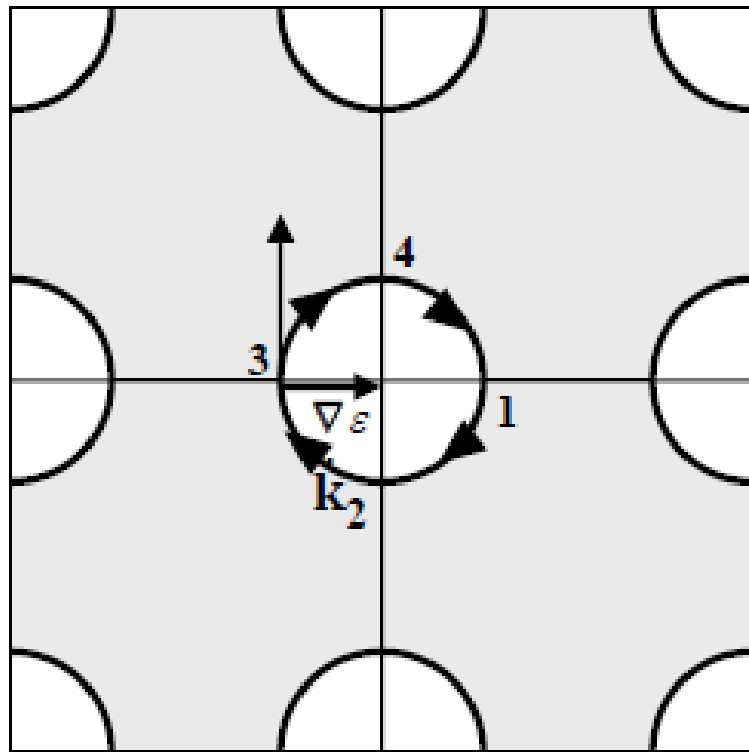
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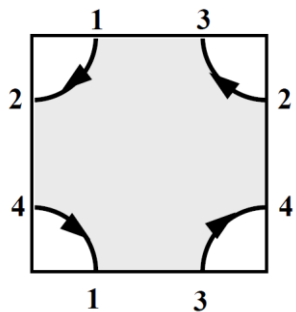
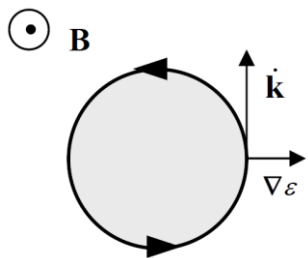
Órbita de elétron



B



Órbitas fechadas

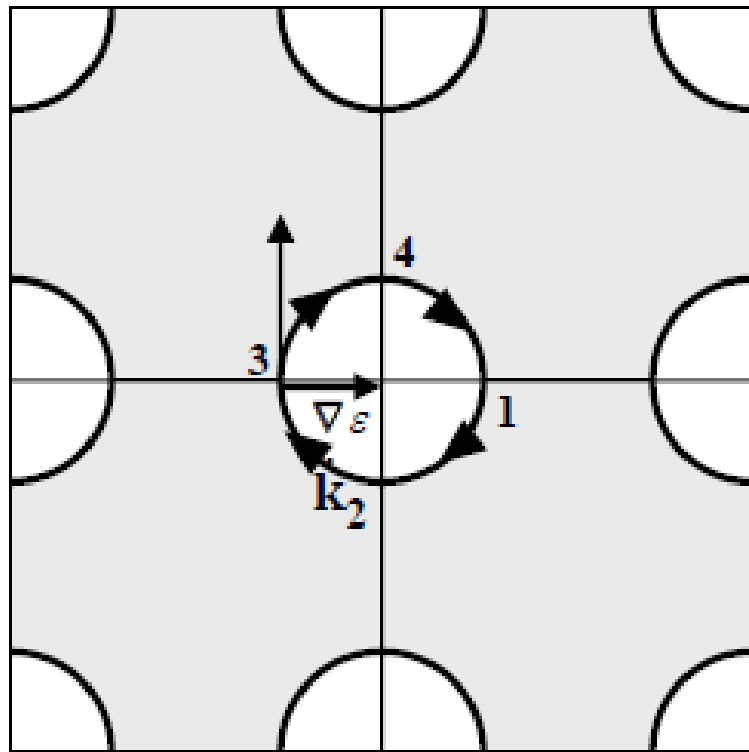


Órbita de elétron

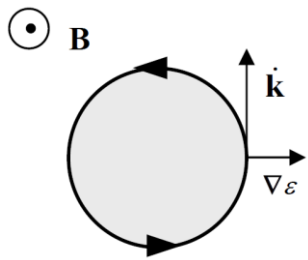


B

Órbita de buraco



Órbitas fechadas

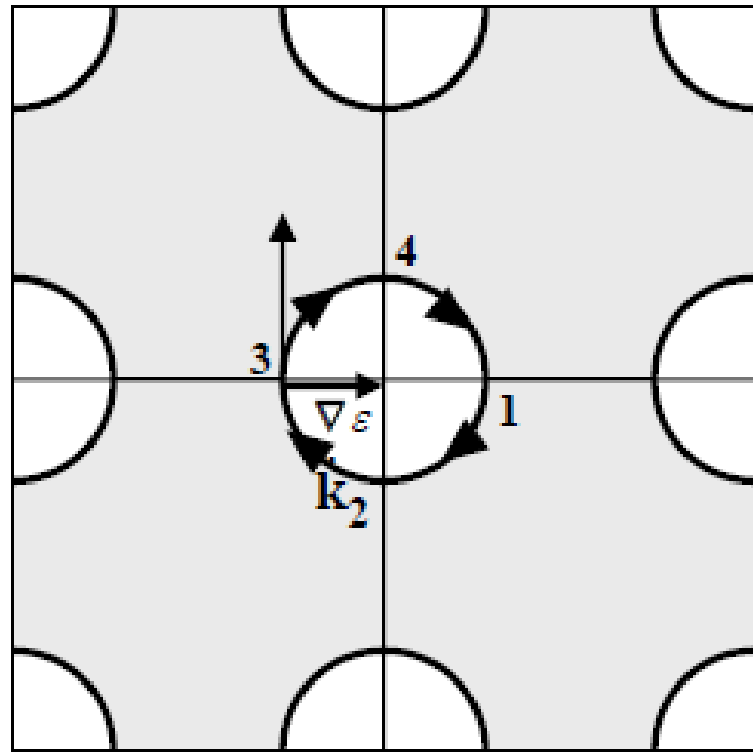


Órbita de elétron



Órbita de buraco

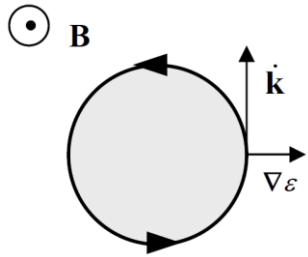
B



$$\omega_c = \frac{eB}{m_c}$$

Freq. de ciclotron

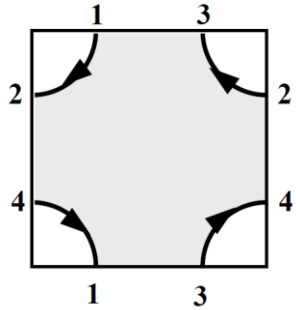
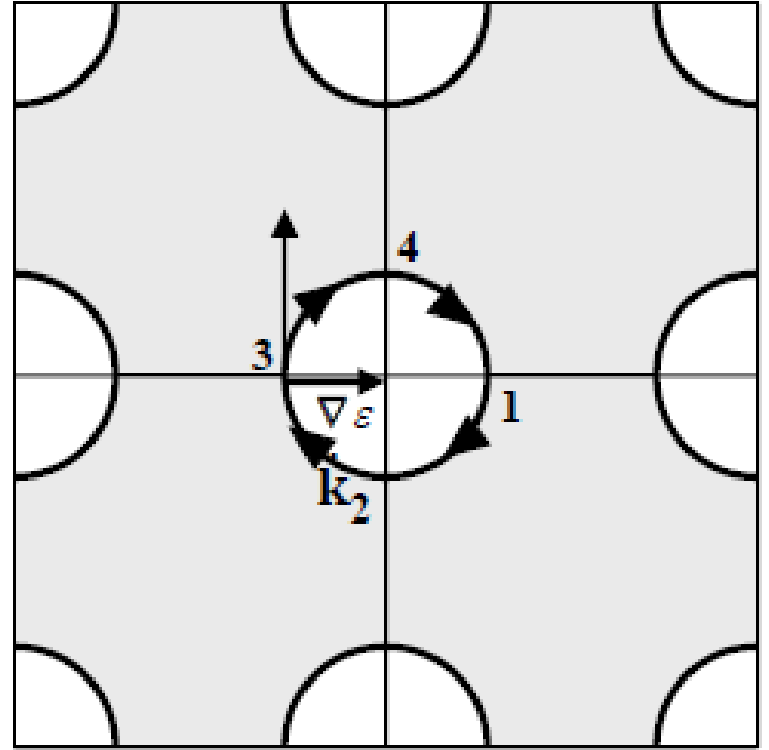
Órbitas fechadas



Órbita de elétron



Órbita de buraco



$$\omega_c = \frac{eB}{m_c}$$

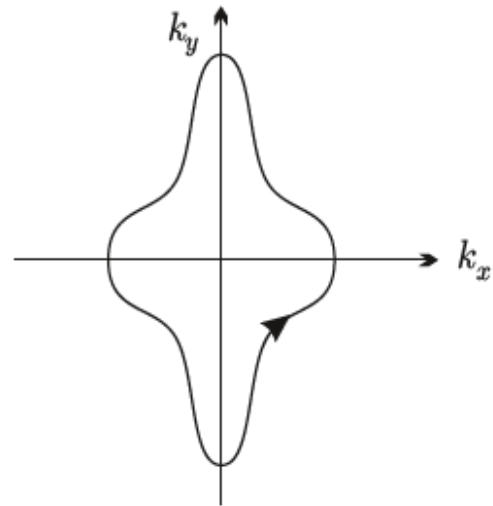
Freq. de ciclotron

$$m_c = \left(\frac{\det M_{ij}^*}{M_{zz}^*} \right)^{1/2}$$

Massa de ciclotron

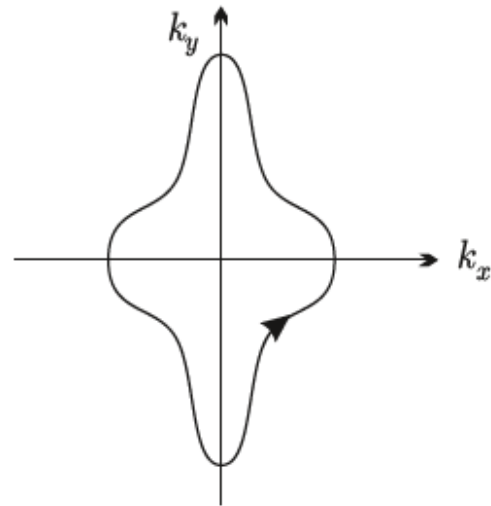
Trajectoria no espaco real:

Trajectoria no espaço real:



Trajetória no espaço real:

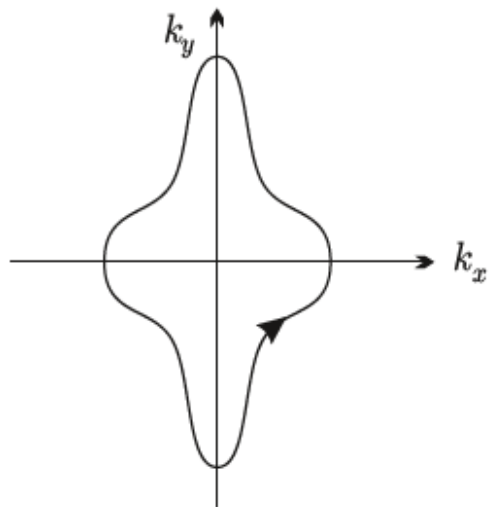
$$\frac{d\mathbf{k}}{dt} = -\frac{e}{\hbar} \left(\frac{d\mathbf{r}}{dt} \times \mathbf{B} \right)$$



Trajetória no espaço real:

$$\frac{d\mathbf{k}}{dt} = -\frac{e}{\hbar} \left(\frac{d\mathbf{r}}{dt} \times \mathbf{B} \right)$$

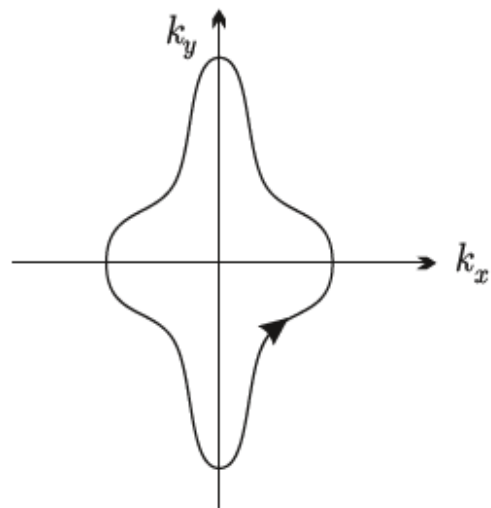
$$\mathbf{k}(t) - \mathbf{k}(0) = -\frac{e}{\hbar} [\mathbf{r}(t) - \mathbf{r}(0)] \times \mathbf{B}.$$



Trajetória no espaço real:

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$$\mathbf{k}(t) - \mathbf{k}(0) = -\frac{e}{\hbar} [\mathbf{r}(t) - \mathbf{r}(0)] \times \mathbf{B}.$$



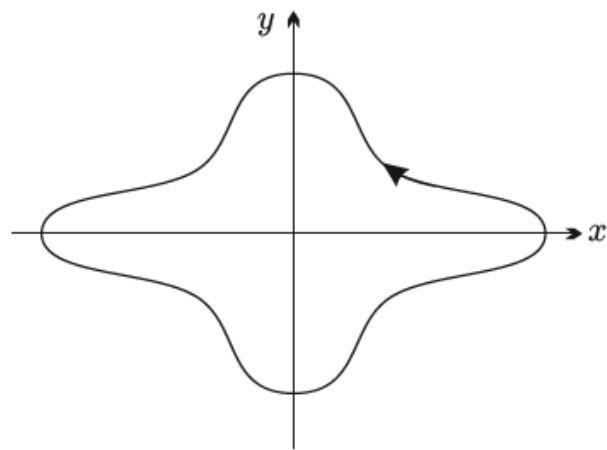
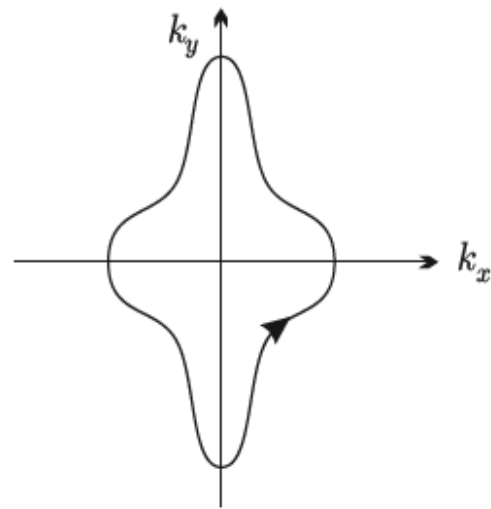
$$\left\{ \begin{array}{l} x(t) - x(0) = \frac{\hbar}{eB} [k_y(t) - k_y(0)], \\ y(t) - y(0) = -\frac{\hbar}{eB} [k_x(t) - k_x(0)]. \end{array} \right.$$

Trajetória no espaço real:

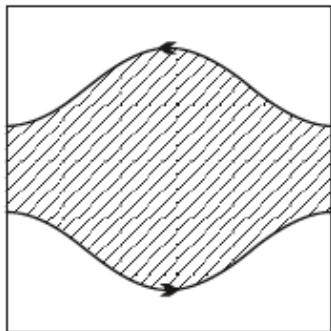
$$\frac{d\mathbf{k}}{dt} = -\frac{e}{\hbar} \left(\frac{d\mathbf{r}}{dt} \times \mathbf{B} \right)$$

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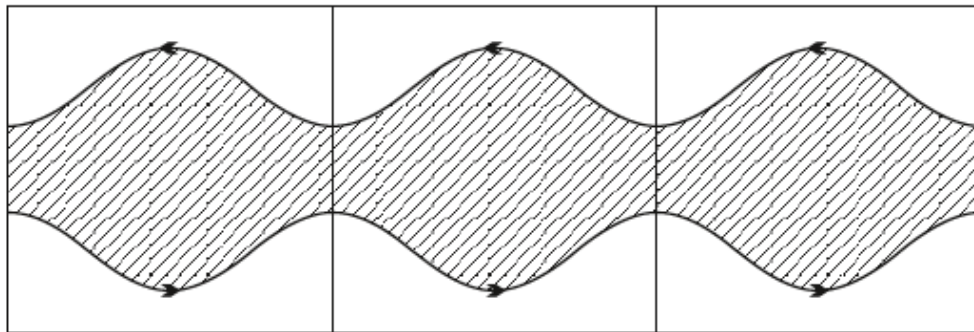
Órbitas abertas



Zona reduzida

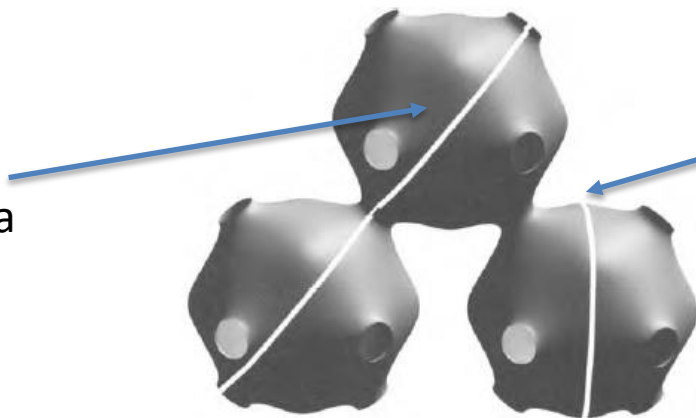


B



Zona estendida

Órbita aberta



Órbita fechada

