

Estrutura de bandas

Para cada valor de \mathbf{q} permitido (discreto), podemos ter mais de uma solução possível. Usamos um índice “j” para diferenciar.

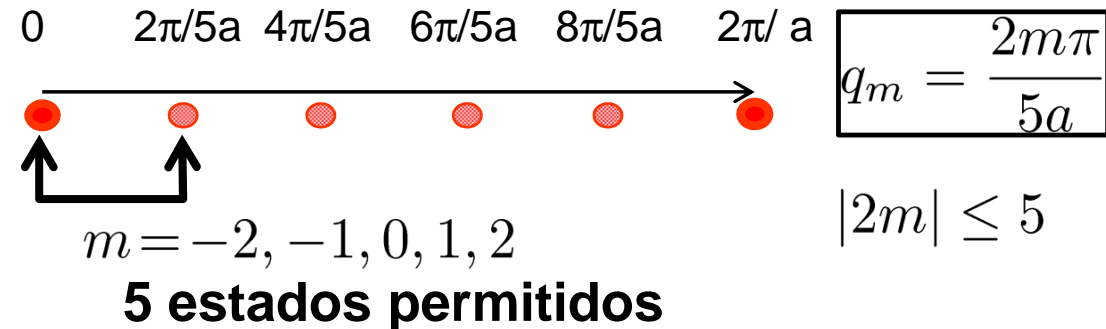
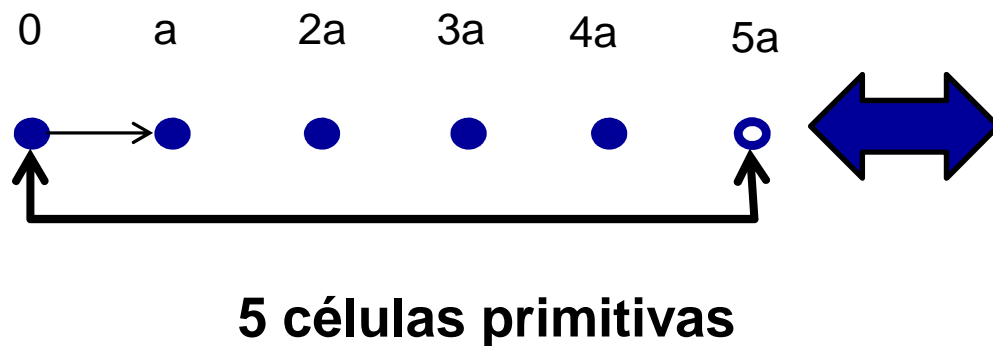
$$\Psi_{\mathbf{q}}^{(j)}(\mathbf{r}) = e^{i\mathbf{q}\cdot\mathbf{r}} u_{j,\mathbf{q}}(\mathbf{r})$$

Cada valor de j representa uma *banda de energia*.

O número de valores de \mathbf{q} permitidos é igual ao número de células primitivas do cristal.

MAS o número de soluções independentes pode ser maior que N.

■ Exemplo para uma cadeia com $N=5$:



Estrutura de bandas

- Função de onda (Bloch) :

$$\Psi_{\mathbf{q}}^{(j)}(\mathbf{r}) = e^{i\mathbf{q}\cdot\mathbf{r}} u_{j,\mathbf{q}}(\mathbf{r})$$

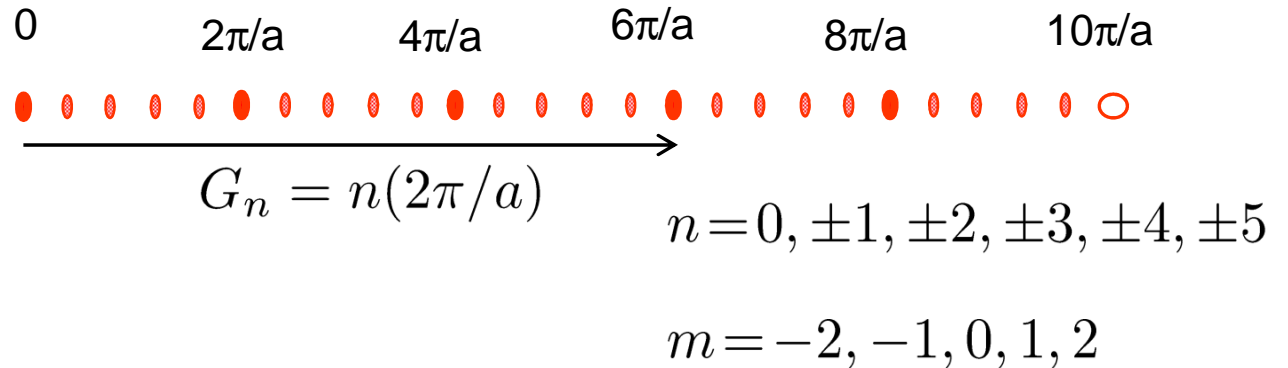
$$u_{j,\mathbf{q}}(\mathbf{r}) = \sum_{\mathbf{G}'} C_{\mathbf{q}-\mathbf{G}'} e^{-i\mathbf{G}'\cdot\mathbf{r}}$$

$$\Psi_m(x) = e^{i\frac{2m\pi x}{5a}} u_m(x)$$

$$q_m - G_n = (m - 5n) \left(\frac{2\pi}{5a} \right)$$

$$|m - 5n| \leq 25$$

$$u_m(x) = \sum_{n=-5}^5 C_{(m-5n)} e^{-i2n\pi x/a}$$



C_{m-5n} $q_m = \frac{2m\pi}{5a}$ **51 coeficientes !**

$n \setminus m$	-2	-1	0	1	2
0	-2	-1	0	1	2
±1	-7,+3	-6,+4	-5,+5	-4,+6	-3,+7
±2	-12,+8	-11,+9	-10,+10	-9,+11	-8,+12
±3	-17,+13	-16,+14	-15,+15	-14,+16	-13,+17
±4	-22,+18	-21,+19	-20,+20	-19,+21	-18,+22
±5	+23	+24	-25,+25	-24	-23

Elétrons livres

- Elétrons livres ($V(r)=0$) :

$$-\frac{\hbar^2}{2m^*} \nabla^2 \Psi(\mathbf{r}) = \varepsilon \Psi(\mathbf{r})$$

Solução (ondas planas):

$$\Psi(\mathbf{r}) = \sum_{\mathbf{k}} C_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}}$$

$$\mathbf{G} = m_1 \mathbf{A}_1 + m_2 \mathbf{A}_2 + m_3 \mathbf{A}_3$$

$$\mathbf{k} = \sum_{j=1}^3 \frac{m_j}{N_j} \mathbf{A}_j$$

- Substituindo na Eq. de Schrodinger:

$$\left(\frac{\hbar^2 k^2}{2m^*} - \varepsilon \right) C_{\mathbf{k}} = 0$$

Solução (cada estado!):

$$\varepsilon_{|\mathbf{q}-\mathbf{G}'|}^{(0)} = \frac{\hbar^2 (\mathbf{q} - \mathbf{G}')^2}{2m^*} \quad C_{\mathbf{q}-\mathbf{G}'} \neq 0$$

OU $C_{\mathbf{q}-\mathbf{G}} = 0 \quad (\mathbf{G} \neq \mathbf{G}')$

- Em termos de \mathbf{q} na 1a ZB :

$$\mathbf{q} = \mathbf{k} + \mathbf{G}'$$

$$\left(\frac{\hbar^2 (\mathbf{q} - \mathbf{G}')^2}{2m^*} - \varepsilon \right) C_{\mathbf{q}-\mathbf{G}'} = 0$$

Note que, para um dado \mathbf{q} , existem vários estados possíveis!

São combinações de \mathbf{k} e \mathbf{G}' .

Elétrons quase livres (V pequeno)

- Equação para os coeficientes :
$$\left(\varepsilon_{\mathbf{q}-\mathbf{G}'}^{(0)} - E\right) C_{\mathbf{q}-\mathbf{G}'} + \sum_{\mathbf{G}''} V_{\mathbf{G}''-\mathbf{G}'} C_{\mathbf{q}-\mathbf{G}''} = 0$$

$$\varepsilon_{|\mathbf{q}-\mathbf{G}|}^{(0)} = \frac{\hbar^2(\mathbf{q}-\mathbf{G})^2}{2m^*}$$

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{r}\cdot\mathbf{G}} \quad \text{com } V_0 \equiv 0$$

- Exemplo: vamos considerar apenas dois \mathbf{G} :

$$\left\{ \begin{array}{l} \left(\varepsilon_{\mathbf{q}-\mathbf{G}_1}^{(0)} - E\right) C_{\mathbf{q}-\mathbf{G}_1} + V_{\mathbf{G}_2-\mathbf{G}_1} C_{\mathbf{q}-\mathbf{G}_2} = 0 \\ \left(\varepsilon_{\mathbf{q}-\mathbf{G}_2}^{(0)} - E\right) C_{\mathbf{q}-\mathbf{G}_2} + V_{\mathbf{G}_1-\mathbf{G}_2} C_{\mathbf{q}-\mathbf{G}_1} = 0 \end{array} \right.$$

Simplificando a notação:

$$\varepsilon_{\mathbf{q}-\mathbf{G}_n}^{(0)} \rightarrow \varepsilon_n^{(0)}$$

$$V_{\mathbf{G}_2-\mathbf{G}_1} = (V_{\mathbf{G}_1-\mathbf{G}_2})^* \rightarrow V$$

- Solução:

$$E = \frac{1}{2} \left(\varepsilon_1^{(0)} + \varepsilon_2^{(0)} \pm \sqrt{(\varepsilon_1^{(0)} - \varepsilon_2^{(0)})^2 + 4|V|^2} \right)$$

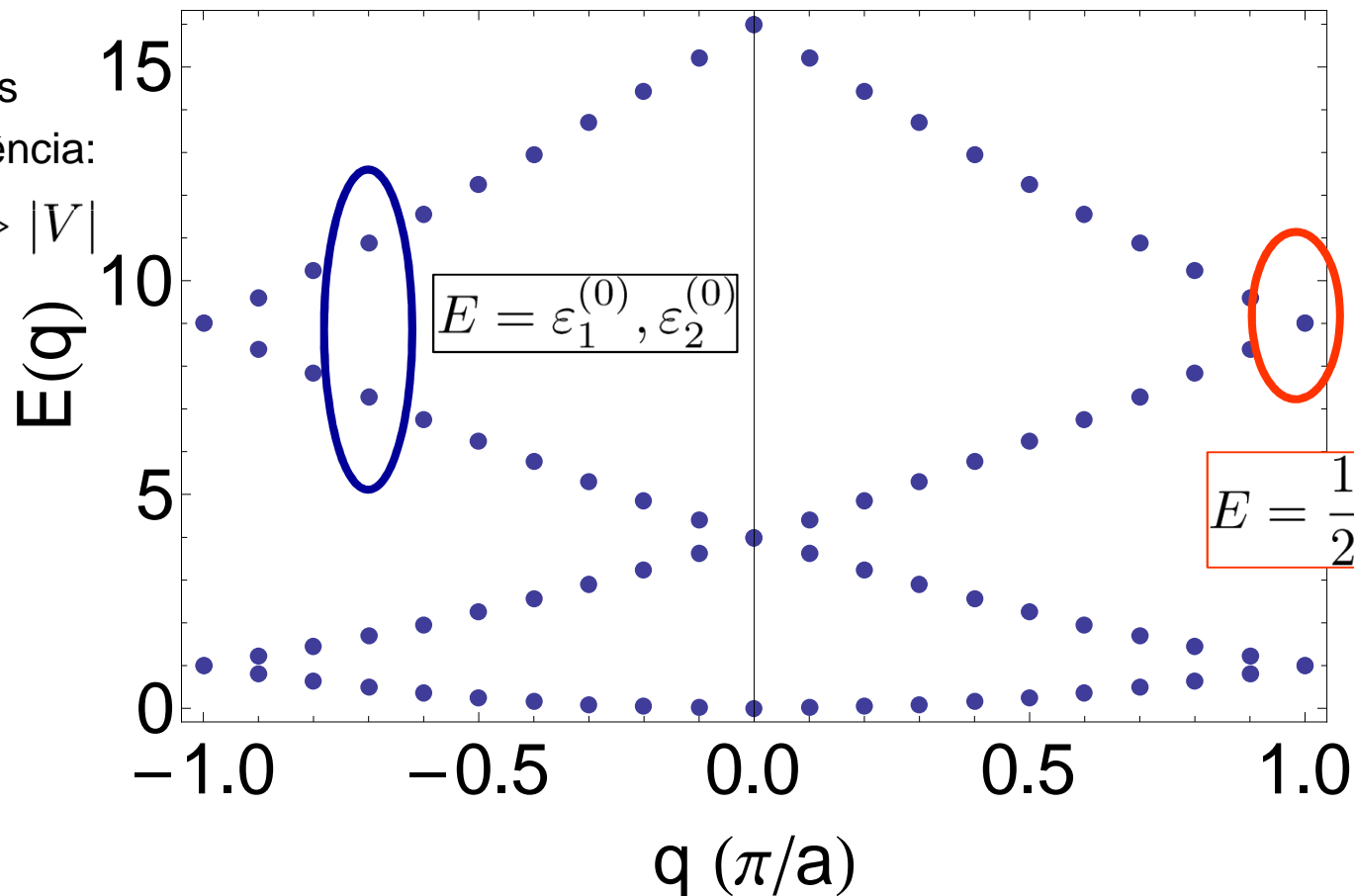
Elétrons quase livres (V pequeno)

$$E = \frac{1}{2} \left(\varepsilon_1^{(0)} + \varepsilon_2^{(0)} \pm \sqrt{(\varepsilon_1^{(0)} - \varepsilon_2^{(0)})^2 + 4|V|^2} \right)$$

■ Limites:

Longe de pontos
de degenerescência:

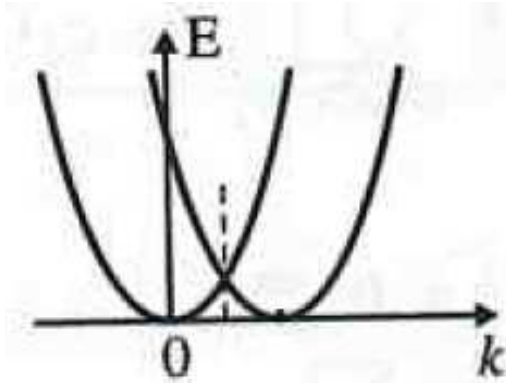
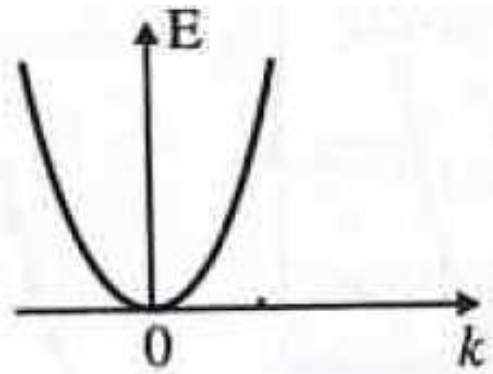
$$|\varepsilon_1^{(0)} - \varepsilon_2^{(0)}| \gg |V|$$



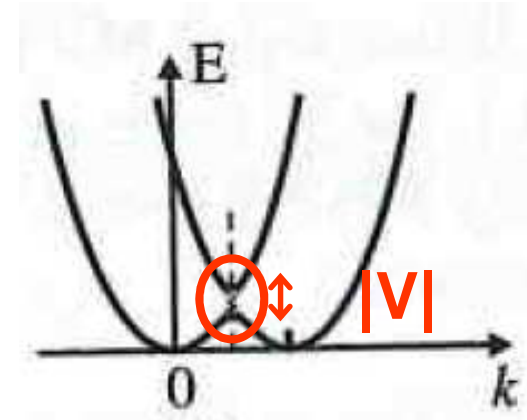
Próximo de pontos
de degenerescência:

$$|\varepsilon_1^{(0)} - \varepsilon_2^{(0)}| \ll |V|$$

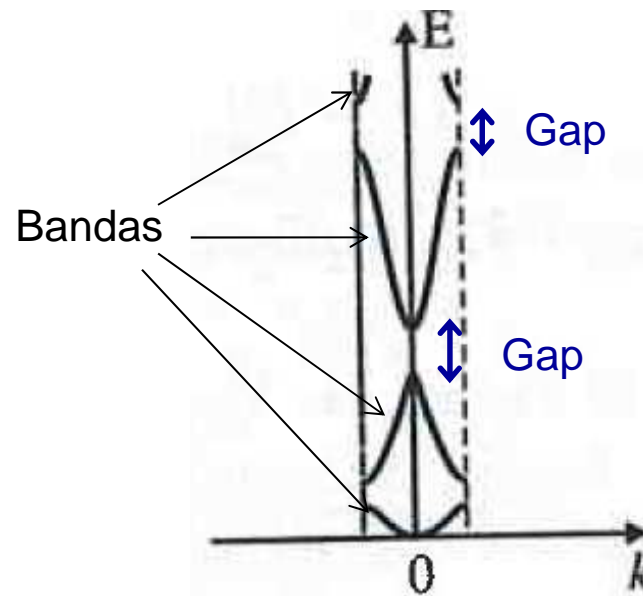
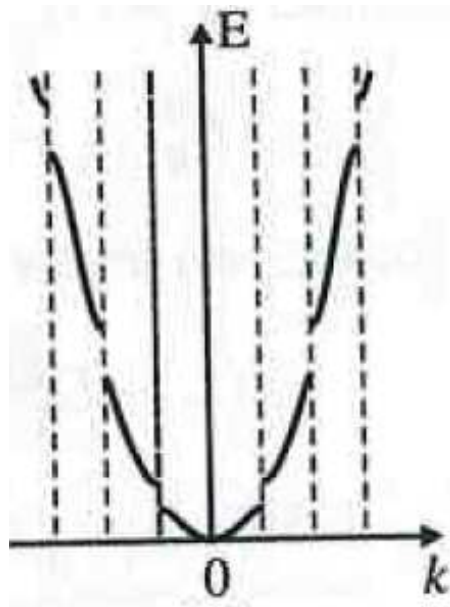
Elétrons quase livres: gaps nas bandas



$$|\varepsilon_1^{(0)} - \varepsilon_2^{(0)}| \ll |V|$$



$$E = \frac{1}{2}(\varepsilon_1^{(0)} + \varepsilon_2^{(0)}) \pm |V|$$



Onde ocorrem os gaps?

$$\varepsilon_{\mathbf{q}-\mathbf{G}_n}^{(0)} \rightarrow \varepsilon_n^{(0)}$$

$$\mathbf{G} \equiv \mathbf{G}_2 - \mathbf{G}_1$$

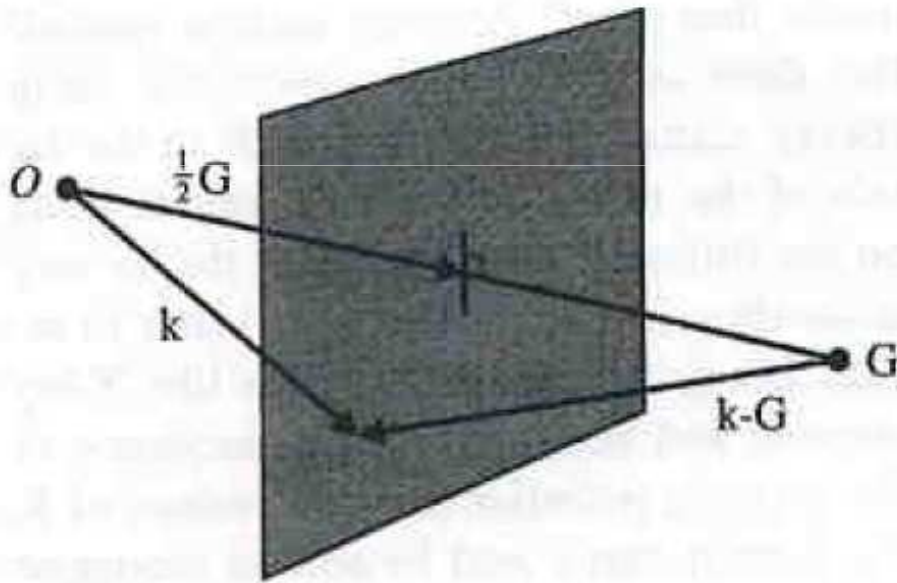
Pontos de degenerescência:

$$|\varepsilon_{\mathbf{k}}^{(0)} - \varepsilon_{\mathbf{k}-\mathbf{G}}^{(0)}| \ll |V|$$

$$V_{\mathbf{G}_2-\mathbf{G}_1} = (V_{\mathbf{G}_1-\mathbf{G}_2})^* \rightarrow V$$

$$\mathbf{k} \equiv \mathbf{q} - \mathbf{G}_1$$

$$|\mathbf{k}| \approx |\mathbf{k} - \mathbf{G}|$$



Planos de Bragg:

$$\mathbf{G} \cdot \left(\mathbf{k} - \frac{1}{2} \mathbf{G} \right) = 0$$

$$G^2 = 2\mathbf{k} \cdot \mathbf{G}$$

Bordas das zonas de Brillouin
são planos de Bragg

Fig. 3.2 The plane defining the points at which $E_{\mathbf{k}}^0 = E_{\mathbf{k}-\mathbf{G}}^0$.