

Elétrons em cristais

Contudo, um sólido contém muitos elétrons e íons, daí a Hamiltoniana (não relativística) deve incluir

Energia cinética dos elétrons

Interação elétron-íon

Interação elétron-íon

$$\hat{H} = -\frac{\hbar^2}{2m_e} \sum_i \nabla_i^2 - \sum_{i,I} \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$
$$- \sum_I \frac{\hbar^2}{2M_I} \nabla_I^2 + \frac{1}{2} \sum_{I \neq J} \frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|}$$

Energia cinética dos íons

Interação íon-íon

$$e^2 \rightarrow e^2 / (4\pi\epsilon_0)$$

\vec{R}_I → posição do I-ésimo íon

\vec{r}_i → posição do i-ésimo elétron

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Pot. Periódico

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Constante

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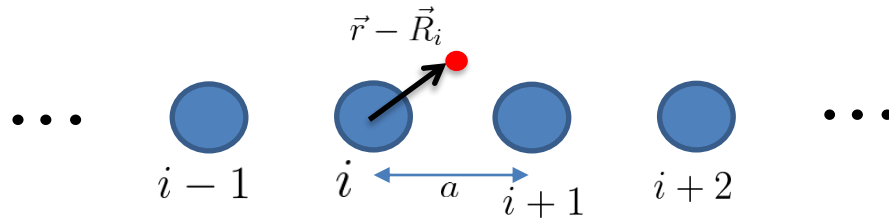
$\vec{r}_i \rightarrow$ posição do i-ésimo elétron

Elétrons em cristais

Sem perda de generalidade, podemos aproximar um problema de elétrons em sólidos como um problema de elétrons em um potencial periódico. Isto é, as autofunções eletrônicas devem satisfazer à Eq. de Schrödinger

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$V(\mathbf{r} + \mathbf{R}) = V(\mathbf{r})$$
$$\forall \mathbf{R} \in \text{Rede de Bravais}$$



Teorema de Bloch

$$\left[-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r})$$

- As autofunções deste Hamiltoniano são da forma:

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

com

$$u_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R})$$

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Alternativamente

$$\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}} \psi_{n\mathbf{k}}(\mathbf{r})$$

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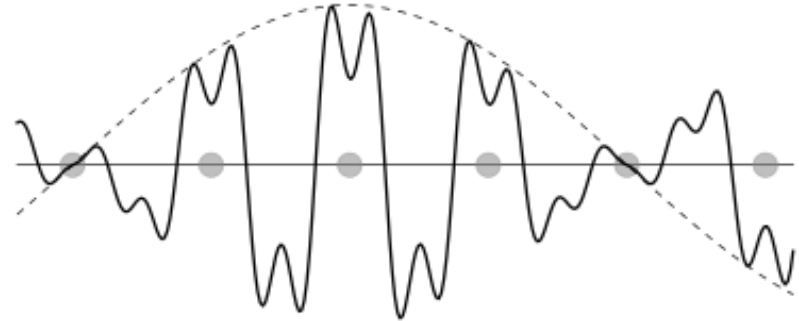
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$$u_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R})$$

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Demonstração:

Seja $T_{\mathbf{R}}$ um operador de translação por \mathbf{R} , i.e. $T_{\mathbf{R}} f(\mathbf{r}) = f(\mathbf{r} + \mathbf{R})$, então

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$$\Rightarrow [T_{\mathbf{R}}, H] = 0$$


$$T_{\mathbf{R}}[H(\mathbf{r})\psi(\mathbf{r})] = H(\mathbf{r} + \mathbf{R})\psi(\mathbf{r} + \mathbf{R})$$

$$T_{\mathbf{R}}[H(\mathbf{r})\psi(\mathbf{r})] = H(\mathbf{r})T_{\mathbf{R}}\psi(\mathbf{r})$$

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$$T_{\mathbf{R}}T_{\mathbf{R}'}\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{R}' + \mathbf{R})$$

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Com isso, $T_{\mathbf{R}}$ e H formam um C.S.C.O

$$\begin{cases} H\psi = \varepsilon\psi \\ T_{\mathbf{R}}\psi = c(\mathbf{R})\psi \end{cases}$$

onde $c(\mathbf{R})$ são os autovalores de $T_{\mathbf{R}}$

Teorema de Bloch

Demonstração:

Contudo, $T_{\mathbf{R}}$ possui propriedades muito particulares

$$\begin{aligned}T_{\mathbf{R}}T_{\mathbf{R}'}\psi &= c(\mathbf{R})c(\mathbf{R}')\psi \\ &= T_{\mathbf{R}+\mathbf{R}'}\psi = c(\mathbf{R} + \mathbf{R}')\psi\end{aligned}$$

Qual função satisfaz essa propriedade?

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$$c(\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}$$

Em princípio, \mathbf{k} pode ser real ou complexo.

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Dado as PBC, temos $\psi(\mathbf{r}) = \psi(\mathbf{r} + N_i \mathbf{a}_i) = e^{i\mathbf{k}\cdot(N_i \mathbf{a}_i)} \psi(\mathbf{r})$, logo \mathbf{k} deve ser real para satisfazer

$$e^{i\mathbf{k}\cdot(N_i \mathbf{a}_i)} = 1$$

Teorema de Bloch

Demonstração:

Como $\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$, então é natural definirmos


$$\mathbf{k} = x_1 \mathbf{b}_1 + x_2 \mathbf{b}_2 + x_3 \mathbf{b}_3$$

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$$x_1 = \frac{n_1}{N_1}; \quad x_2 = \frac{n_2}{N_2}; \quad x_3 = \frac{n_3}{N_3},$$

Com isso, mostramos que $\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{R}} \psi_{n\mathbf{k}}(\mathbf{r})$

Consequências do teorema de Bloch

1. $\hbar\mathbf{k}$ NÃO é autovalor do operador momento linear \mathbf{P}

$$\begin{aligned}\mathbf{p}\psi_{n\mathbf{k}} &= -i\hbar\vec{\nabla}\left[e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})\right] \\ &= \hbar\mathbf{k}\psi_{n\mathbf{k}} - i\hbar e^{i\mathbf{k}\cdot\mathbf{r}}\vec{\nabla}u_{n\mathbf{k}}(\mathbf{r})\end{aligned}$$

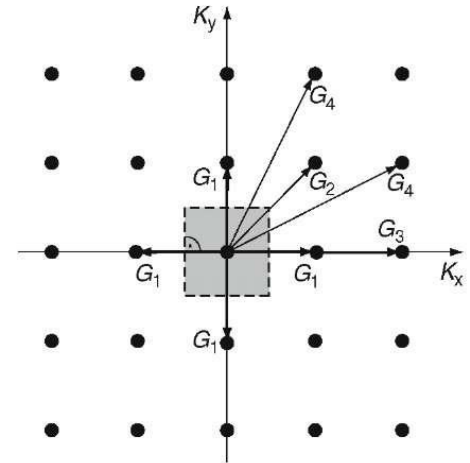
$\hbar\mathbf{k}$ é momento cristalino

2. Valores não repetidos (degenerados) de \mathbf{k} estão sempre dentro da 1ª ZB

$$\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r})$$

$$\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{G}\cdot\mathbf{R}}e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r})$$

$$\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r})$$

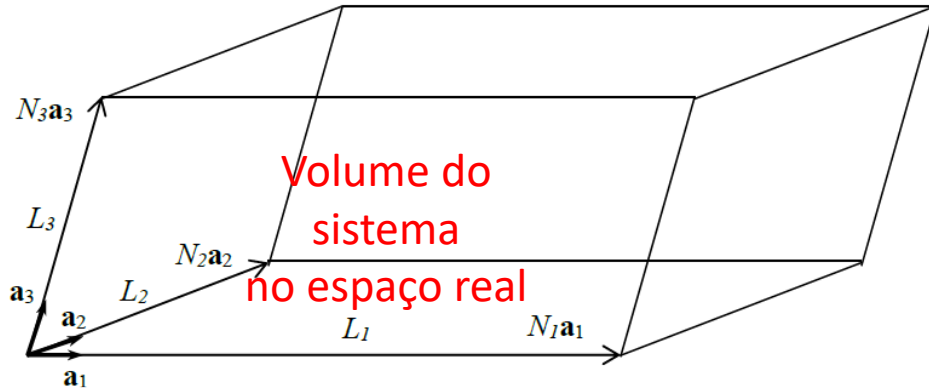
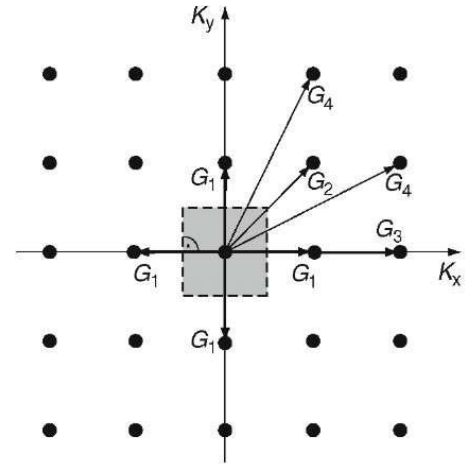


Consequências do teorema de Bloch

$$2. \quad \psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) = \Psi_{n(\mathbf{k}+\mathbf{G})}(\mathbf{r})$$

$$\Psi_{n(\mathbf{k}+\mathbf{G})}(\mathbf{r}) = e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} u_{n(\mathbf{k}+\mathbf{G})}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

$$e^{i\mathbf{G}\cdot\mathbf{r}} u_{n(\mathbf{k}+\mathbf{G})}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r})$$



3. Temos $N_1 \times N_2 \times N_3$ estados de momento na 1ª ZB

4. A velocidade de um elétron de Bloch é $\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar} \vec{\nabla}_{\mathbf{k}} \varepsilon_n(\mathbf{k})$ ($\mathbf{v}_g = d\omega/d\mathbf{k} = \hbar^{-1} d\varepsilon/d\mathbf{k}$)

Equação Central

$$\left[\frac{-\hbar^2 \nabla^2}{2m} + U(\mathbf{r}) \right] \psi = \varepsilon \psi$$

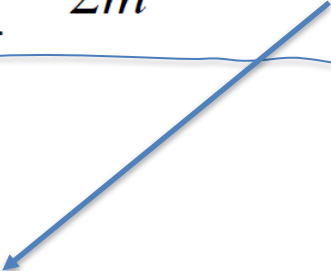
Se buscarmos resolver a Eq. de Schrodinger para um caso genérico, é útil trabalharmos no espaço recíproco.

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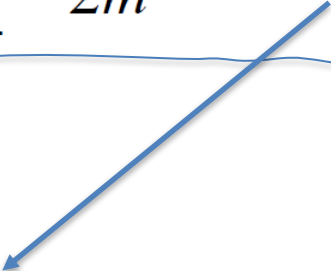
$$\psi_k(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_k(\mathbf{r})$$


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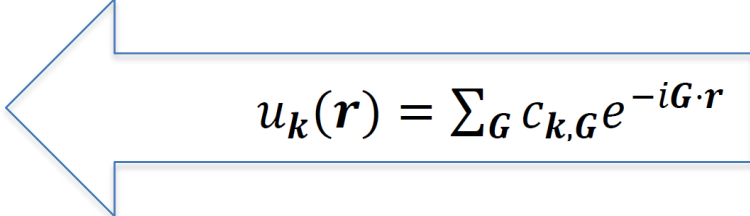
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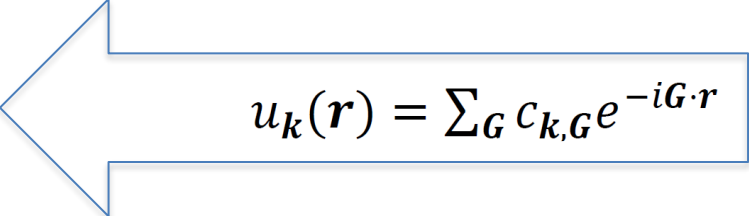
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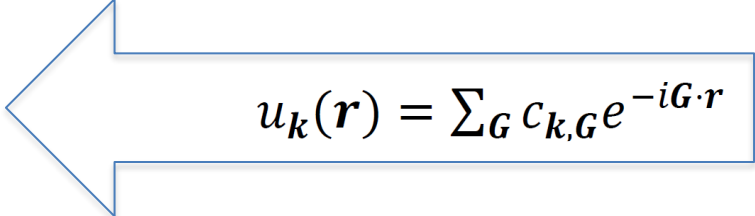
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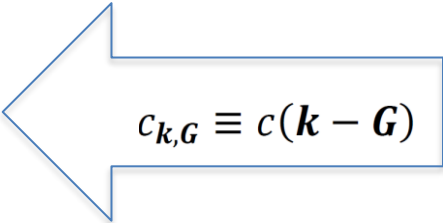
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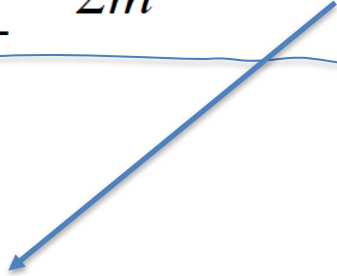
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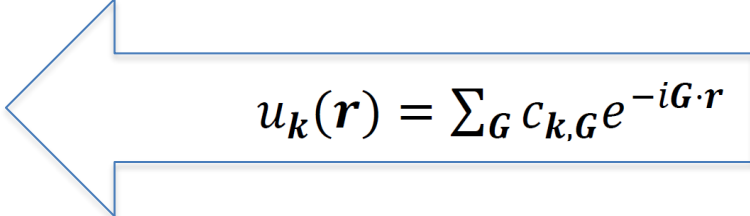
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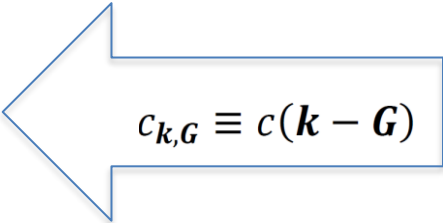
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$$\sum_{\mathbf{G}} \left[\frac{\hbar^2 (\mathbf{k} - \mathbf{G})^2}{2m} - \varepsilon \right] c(\mathbf{k} - \mathbf{G}) e^{i(\mathbf{k} - \mathbf{G}) \cdot \mathbf{r}} + \sum_{\mathbf{G}, \mathbf{G}'} U_{\mathbf{G}'} c(\mathbf{k} - \mathbf{G}) e^{i(\mathbf{k} - \mathbf{G} + \mathbf{G}') \cdot \mathbf{r}} = 0$$

$$\left[\frac{\hbar^2 (\mathbf{k} - \mathbf{G}'')^2}{2m} - \varepsilon \right] c(\mathbf{k} - \mathbf{G}'') + \sum_{\mathbf{G}, \mathbf{G}'} U_{\mathbf{G}'} c(\mathbf{k} - \mathbf{G}) \delta_{\mathbf{G}'', \mathbf{G} - \mathbf{G}'} = 0$$

$$\left[\frac{\hbar^2 (\mathbf{k} - \mathbf{G}'')^2}{2m} - \varepsilon \right] c(\mathbf{k} - \mathbf{G}'') + \sum_{\mathbf{G}'} U_{\mathbf{G}'} c(\mathbf{k} - \mathbf{G}'' - \mathbf{G}') = 0$$

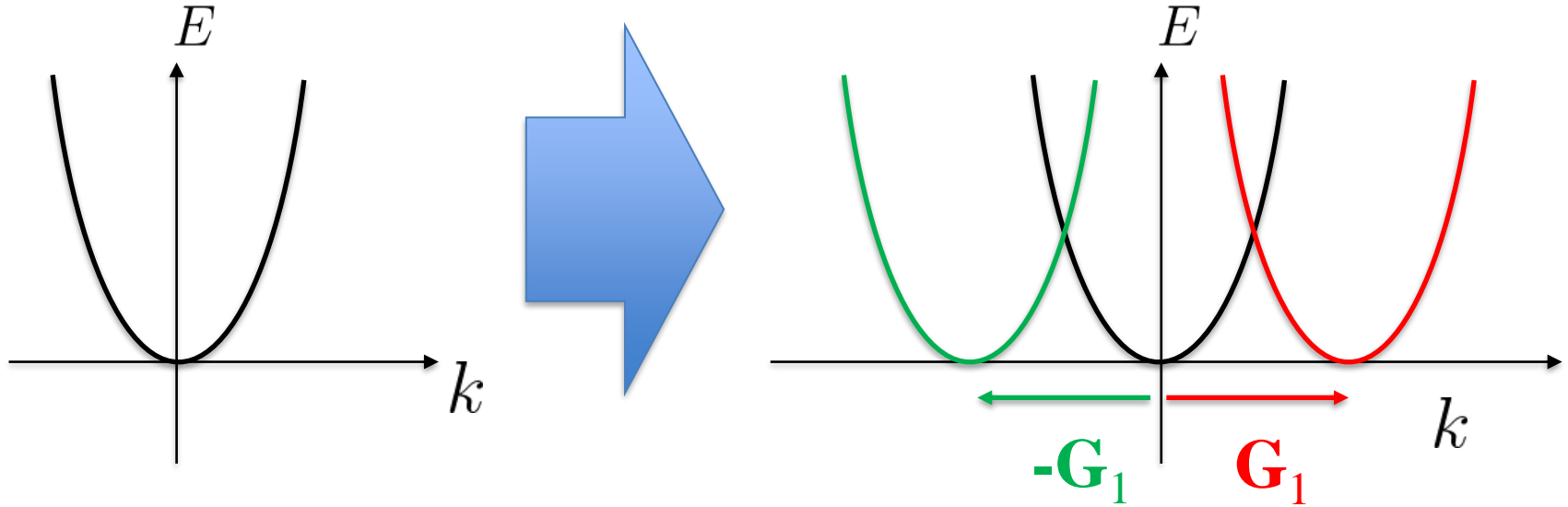
$$\boxed{\left[\frac{\hbar^2 (\mathbf{k} - \mathbf{G})^2}{2m} - \varepsilon \right] c(\mathbf{k} - \mathbf{G}) + \sum_{\mathbf{G}'} U_{\mathbf{G}' - \mathbf{G}} c(\mathbf{k} - \mathbf{G}') = 0}$$

Equação Central

$$\begin{pmatrix} \lambda_{\mathbf{k}-\mathbf{G}_1} - \varepsilon + U_0 & U_{\mathbf{G}_2-\mathbf{G}_1} & U_{\mathbf{G}_3-\mathbf{G}_1} & \dots \\ U_{\mathbf{G}_1-\mathbf{G}_2} & \lambda_{\mathbf{k}-\mathbf{G}_2} - \varepsilon + U_0 & U_{\mathbf{G}_3-\mathbf{G}_2} & \dots \\ U_{\mathbf{G}_1-\mathbf{G}_3} & U_{\mathbf{G}_2-\mathbf{G}_3} & \lambda_{\mathbf{k}-\mathbf{G}_3} - \varepsilon + U_0 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c(\mathbf{k}-\mathbf{G}_1) \\ c(\mathbf{k}-\mathbf{G}_2) \\ c(\mathbf{k}-\mathbf{G}_3) \\ \vdots \end{pmatrix} = 0$$

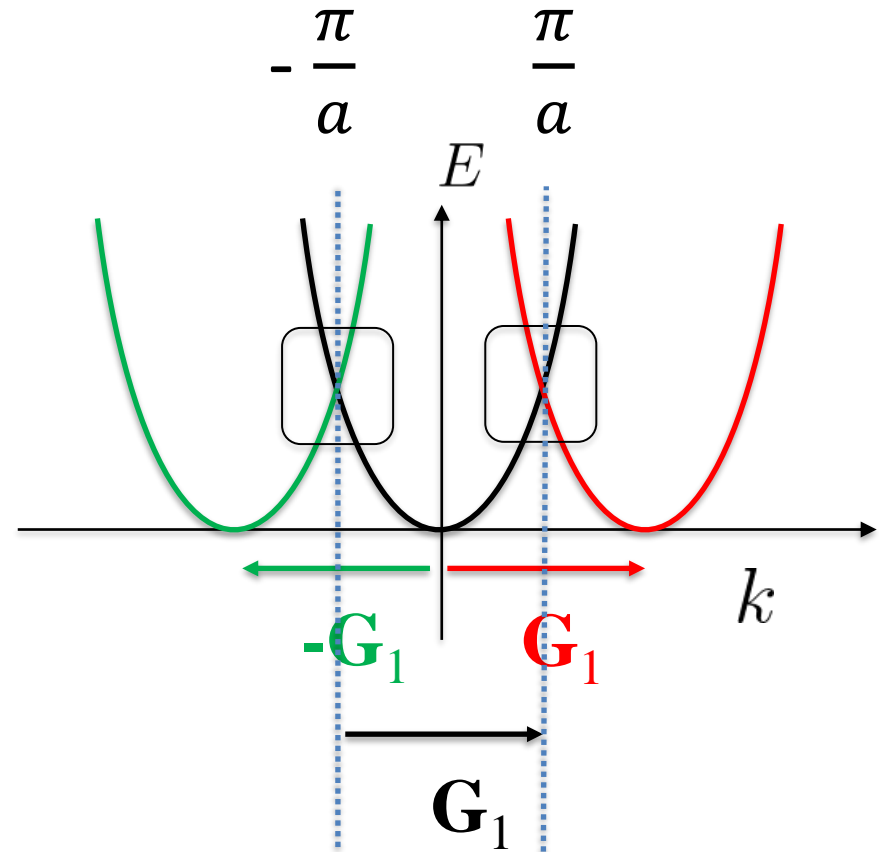
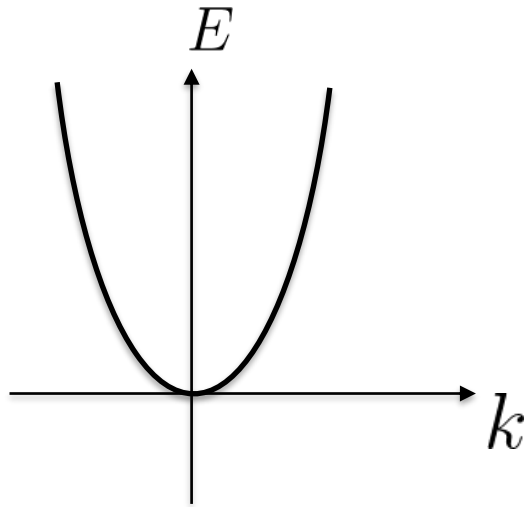
Potencial Periódico Fraco

$$V(x) = 0$$



Potencial Periódico Fraco

$$V(x) = 0$$



Potencial Periódico Fraco

$$V(x) \neq 0$$

Teoria de Perturbação de 1ª ordem

$$\varepsilon_n(\mathbf{k}) = \lambda_{\mathbf{k}-\mathbf{G}_n} + \langle \mathbf{k} - \mathbf{G}_n | U | \mathbf{k} - \mathbf{G}_n \rangle$$



$$\langle \mathbf{k} - \mathbf{G}_n | U | \mathbf{k} - \mathbf{G}_n \rangle = \frac{1}{v_{cel}} \int_{v_{cel}} d\mathbf{r} e^{-i(\mathbf{k}-\mathbf{G}_n)\cdot\mathbf{r}} U(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{G}_n)\cdot\mathbf{r}} = U_0$$



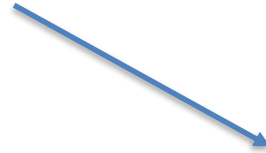
Constante!!

Potencial Periódico Fraco

$$V(x) \neq 0$$

Teoria de Perturbação de 2ª ordem (não degenerado)

$$\varepsilon_n(\mathbf{k}) = \lambda_{\mathbf{k}-\mathbf{G}_n} + \sum_{j \neq n} \frac{|U_{\mathbf{G}_j - \mathbf{G}_n}|^2}{\lambda_{\mathbf{k}-\mathbf{G}_n} - \lambda_{\mathbf{k}-\mathbf{G}_j}}$$



Só é adequado longe das bordas das ZB

Potencial Periódico Fraco

$$V(x) \neq 0$$

Teoria de Perturbação de 2ª ordem (degenerado)

- Para k próximo de $k = \frac{\pi n}{a}$ temos

$$|E^{(0)}(k) - E^{(0)}(k')| \lesssim V$$

Logo, podemos nos limitar aos subspaços de k e k' , de modo que as energias neste são dadas pelos autovalores da matriz secular

$$\begin{pmatrix} \langle k | H | k \rangle & \langle k | H | k' \rangle \\ \langle k' | H | k \rangle & \langle k' | H | k' \rangle \end{pmatrix} = \begin{pmatrix} E^{(0)}(k) & V_{(k-k')} \\ V_{(k-k')} & E^{(0)}(k') \end{pmatrix}$$

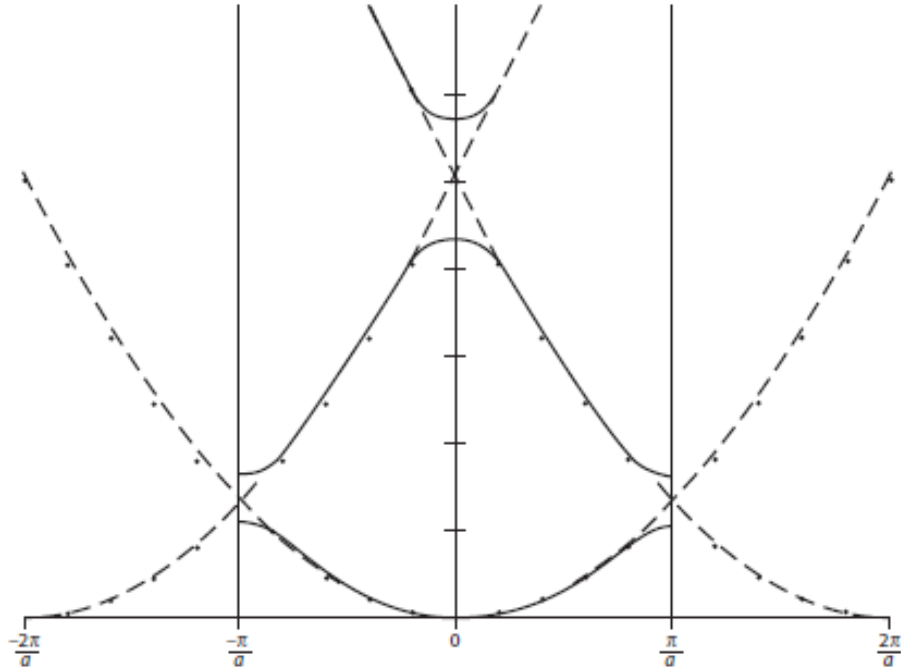
No caso em que k está na borda de alguma zona de Brillouin ($E^{(0)}(k) = E^{(0)}(k')$)

$$E_{\pm}(k) = E^{(0)}(k) \pm |V_{(k-k')}|$$

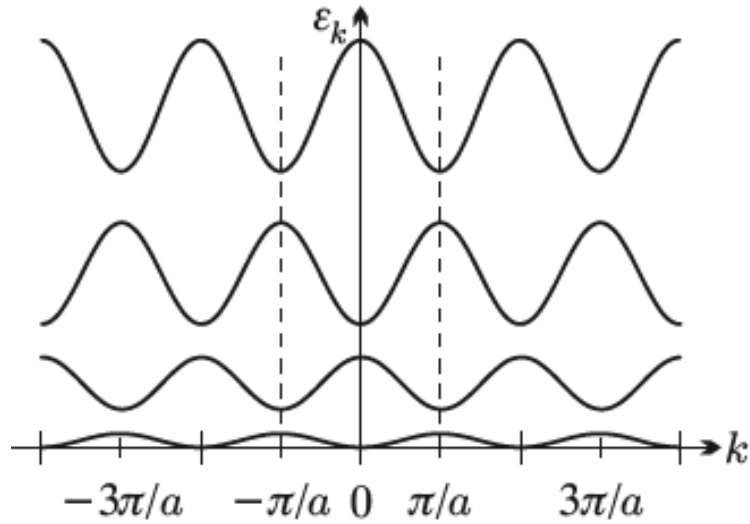
Potencial Periódico Fraco

$$V(x) \neq 0$$

Teoria de Perturbação de 2ª ordem (degenerado)

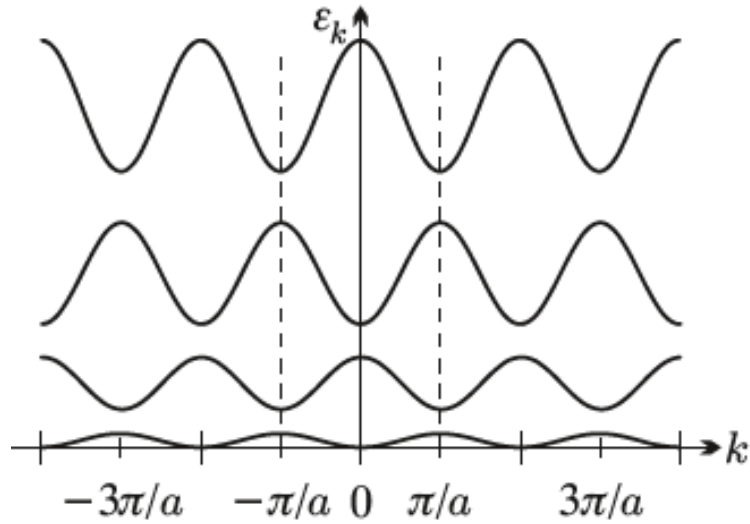


Potencial Periódico Fraco

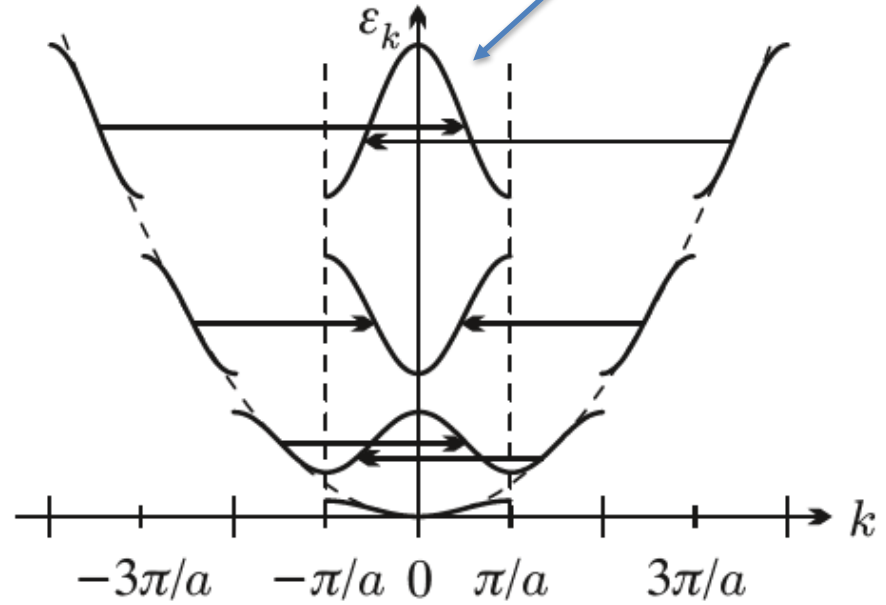


Zona repetida

Potencial Periódico Fraco

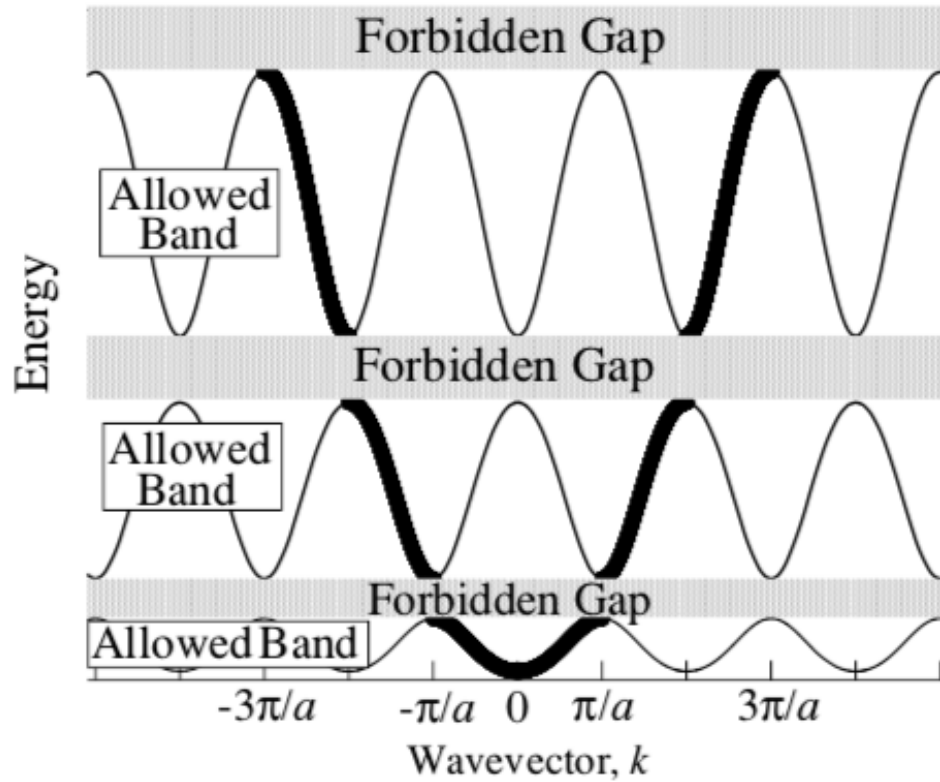


Zona repetida

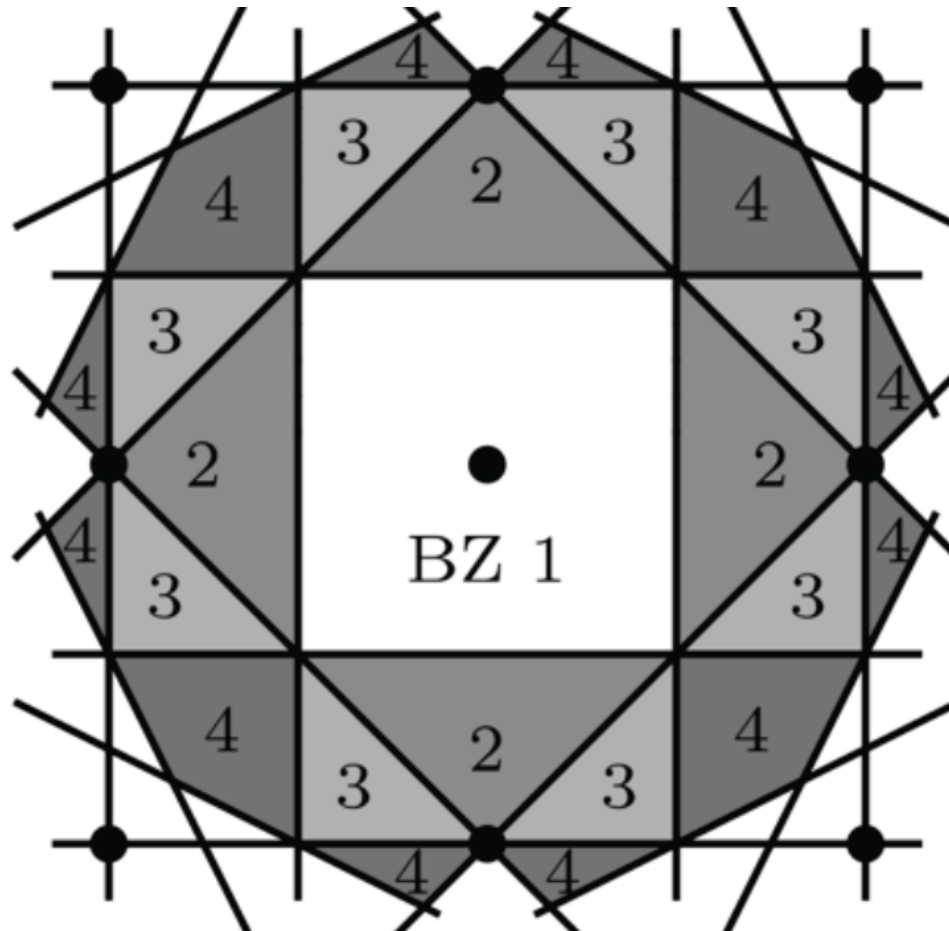


Zona estendida

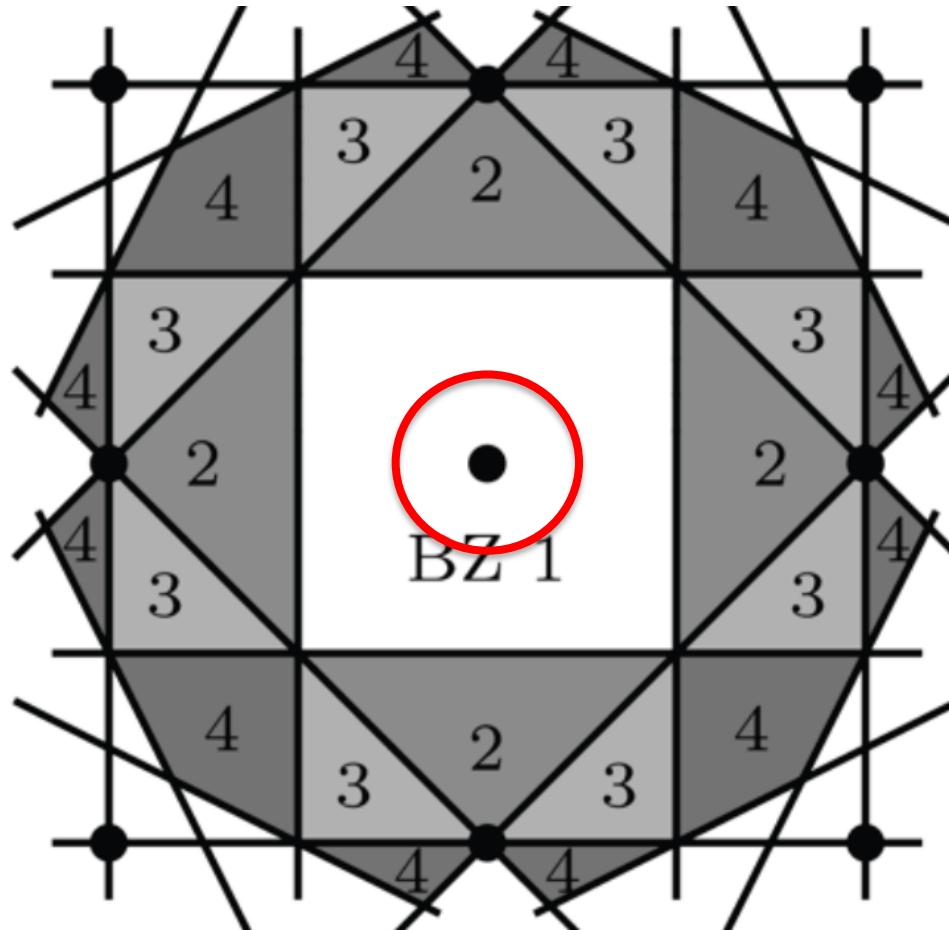
Potencial Periódico Fraco



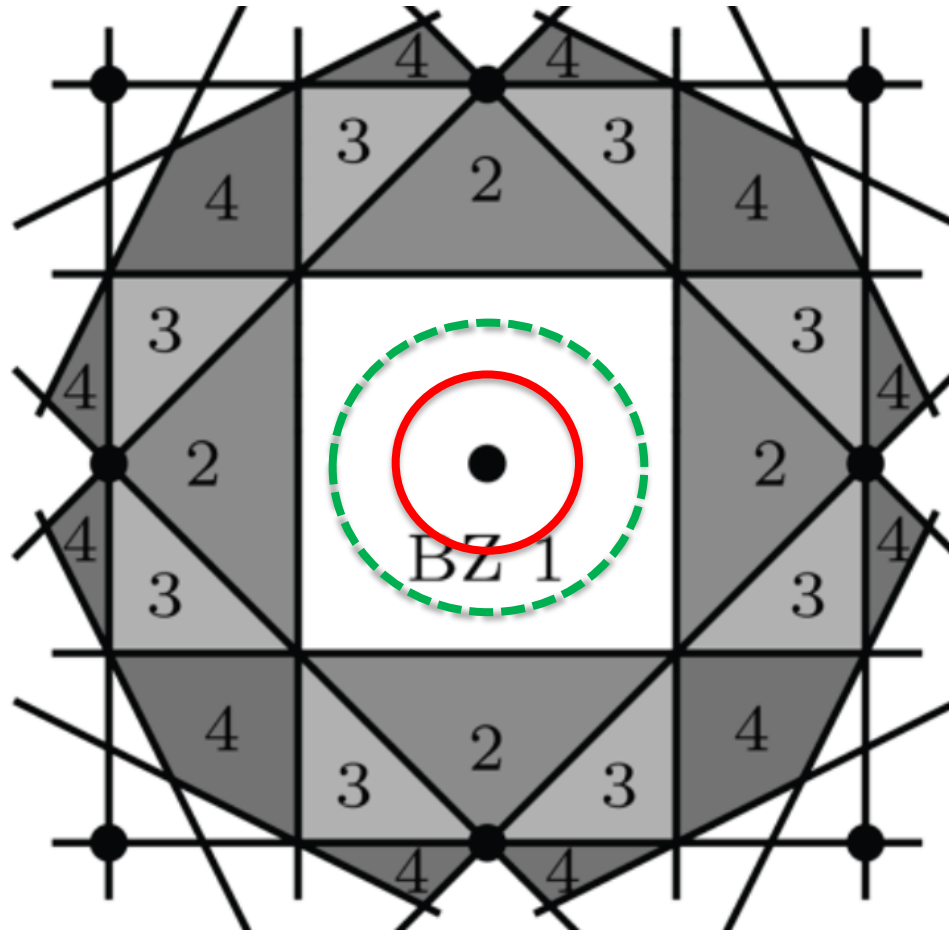
Zonas de Brillouin e sup. de Fermi



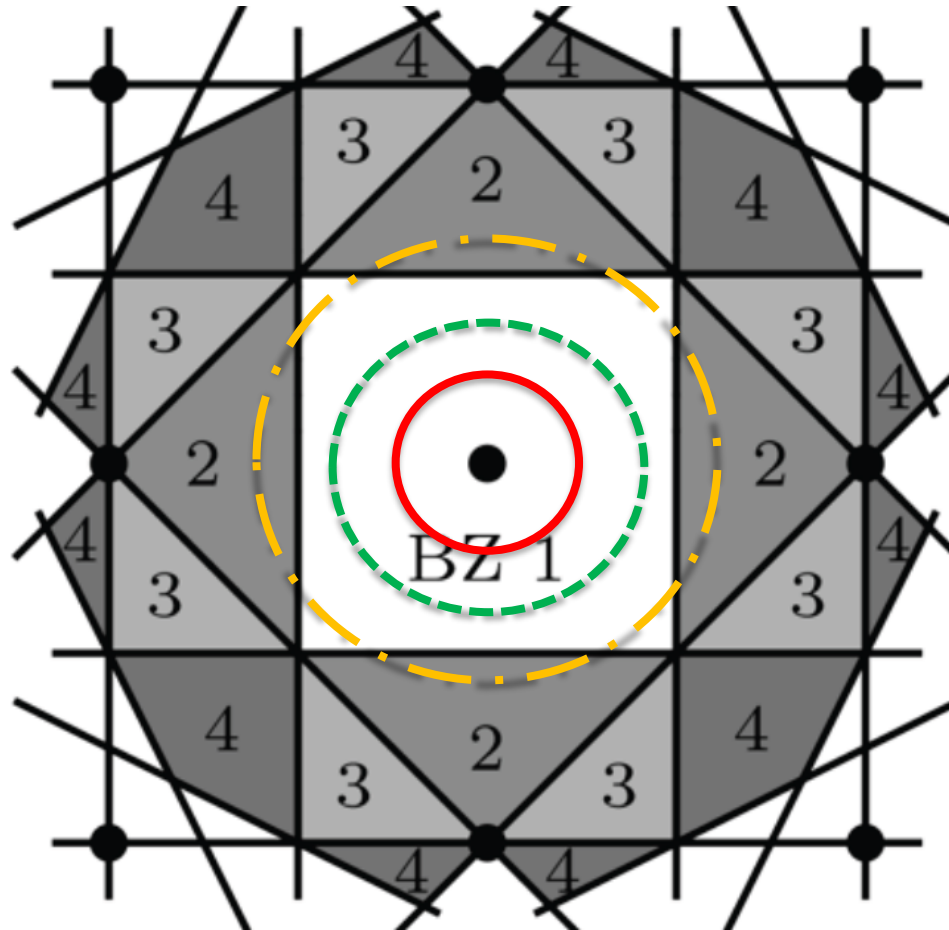
Zonas de Brillouin e sup. de Fermi



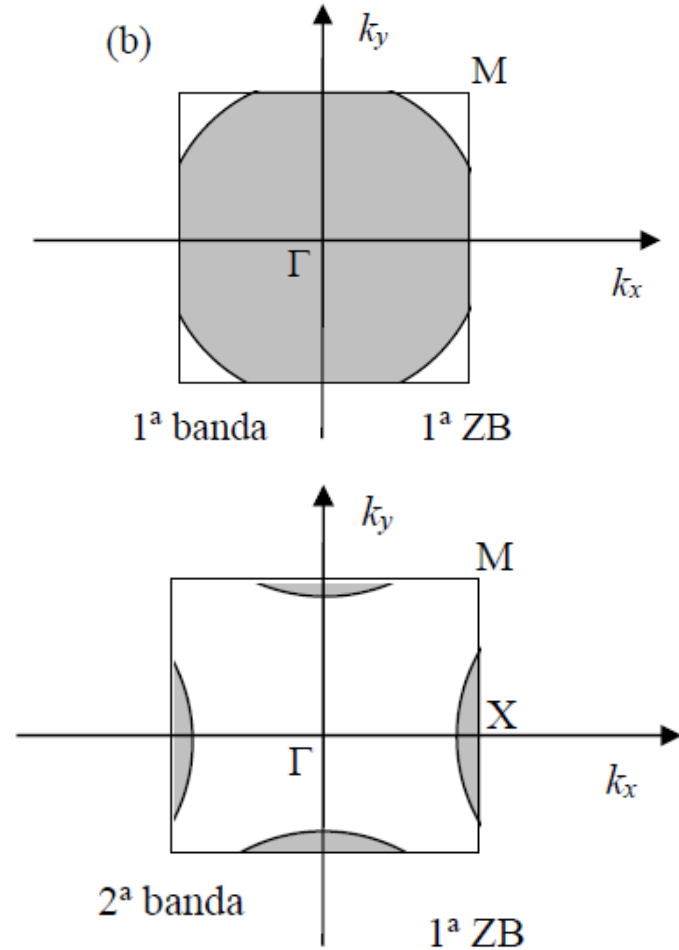
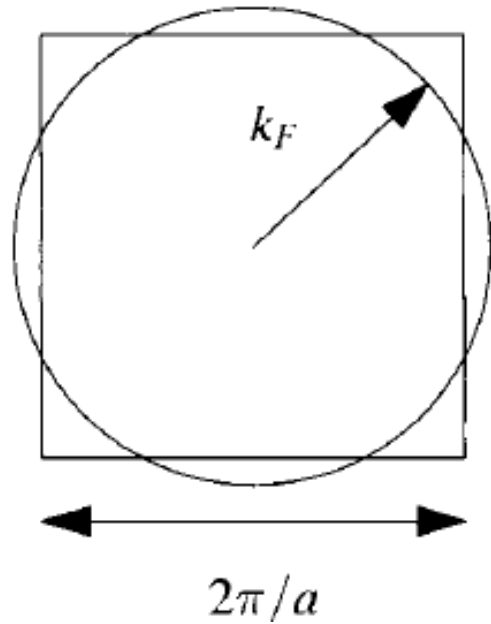
Zonas de Brillouin e sup. de Fermi



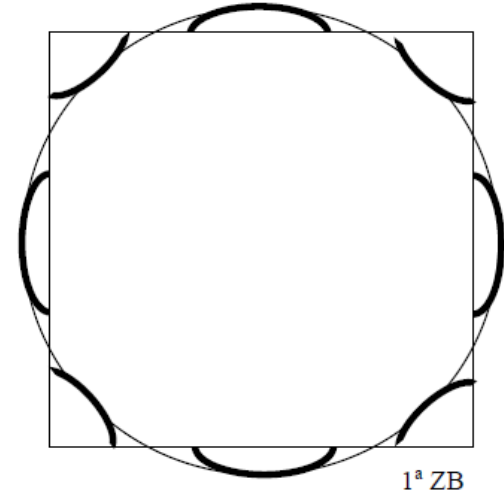
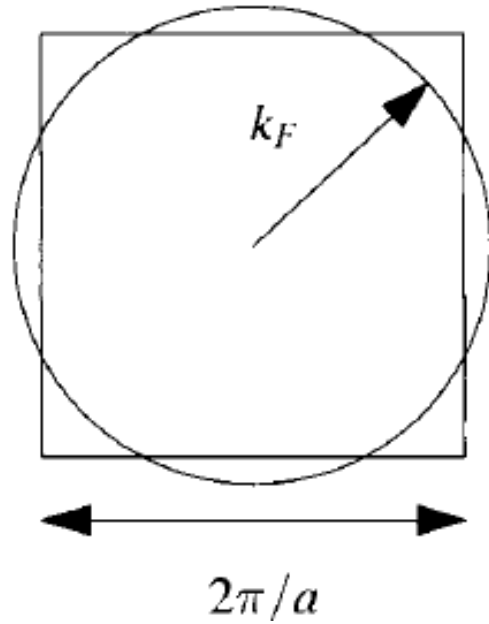
Zonas de Brillouin e sup. de Fermi



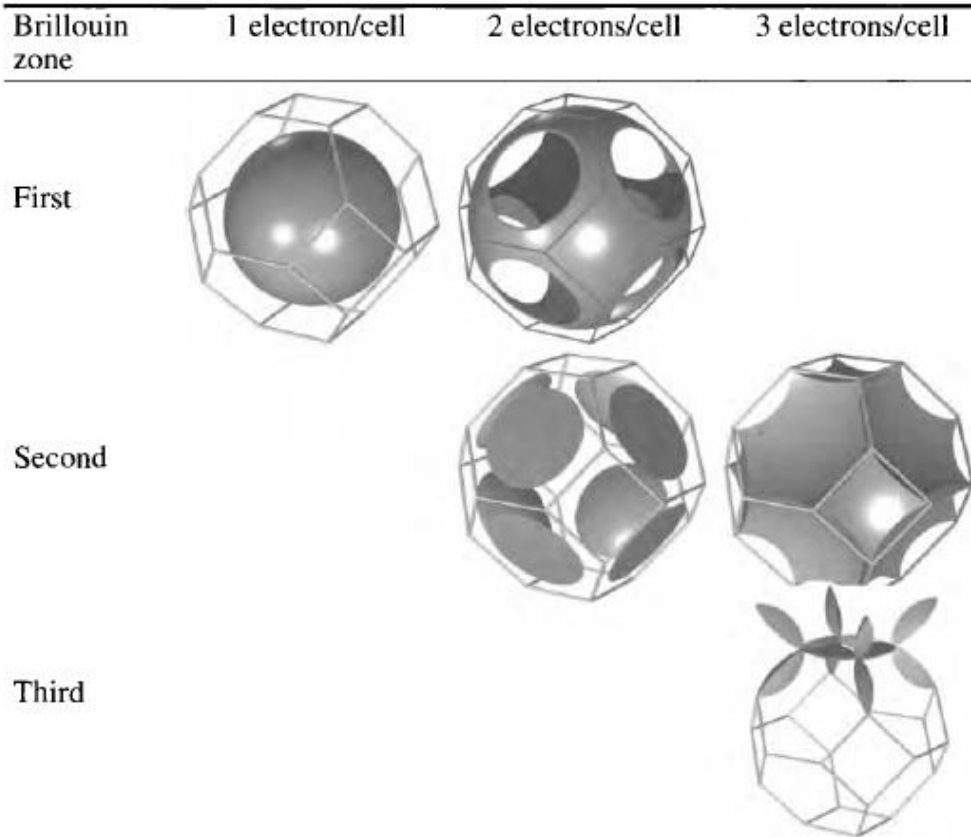
Zonas de Brillouin e sup. de Fermi



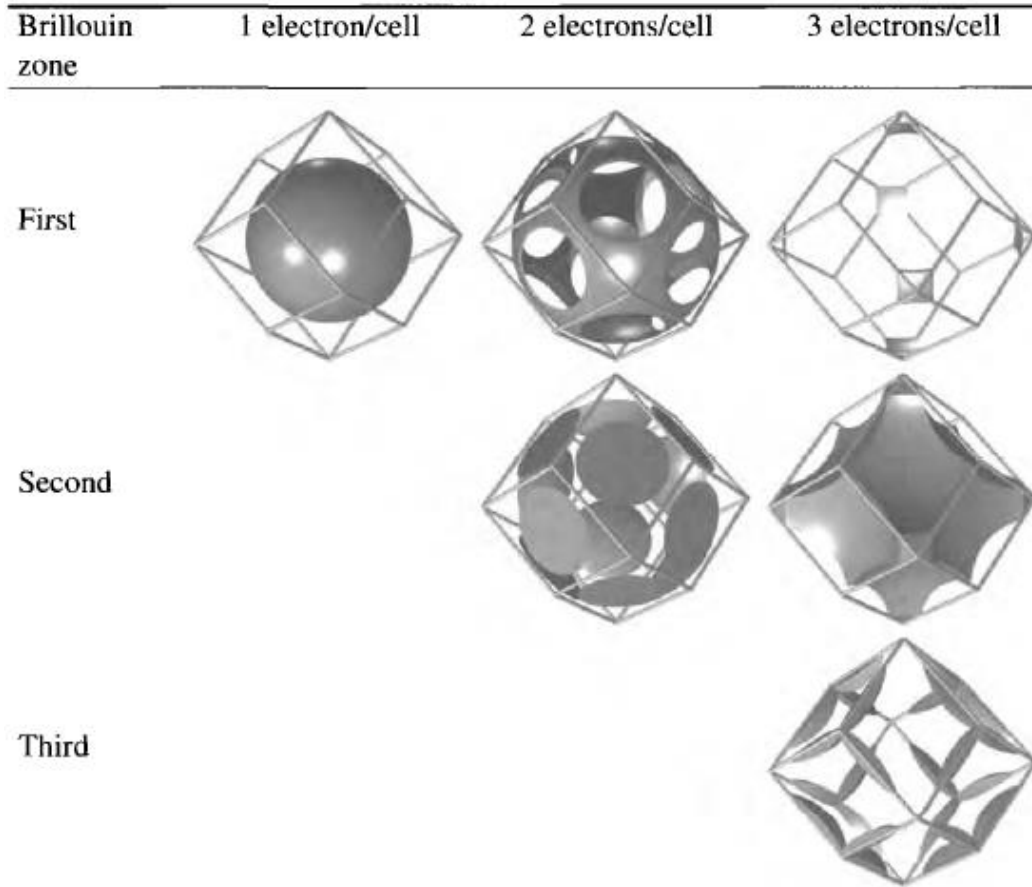
Zonas de Brillouin e sup. de Fermi



Superfícies de Fermi para um cristal FCC



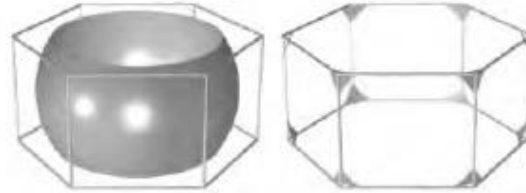
Superfícies de Fermi para um cristal BCC



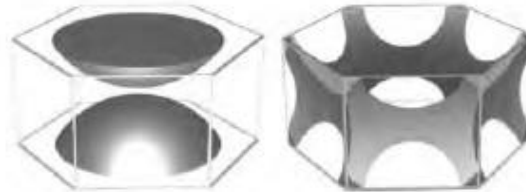
Superfícies de Fermi para um cristal HEX

Brillouin zone	2 electrons/cell	4 electrons/cell
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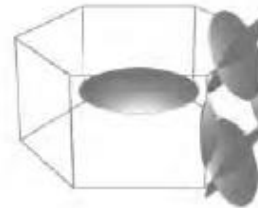
First



Second











Third



Zonas de Brillouin e sup. de Fermi

The Atomic Mac™ Registered to: GREGORY TETRAULT
For use only on a single machine

 Hexagonal
 Cubic body centered
 Rhombohedral
 Cubic
 Cubic face centered
 Monoclinic
 Orthorhombic
 Tetragonal

H	The Atomic Mac™																He																														
Li	Be															B	C	N	O	F	Ne																										
Na	Mg															Al	Si	P	S	Cl	Ar																										
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr																														
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe																														
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn																														
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub	Uut	Uuq	Uup	Uuh	Uus	Uuo																														
<table border="1"> <tbody> <tr> <td>La</td> <td>Ce</td> <td>Pr</td> <td>Nd</td> <td>Pm</td> <td>Sm</td> <td>Eu</td> <td>Gd</td> <td>Tb</td> <td>Dy</td> <td>Ho</td> <td>Er</td> <td>Tm</td> <td>Yb</td> <td>Lu</td> </tr> <tr> <td>Ac</td> <td>Th</td> <td>Pa</td> <td>U</td> <td>Np</td> <td>Pu</td> <td>Am</td> <td>Cm</td> <td>Bk</td> <td>Cf</td> <td>Es</td> <td>Fm</td> <td>Md</td> <td>No</td> <td>Lr</td> </tr> </tbody> </table>																		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu																																	
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr																																	

The Fermi Surface Database

(click icons)

