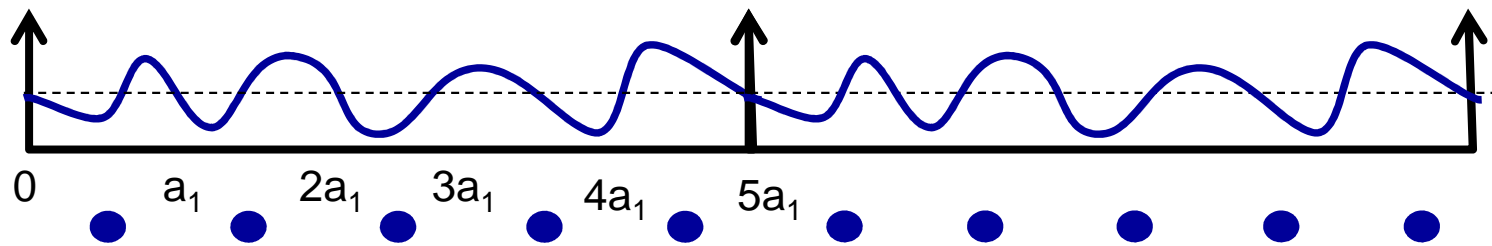


Condições de contorno de Born-von Karman

- Tamanho do sistema = número de células primitivas:



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

$$\phi_{\mathbf{k}}(\mathbf{r}) = A e^{i\mathbf{k} \cdot \mathbf{r}}$$

Tamanho do sistema:

$$\mathbf{L} = N_1 \mathbf{a}_1 + N_2 \mathbf{a}_2 + N_3 \mathbf{a}_3$$

Volume do sistema:

$$V_{\mathbf{r}} = N_1 N_2 N_3 (\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3)$$

Condições periódicas de contorno:

$$\phi(\mathbf{r} + \mathbf{L}) = \phi(\mathbf{r}) \Rightarrow e^{i \sum_j N_j \mathbf{a}_j \cdot \mathbf{k}} = 1$$

$$\mathbf{a}_\ell \cdot \mathbf{A}_j = 2\pi \delta_{\ell j}$$

Quantização de \mathbf{k} :

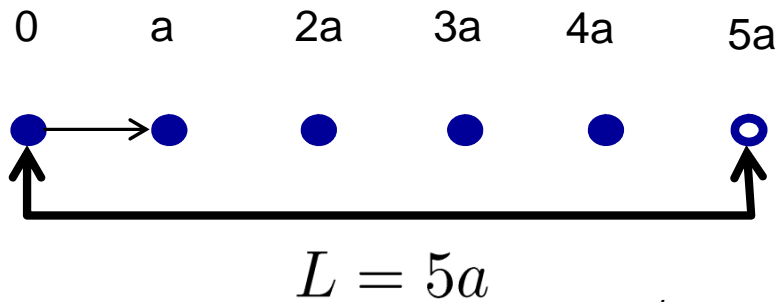
$$\mathbf{k} = \sum_{j=1}^3 \frac{m_j}{N_j} \mathbf{A}_j$$

Volume ocupado por cada estado no espaço \mathbf{k} :

$$V_{\mathbf{k}}^{1st} = \frac{\mathbf{A}_1}{N_1} \cdot \frac{\mathbf{A}_2}{N_2} \times \frac{\mathbf{A}_3}{N_3} = \frac{1}{N} \mathbf{A}_1 \cdot \mathbf{A}_2 \times \mathbf{A}_3$$

Exemplo: rede 1D

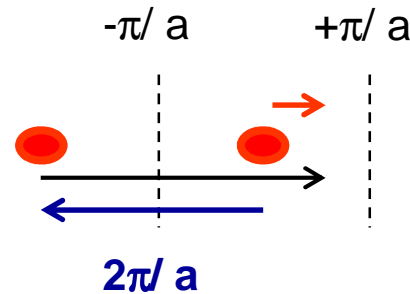
- Rede direta (N=5):



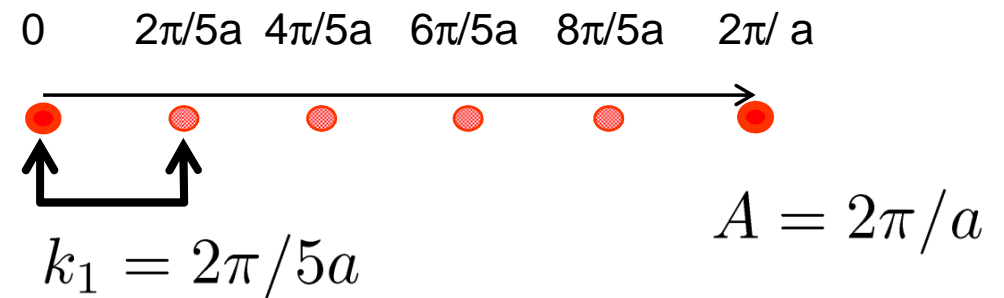
- 1ª Zona de Brillouin:

$$k = q - G$$

$$-\frac{\pi}{a} \leq q \leq +\frac{\pi}{a}$$



- Rede recíproca: $\mathbf{a}_1 \cdot \mathbf{A}_1 = 2\pi$

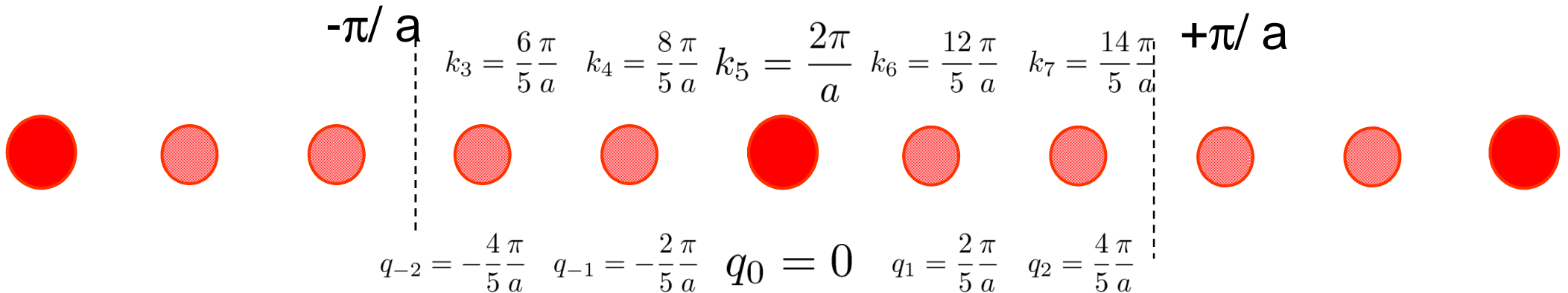


- Quantização de k e q :

$$k_m = \frac{m}{N} \left(\frac{2\pi}{a} \right)$$

$$q_{m'} = \frac{2m'}{N} \left(\frac{\pi}{a} \right)$$

$$|2m'| \leq N$$



Eq. de Schrödinger em um potencial periódico

- Eq. de Schrödinger:

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

Solução (ondas planas):

$$\Psi(\mathbf{r}) = \sum_{\mathbf{k}} C_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \quad \mathbf{k} = \sum_{j=1}^3 \frac{m_j}{N_j} \mathbf{A}_j$$

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{r} \cdot \mathbf{G}}$$

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

- Substituindo na Eq. de Schrodinger (Tarefa):

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

- Escrevendo em termos de um vetor \mathbf{q} na 1a ZB (Tarefa): $\mathbf{k} = \mathbf{q} - \mathbf{G}'$

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

Equação de auto-valores $\varepsilon(\mathbf{q})$.
 Note que $\varepsilon(\mathbf{q}) = \varepsilon(\mathbf{q} + \mathbf{G})!!$

Teorema de Bloch

$$\Psi(\mathbf{r}) = \sum_{\mathbf{k}} C_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \quad \text{Equação para os coeficientes:}$$

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

- Soluções da Eq. de Schrodinger: $\Psi_{\mathbf{q}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{q}-\mathbf{G}} e^{i(\mathbf{q}-\mathbf{G})\cdot\mathbf{r}}$

$$\Psi_{\mathbf{q}}(\mathbf{r}) = e^{i\mathbf{q}\cdot\mathbf{r}} \left(\sum_{\mathbf{G}} C_{\mathbf{q}-\mathbf{G}} e^{-i\mathbf{G}\cdot\mathbf{r}} \right) \equiv e^{i\mathbf{q}\cdot\mathbf{r}} u_{\mathbf{q}}(\mathbf{r})$$

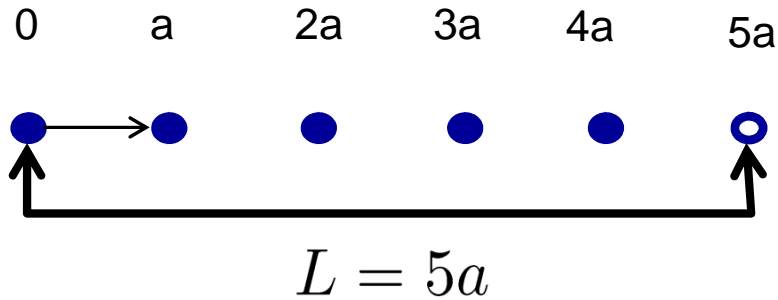
- **Teorema de Bloch:** as soluções da Eq. de Schroedinger podem ser escritas na forma:

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

onde $u_{j,\mathbf{q}}(\mathbf{r})$ é uma função periódica (com mesmo período do potencial): $u_{j,\mathbf{q}}(\mathbf{r} + \mathbf{R}) = u_{j,\mathbf{q}}(\mathbf{r})$

Exemplo: Teorema de Bloch em 1D.

- Rede direta (N=5):

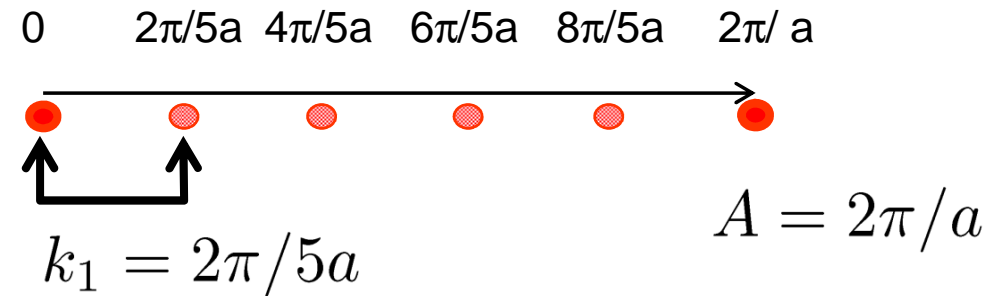


$$\Psi_{m'}(x) = e^{iq_{m'}x} u_{m'}(x)$$

$$u_{m'}(x) = \sum_{n=-5}^5 C_{m'-n} e^{-i\frac{2\pi n}{a}x}$$

$$u_{m'}(x+a) = \sum_{n=-5}^5 C_{m'-n} e^{-i\frac{2\pi n}{a}x} e^{-i2\pi n} = u_{m'}(x)$$

- Rede recíproca: $\mathbf{a}_1 \cdot \mathbf{A}_1 = 2\pi$



$$q_{m'} = \frac{2m'}{N} \left(\frac{\pi}{a} \right)$$

$$|2m'| \leq N$$

$$k_m = \frac{m}{N} \left(\frac{2\pi}{a} \right)$$

$$G = n \left(\frac{2\pi}{a} \right)$$

