

Estrutura de bandas

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

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

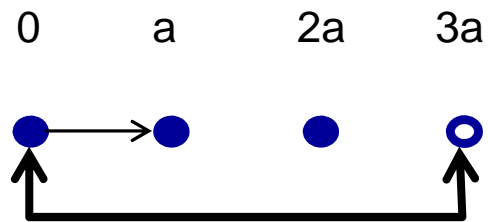
Cada valor de j representa uma *banda de energia*.

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

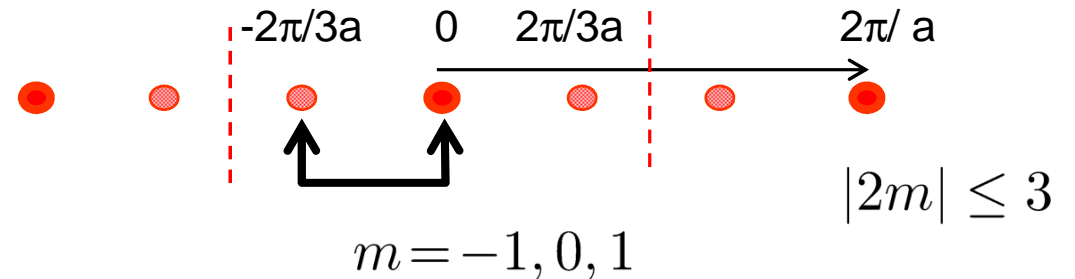
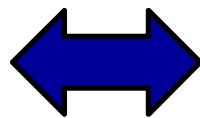
MAS o número de soluções independentes pode ser maior que N.

- Exemplo para uma cadeia com $N=3$:

$$q_m = \frac{2m\pi}{3a}$$



3 células primitivas

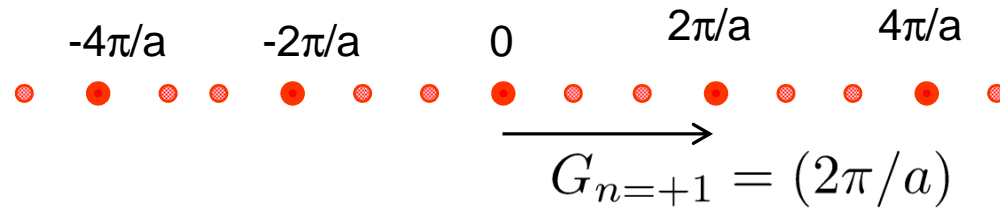


**3 estados permitidos
na 1a ZB**

Exemplo para N=3

■ Função de onda (Bloch) :

$$\left\{ \begin{array}{l} \Psi_m^{(j)}(x) = e^{iq_m x} u_{j,m}(x) \\ u_{j,m}(x) = \sum_{n'} \mathcal{C}_{q_m - G_{n'}} e^{-iG_{n'} x} \\ V(x) = \sum_n V_n e^{iG_n x} \end{array} \right.$$



$$G_n = n(2\pi/a) \quad q_m = \frac{2m\pi}{3a} \quad m = -1, 0, 1$$

$$n = 0, \pm 1, \pm 2, \pm 3, \dots$$

$$\Psi_m(x) = e^{i \frac{2m\pi x}{3a}} u_m(x)$$

$$q_m - G_n = (m - 3n) \left(\frac{2\pi}{3a} \right)$$

Usando $|n_{\max}|=1$, temos **9 coeficientes**.

m	n	m-3n
-1	-1	+2
	0	-1
	+1	-4
0	-1	+3
	0	0
	1	-3
+1	-1	+4
	0	+1
	+1	-2

$$\mathcal{C}_{m-3n}$$

$$\mathcal{C}_{-4}, \mathcal{C}_{-3}, \dots, \mathcal{C}_0 \dots \mathcal{C}_{-3}, \mathcal{C}_{+4}$$

$$u_m(x) = \sum_n \mathcal{C}_{(m-3n)} e^{-i2n\pi x/a}$$

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 :

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

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

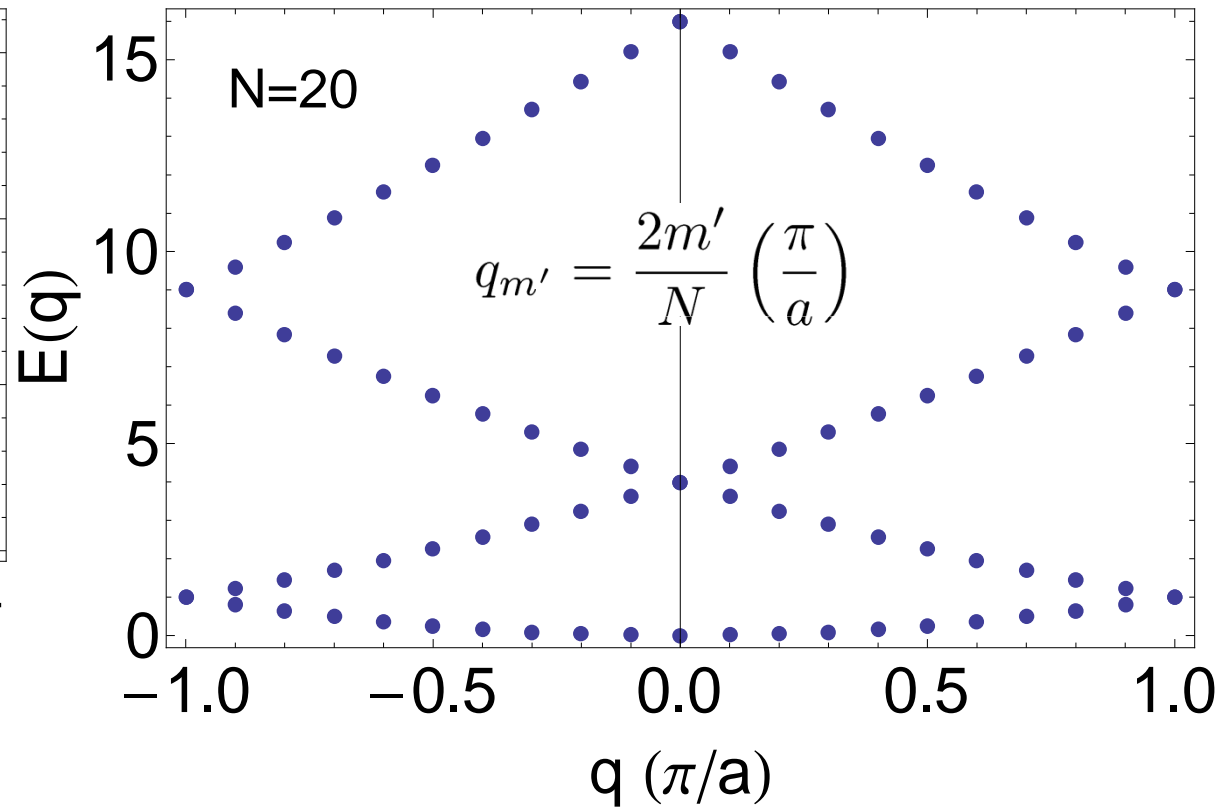
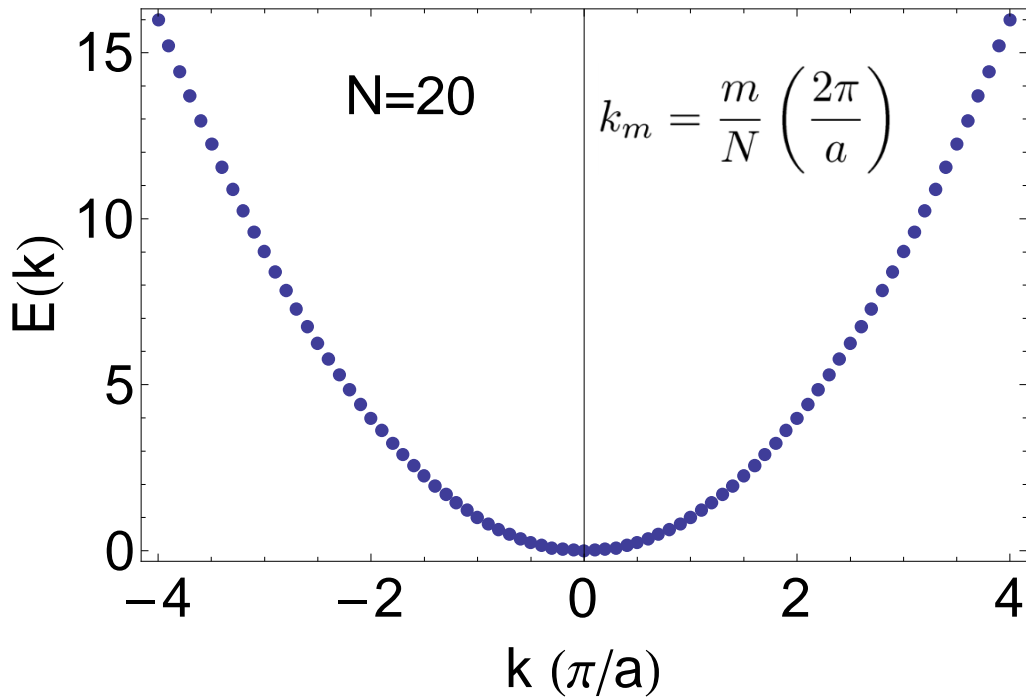
Note que, para um dado \mathbf{q} , existem vários estados possíveis!

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

Bandas dos elétrons livres

$$\varepsilon_{\mathbf{k}}^{(0)} = \frac{\hbar^2 \mathbf{k}^2}{2m^*}$$

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



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)

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

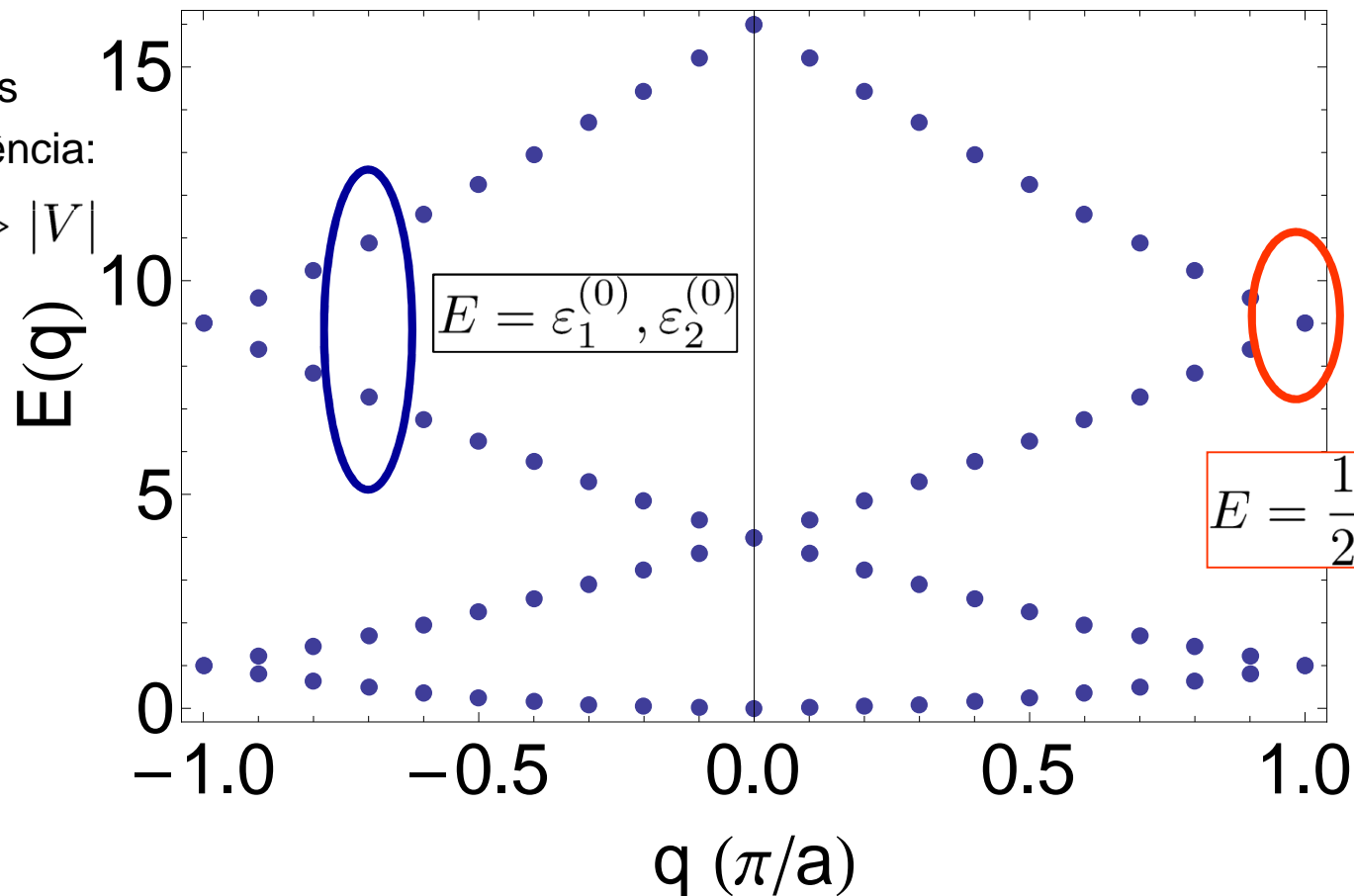
■ Limites:

Longe de pontos
de degenerescência:

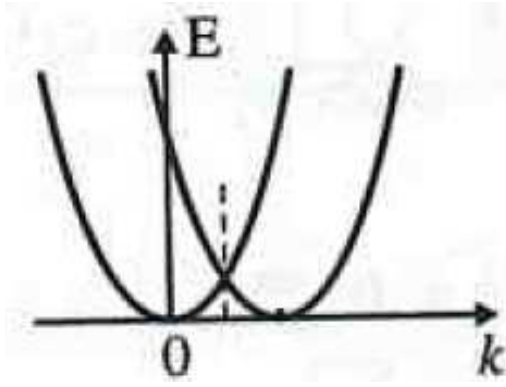
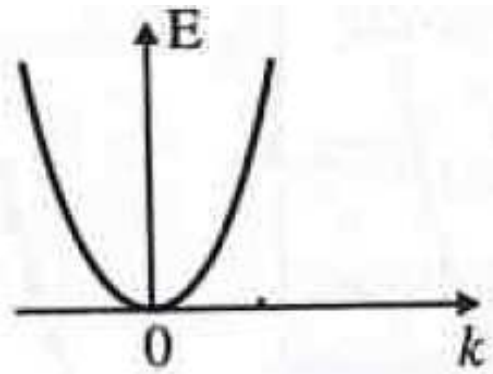
$$|\varepsilon_1^{(0)} - \varepsilon_2^{(0)}| \gg |V|$$

Próximo de pontos
de degenerescência:

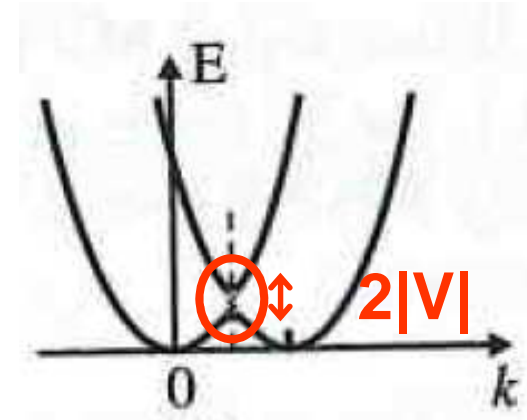
$$|\varepsilon_1^{(0)} - \varepsilon_2^{(0)}| \ll |V|$$



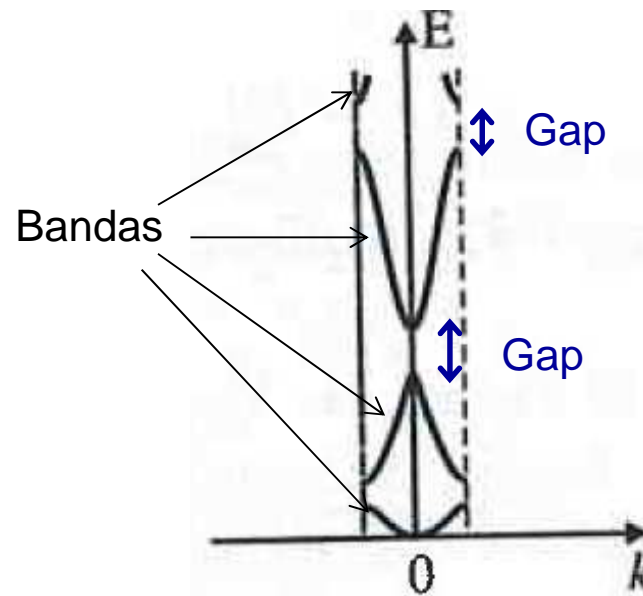
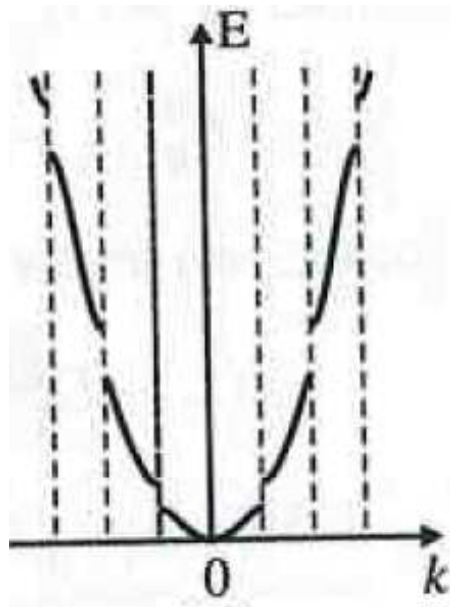
Elétrons quase livres: gaps nas bandas



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



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



Onde ocorrem os gaps?

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

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

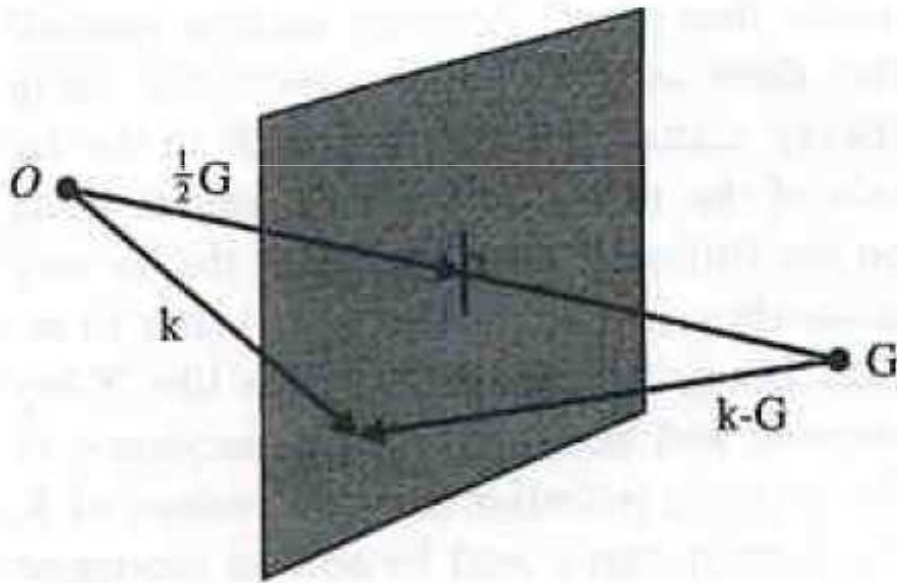
Pontos de degenerescência:

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

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

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

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



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 $E_{\mathbf{k}}^0 = E_{\mathbf{k}-\mathbf{G}}^0$.