

# AULA 2: TIGHT-BINDING

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CBPF

<https://tgrappoport.github.io/page>



<https://github.com/tgrappoport/2dmat>

# FERRAMENTAS

Referência:

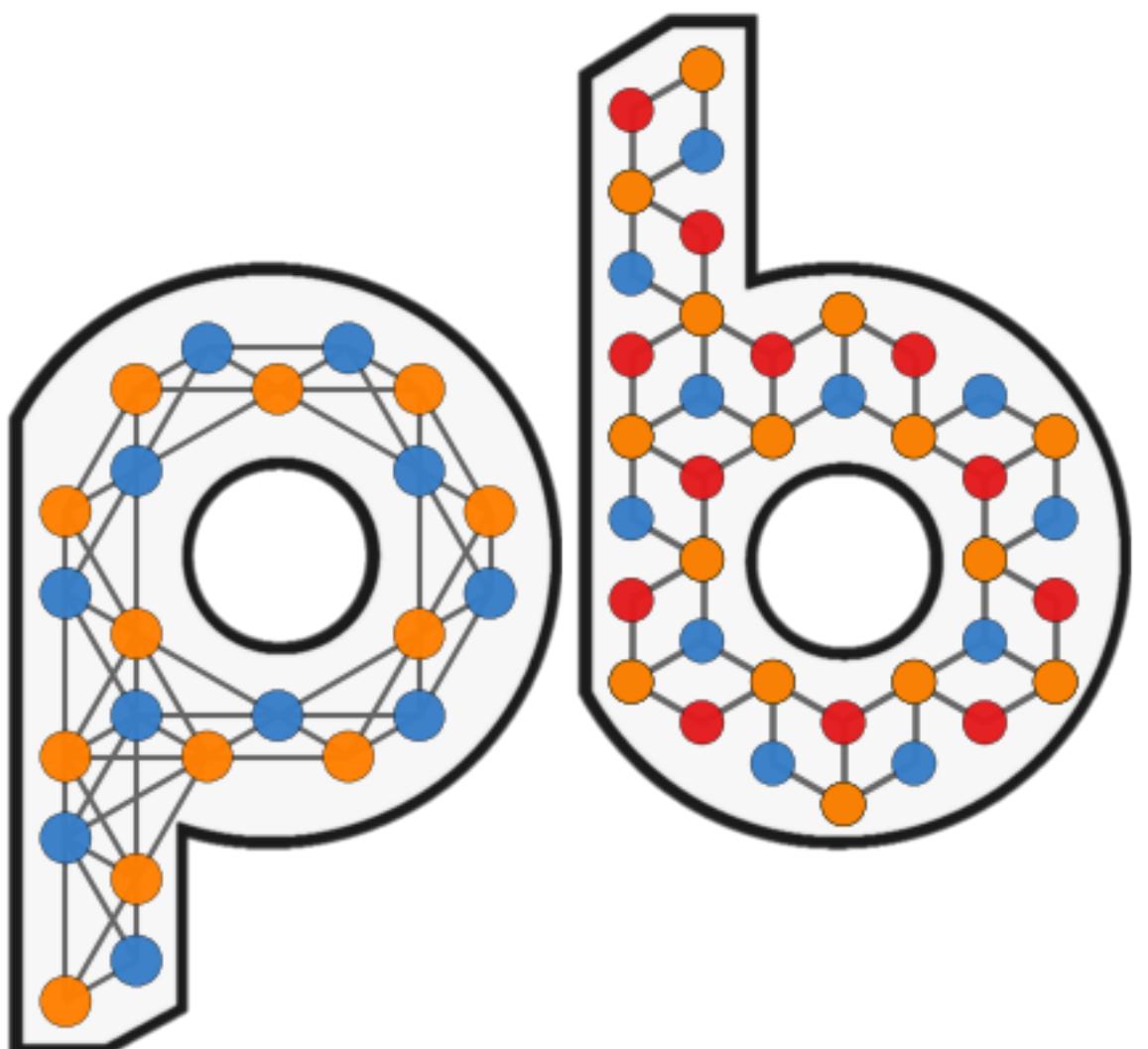
**Quantum Transport: Atom to Transistor**  
**Supriyo Datta**

**<https://solidstate.quantumtinkerer.tudelft.nl/>**

**<https://podcasts.ox.ac.uk/series/oxford-solid-state-basics>**

Framework:

**Python**



Bibliotecas python

**numpy, matplotlib, pybinding**

**<https://docs.pybinding.site/>**

**pip install pybinding**

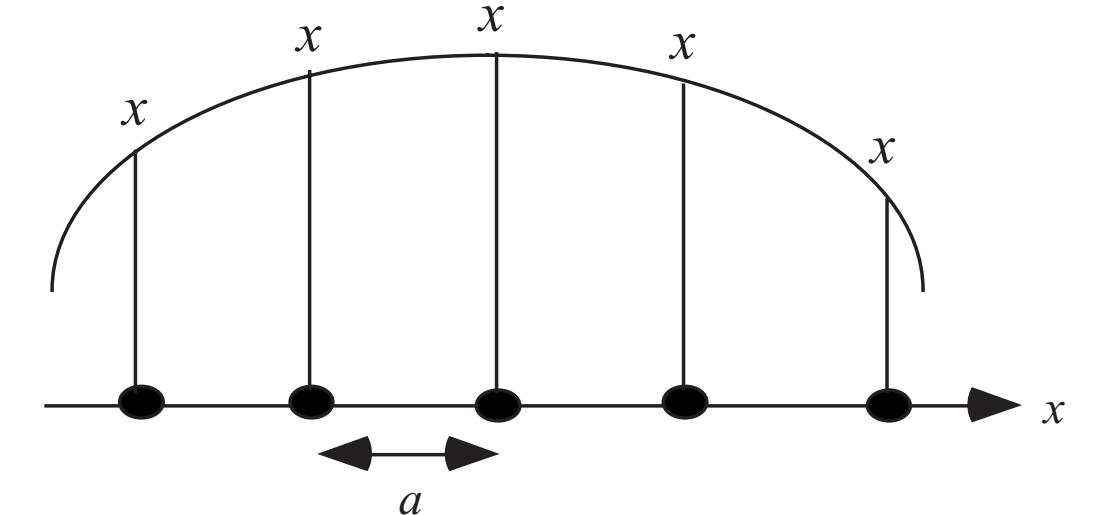
# EQUAÇÃO DE SCHRÖDINGER

## Solução Numérica

De uma equação diferencial parcial a uma equação matricial:

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = H_{\text{op}} \Psi(\vec{r}, t)$$

$$i\hbar \frac{d}{dt} \{\psi(t)\} = [H] \{\psi(t)\}$$



Solução estacionária  $H_{\text{op}}\psi(x)=E\psi(x)$

$$H_{\text{op}} \equiv -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x)$$

$$\left( \frac{\partial^2 \Psi}{\partial x^2} \right)_{x=x_n} \rightarrow \frac{1}{a^2} [\Psi(x_{n+1}) - 2\Psi(x_n) + \Psi(x_{n-1})]$$

$$t_0 \equiv \hbar^2 / 2ma^2$$

and

$$H_{n,m} = [U_n + 2t_0] \delta_{n,m} - t_0 \delta_{n,m+1} - t_0 \delta_{n,m-1}$$

$$U(x) \Psi(x) \rightarrow U(x_n) \Psi(x_n)$$

# HAMILTONIANA COMO UMA MATRIZ

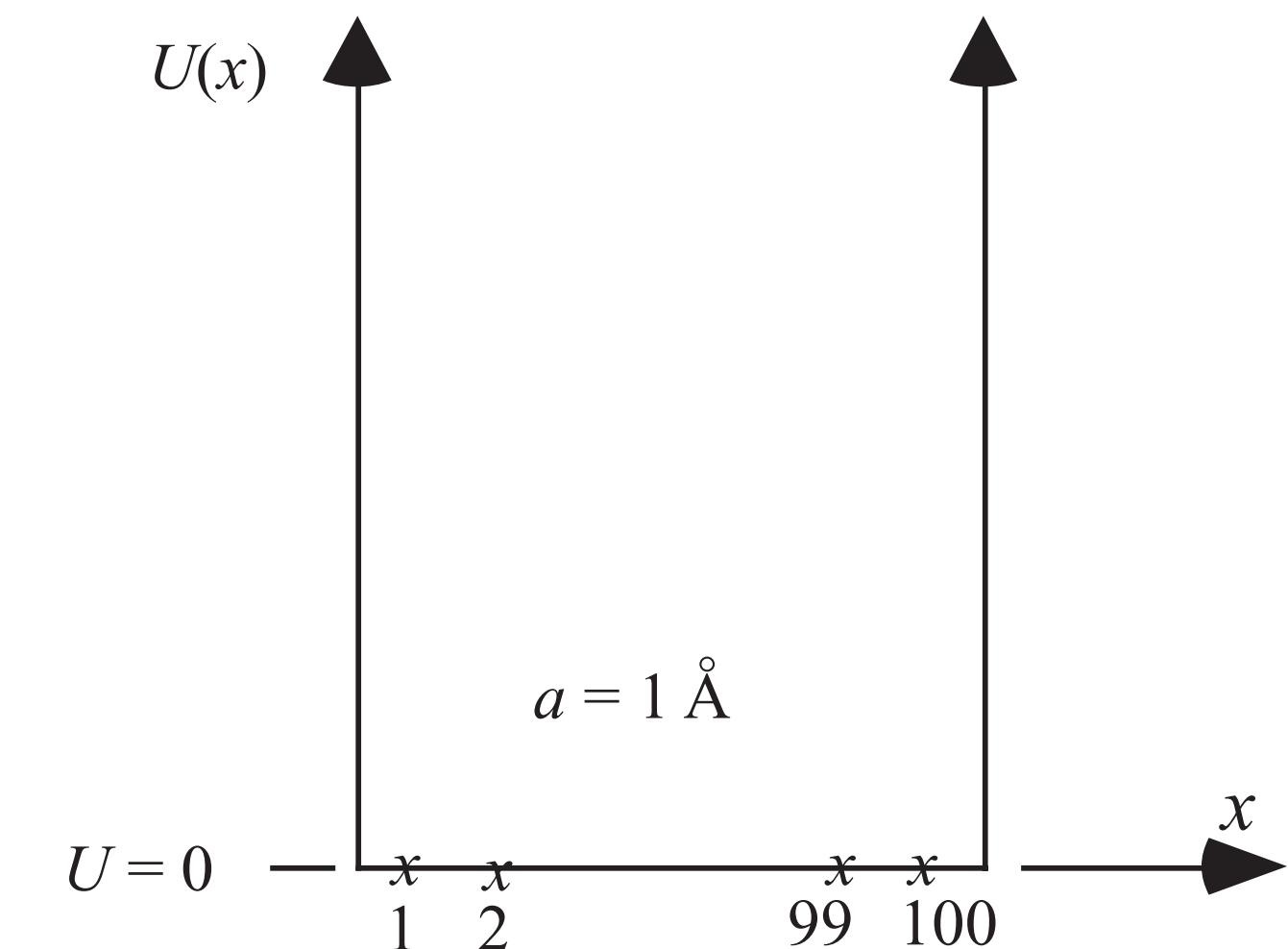
$$H_{n,m} = [U_n + 2t_0] \delta_{n,m} - t_0 \delta_{n,m+1} - t_0 \delta_{n,m-1}$$

$$\begin{array}{cccccc} H = & & 1 & & 2 & & \dots & N-1 & & N \\ & 1 & & 2t_0 + U_1 & & -t_0 & & 0 & & 0 \\ & 2 & & -t_0 & & 2t_0 + U_2 & & 0 & & 0 \\ & & & & \dots & & \dots & & \dots & \\ N-1 & & 0 & & 0 & & & 2t_0 + U_{N-1} & & -t_0 \\ N & & 0 & & 0 & & & -t_0 & & 2t_0 + U_N \end{array} \quad ($$

# POÇO INFINITO

$$-\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi}{\partial x^2} \right)_{x=x_n} \rightarrow t_0 [\Psi(x_{n+1}) - 2\Psi(x_n) + \Psi(x_{n-1})]$$

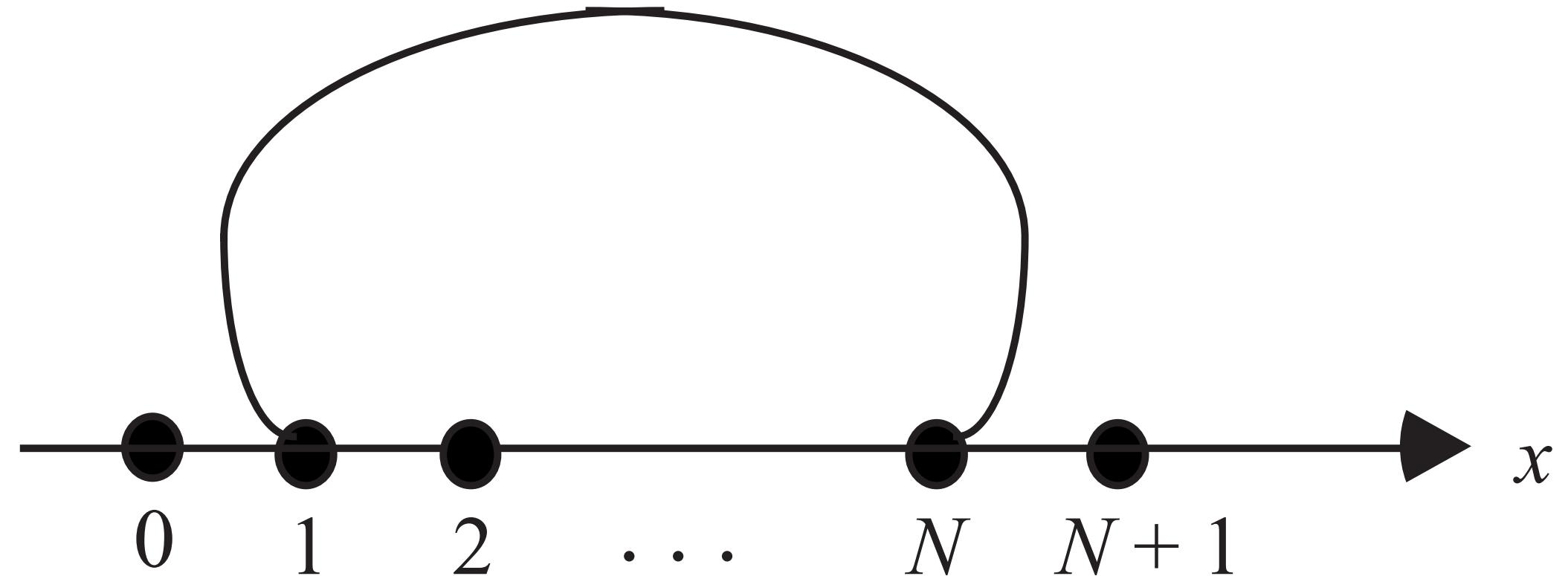
$$H = \begin{matrix} & 1 & 2 & \dots & 99 & 100 \\ 1 & 2t_0 & -t_0 & 0 & 0 \\ 2 & -t_0 & 2t_0 & 0 & 0 \\ & \dots & \dots & \dots & \dots \\ 99 & 0 & 0 & 2t_0 & -t_0 \\ 100 & 0 & 0 & -t_0 & 2t_0 \end{matrix}$$



$\psi_0 = 0$  and  $\psi_{N+1} = 0$

# CONDIÇÕES PERIÓDICAS DE FRONTEIRA

$$H = \begin{matrix} & 1 & 2 & \dots & 99 & 100 \\ 1 & 2t_0 & -t_0 & 0 & -t_0 & \\ 2 & -t_0 & 2t_0 & 0 & 0 & \\ & \dots & \dots & \dots & & \\ 99 & 0 & 0 & 2t_0 & -t_0 & \\ 100 & -t_0 & 0 & -t_0 & 2t_0 & \end{matrix}$$



# MOLÉCULAS

H       $\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}^2} - \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}|}.$

Molécula diatômica

átomos estão suficientemente afastados  
forma dos orbitais não se altera devido à presença do outro

$$\hat{H} = \hat{V}_1 + \hat{V}_2 + \hat{K},$$

$$(\hat{V}_1 + \hat{K})|1\rangle = \varepsilon_0|1\rangle,$$

$$(\hat{V}_2 + \hat{K})|2\rangle = \varepsilon_0|2\rangle.$$

Ideia chave: para encontrar a função de onda do elétron na molécula — o orbital molecular —, procuramos uma solução que seja uma combinação linear dos orbitais atômicos (LCAO):

$$|\psi\rangle = c_1|1\rangle + c_2|2\rangle. \quad H|\psi\rangle = E|\psi\rangle = c_1H|1\rangle + c_2H|2\rangle.$$

$$\langle 1|E|\psi\rangle = c_1\langle 1|\hat{H}|1\rangle + c_2\langle 1|\hat{H}|2\rangle = E\phi_1 \quad E\phi_2 = c_1\langle 2|\hat{H}|1\rangle + c_2\langle 2|\hat{H}|2\rangle.$$

# MOLÉCULAS

$$\langle 1 | \hat{H} | 1 \rangle = \langle 2 | \hat{H} | 2 \rangle \equiv E_0 \quad E_0 = \langle 1 | \hat{H} | 1 \rangle = \langle 1 | \hat{V}_1 + \hat{V}_2 + \hat{K} | 1 \rangle = \varepsilon_0 + \langle 1 | \hat{V}_2 | 1 \rangle,$$

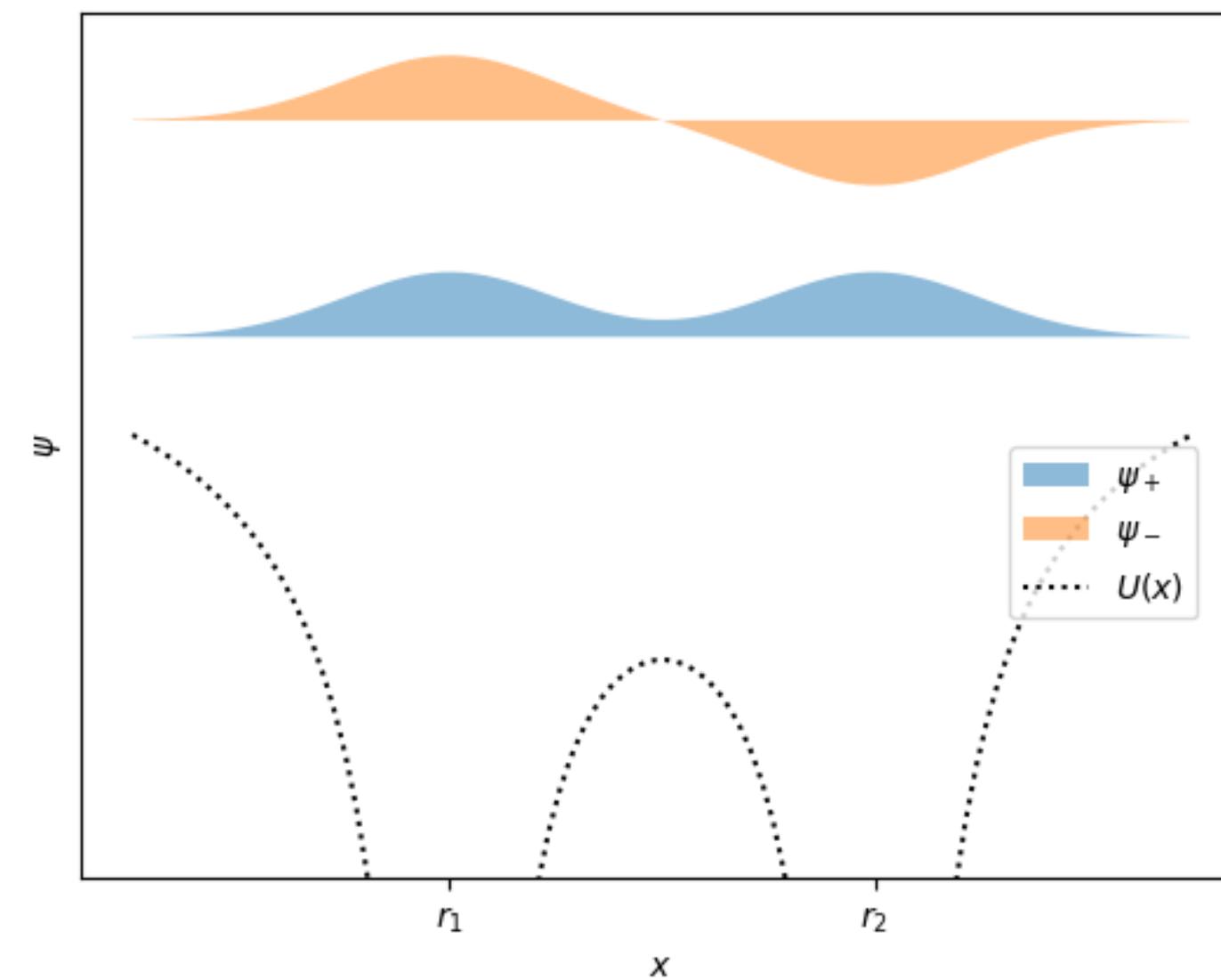
$$\langle 1 | \hat{H} | 2 \rangle \equiv -t, \quad t = -\langle 1 | \hat{H} | 2 \rangle = -\langle 1 | \hat{V}_1 + \hat{V}_2 + \hat{K} | 2 \rangle = -\langle 1 | \hat{V}_1 | 2 \rangle.$$

integral de hopping (hopping) que é energia associada ao movimento do elétron entre os dois orbitais.

$$H = \begin{pmatrix} E_0 & -t \\ -t & E_0 \end{pmatrix}. \quad E_{\pm} = E_0 \mp t.$$

$$|\psi_+\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle),$$

$$|\psi_-\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle),$$



# DA MOLÉCULA AO SÓLIDO

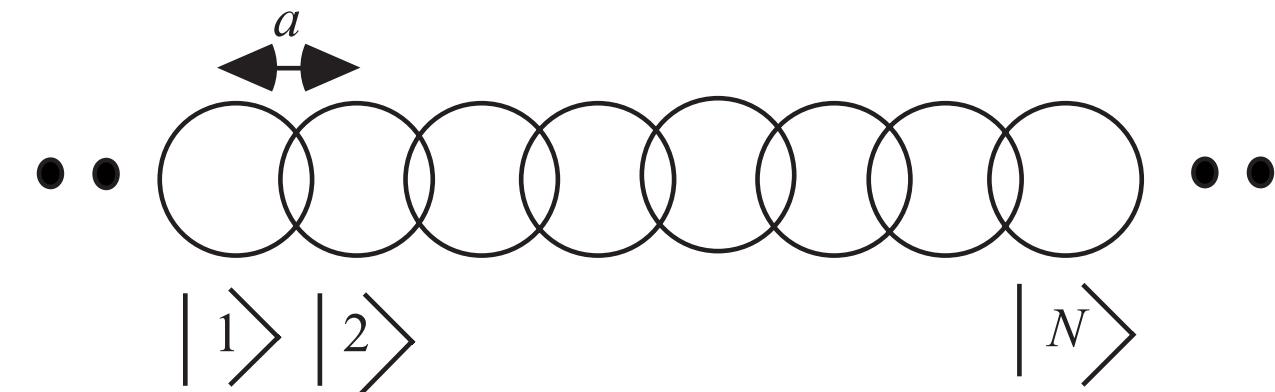
Três átomos:

$$|\psi\rangle = c_1|1\rangle + c_2|2\rangle + c_3|3\rangle. \quad \langle 1|H|1\rangle = \langle 2|H|2\rangle = \langle 3|H|3\rangle = E_0.$$

$$\langle 1|H|2\rangle = \langle 2|H|3\rangle = -t.$$

$$E \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} E_0 & -t & 0 \\ -t & E_0 & -t \\ 0 & -t & E_0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}.$$

Cadeia com N átomos:



$$|\Psi\rangle = \sum_n c_n |n\rangle.$$

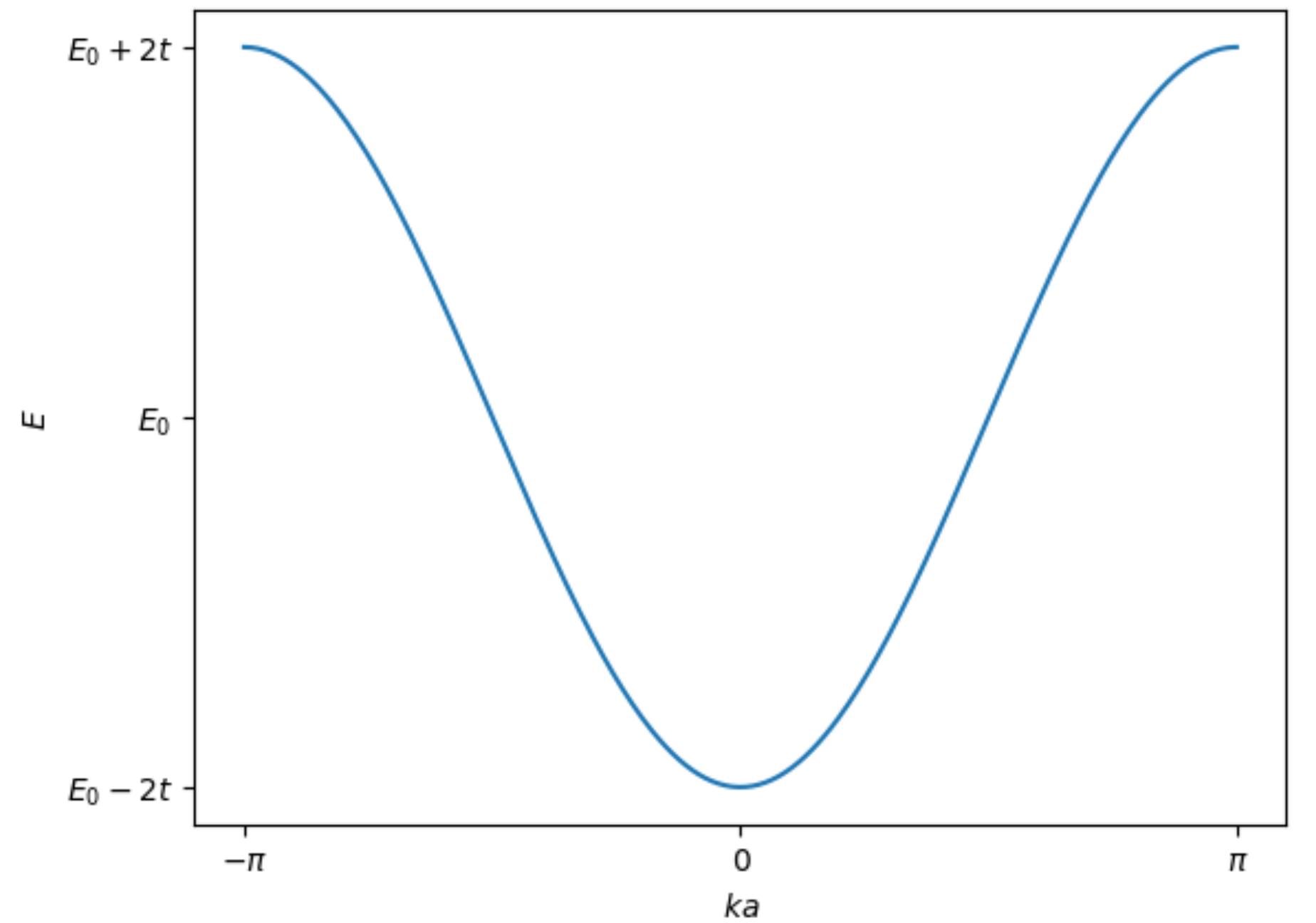
$$Ec_n = E_0 c_n - t c_{n+1} - t c_{n-1}.$$

$$EAe^{-ikna} = E_0 Ae^{-ikna} - t Ae^{-ik(n+1)a} - t Ae^{-ik(n-1)a},$$

$$1 = e^{ik0} = e^{ikNa}.$$

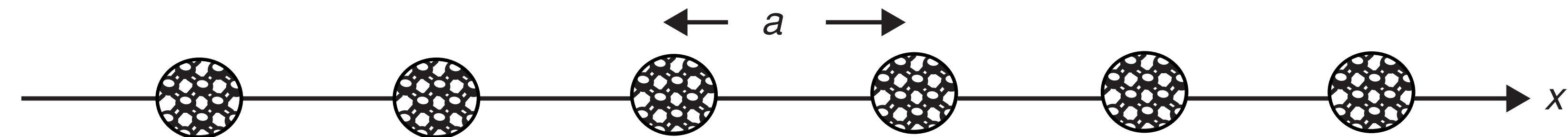
# DISPERSÃO OU DIAGRAMA DE BANDAS

$$E = E_0 - te^{-ika} - te^{ika} = E_0 - 2t \cos(ka),$$

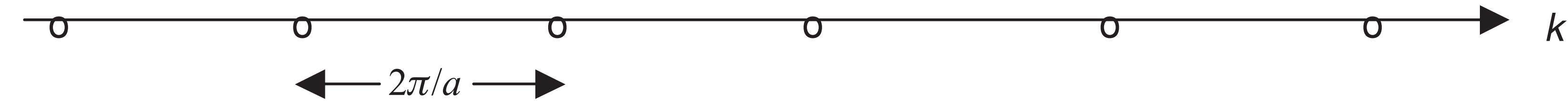


# ESPAÇO RECÍPROCO

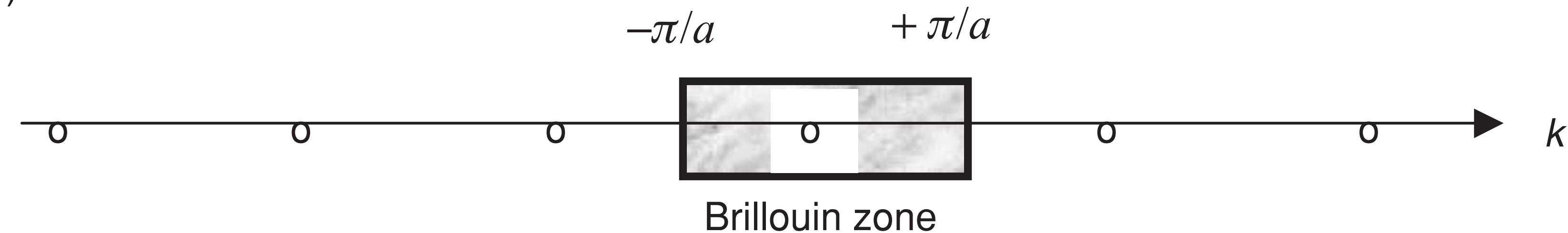
(a) Direct lattice



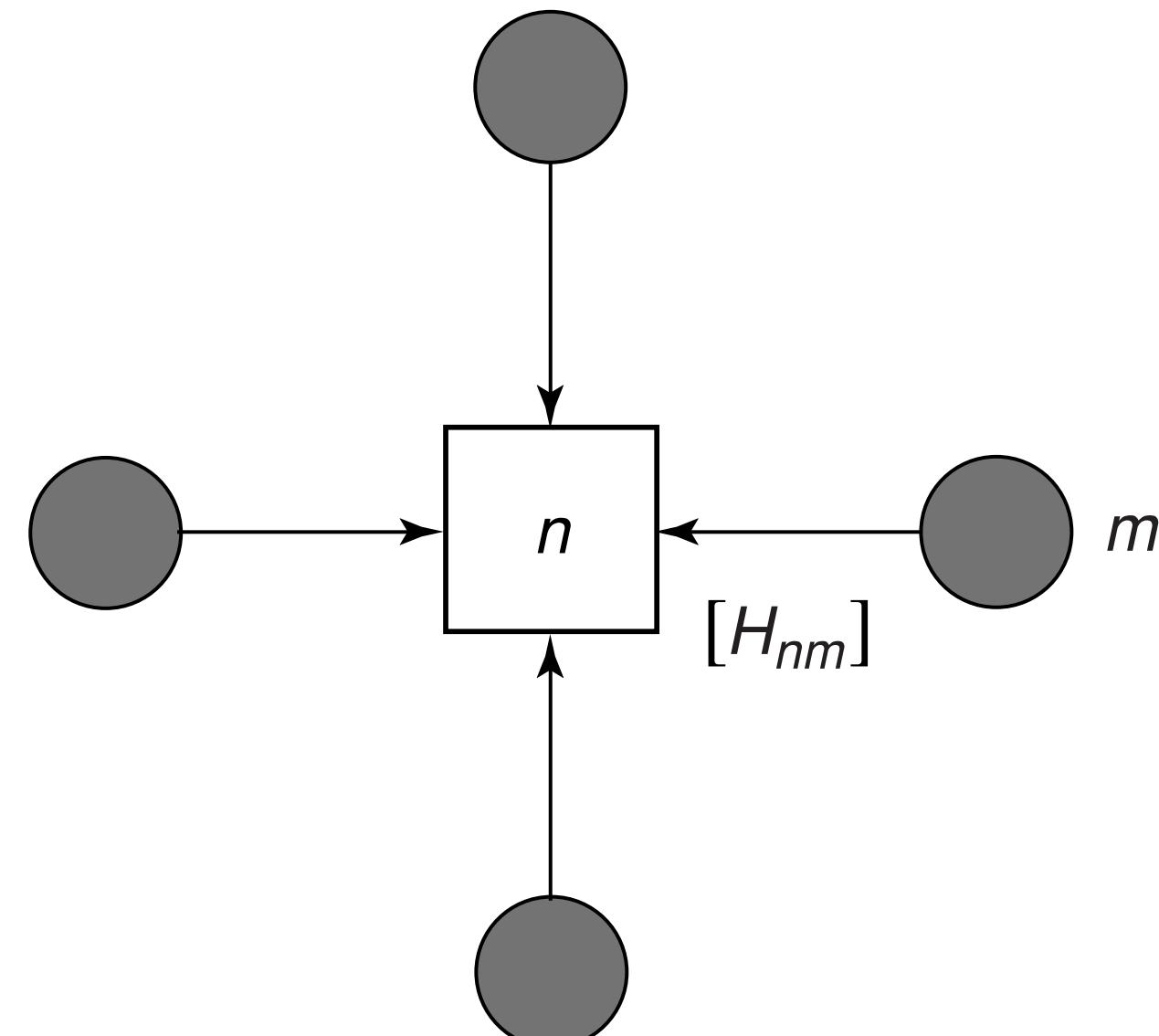
(b) Reciprocal lattice



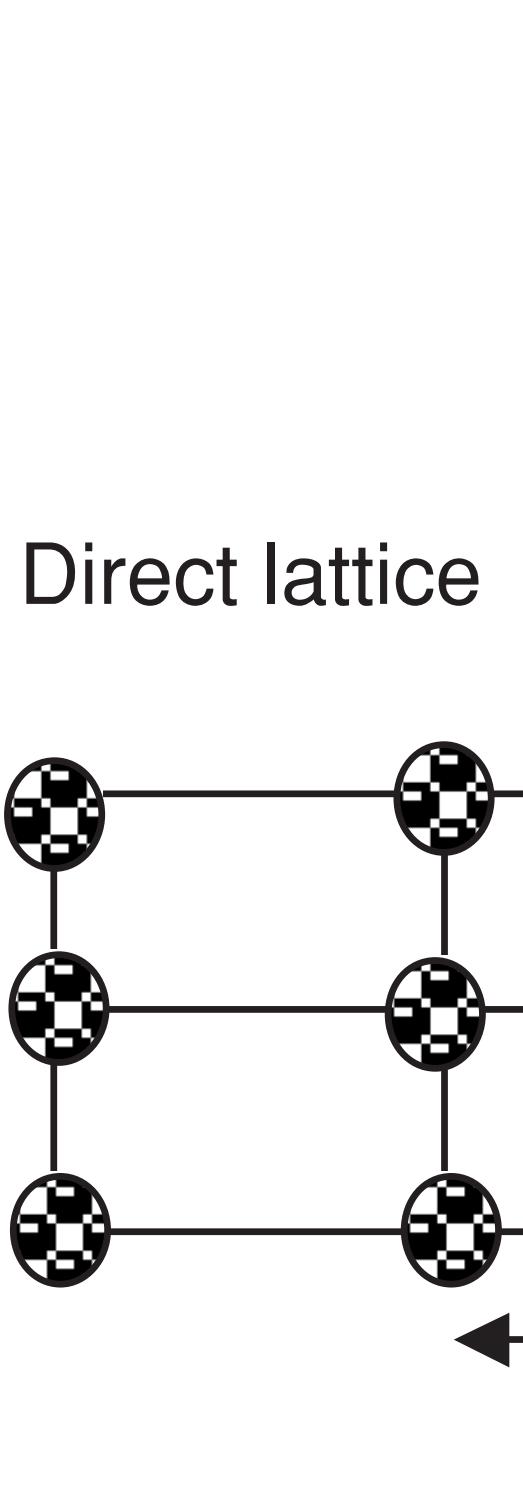
(c)



2D



(a)



Direct lattice

(b)

Reciprocal  
lattice

