Electric dipole moment, topology and quantization of the Su-Schiefer-Heeger model

Physics Department
EPN

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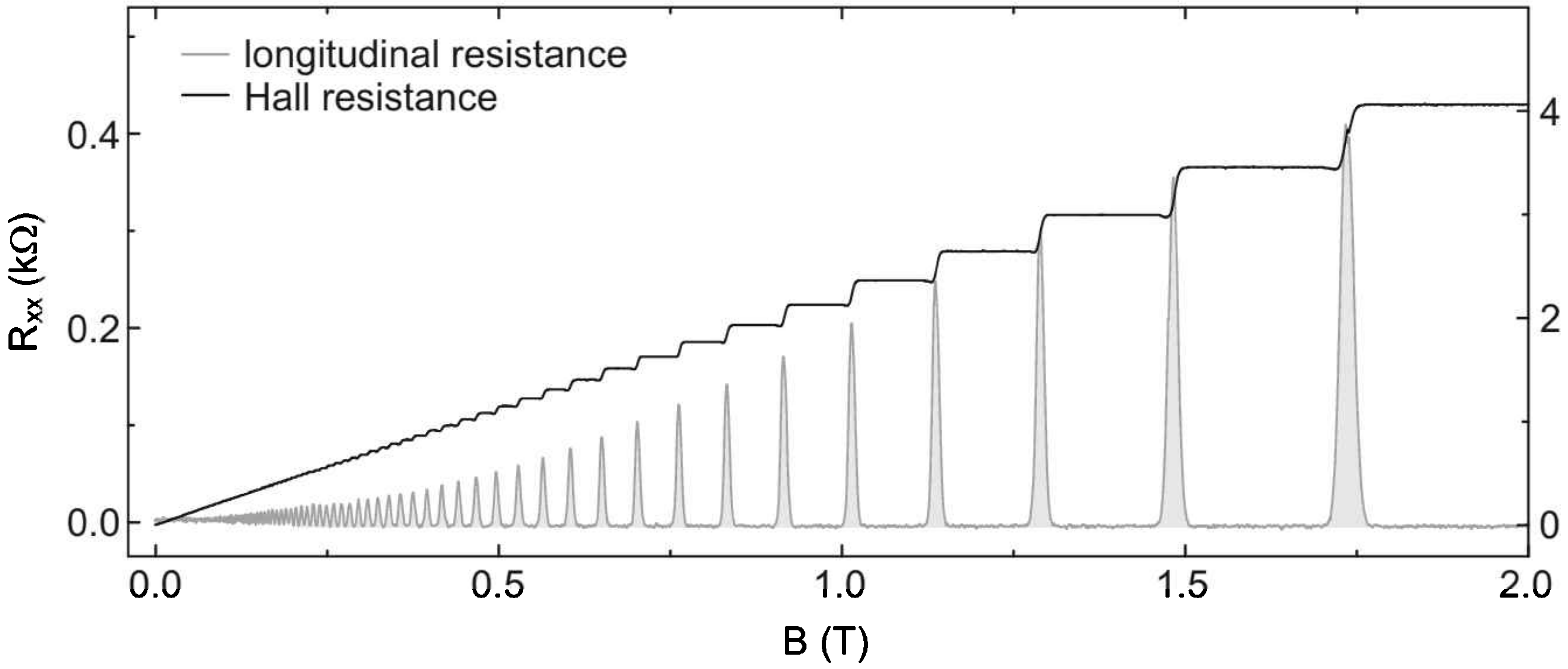
Motivation

Quantum Hall effect

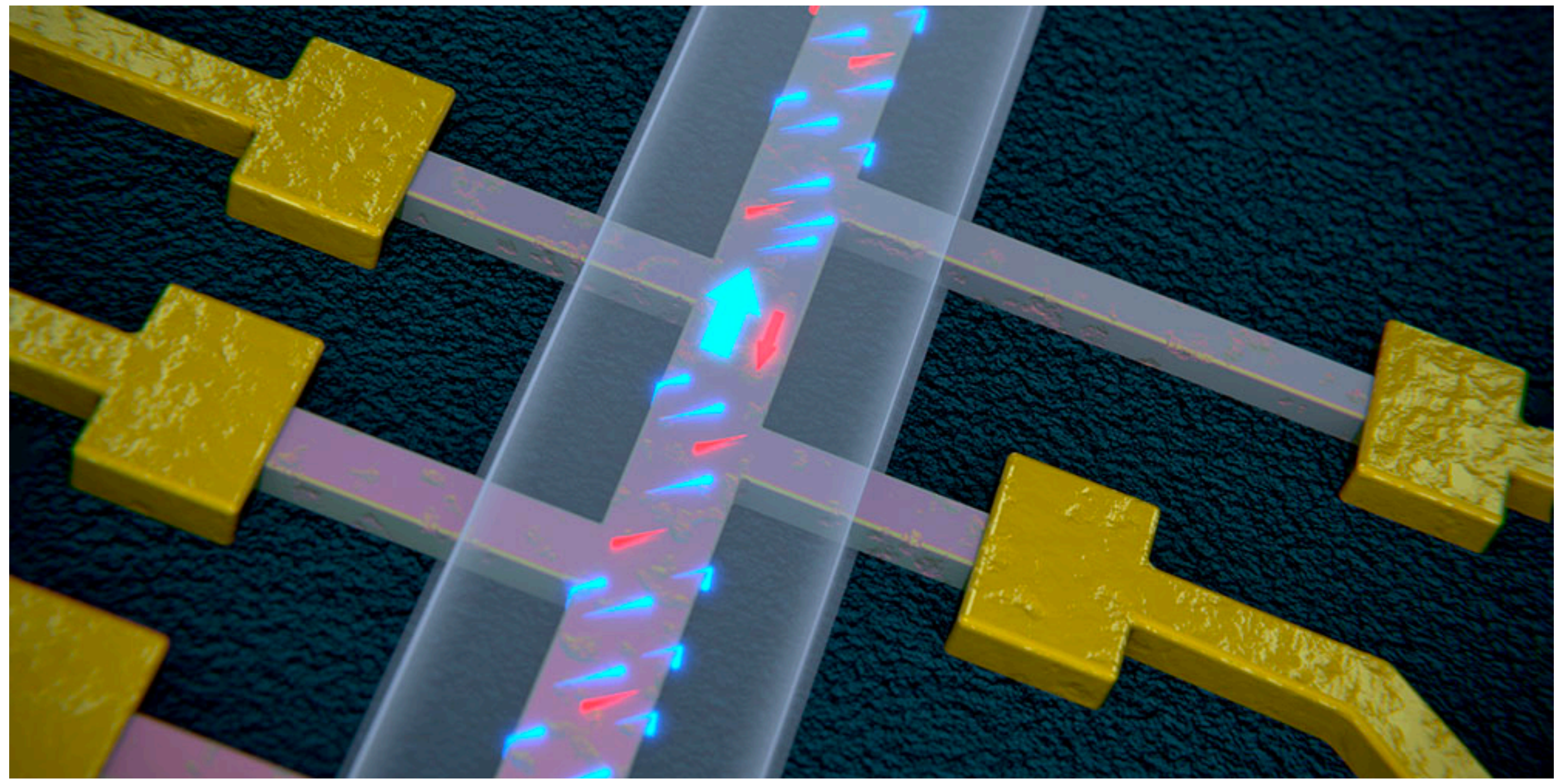


Longitudinal Hall Resistance of a two-dimensional electron gas

$$G_{xy} \equiv \frac{I_x}{V_y} = ne^2/h = \frac{n}{25812.807\Omega}$$

Topological Phases of Matter, New particles, Phenomena and Ordering Principles, Roderich Messier and Joel Moore

Quantum one-way street in topological insulator nanowires



Topological qubits
Robust quantum information

Nature Nanotechnology (2022); dot: 10.1038/s41565-022-02224-1
https://www.unibas.ch/en/News-Events/News/Uni-Research/

Electric monopole

$$|\phi(\mathbf{r},t)|^2 d^3r = dP(\mathbf{r},t)$$

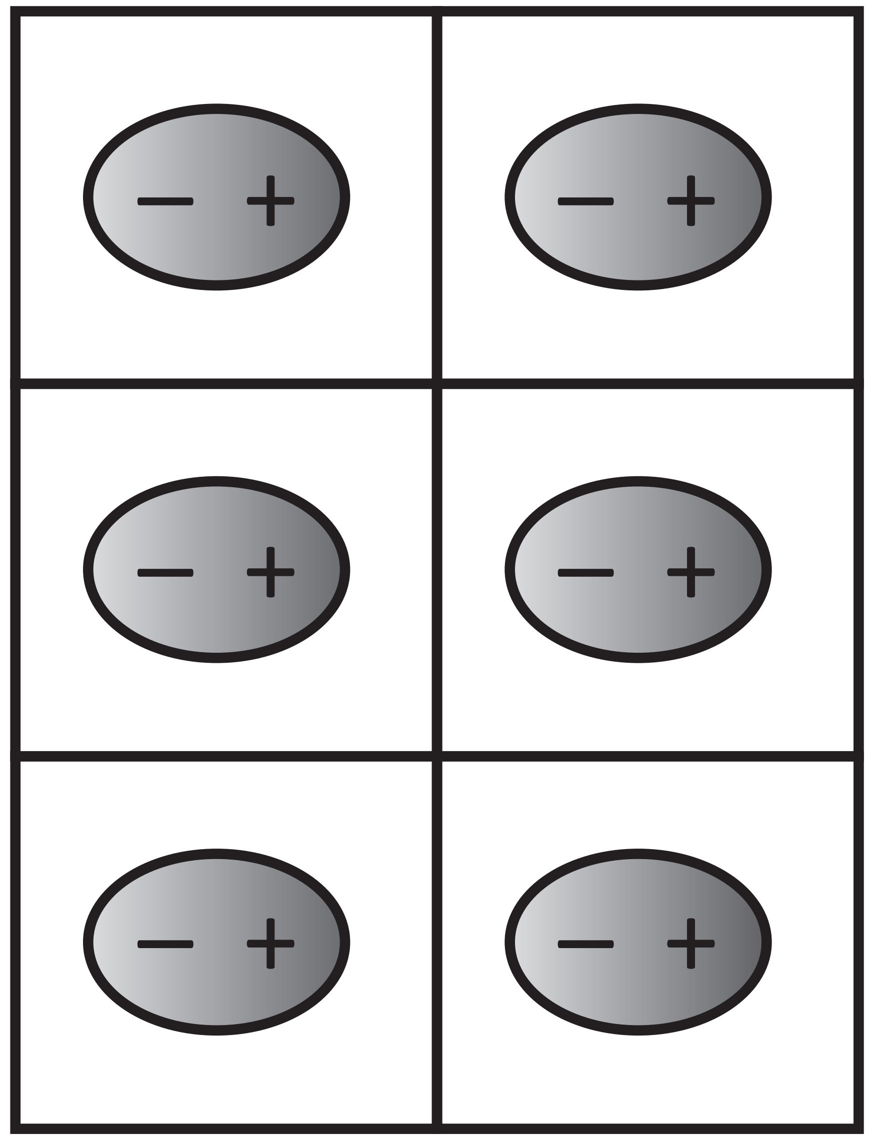
$$\rho^{\text{elec}} = \sum_{i=1}^{N_{\text{occ}}} |\psi_i^{\text{elec}}|^2$$

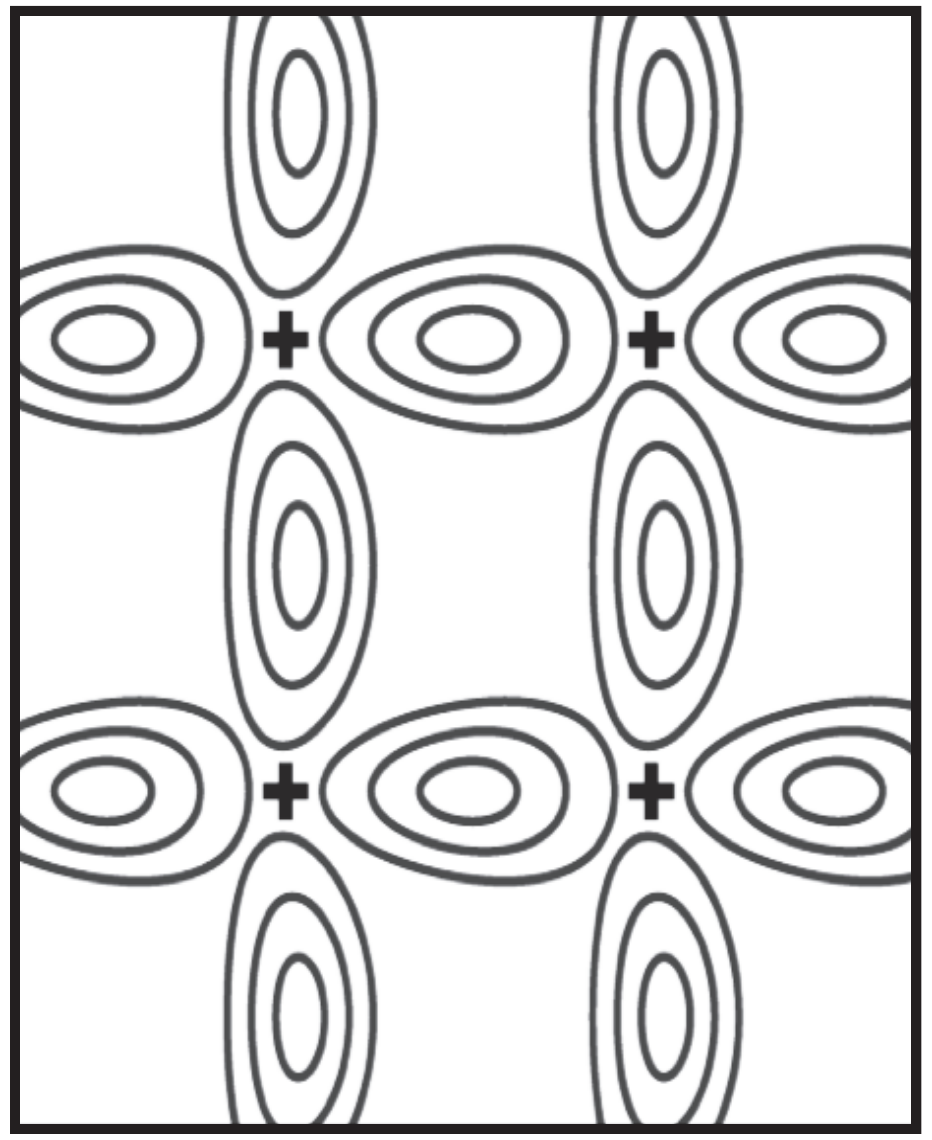
$$Q^{\text{tot}} = \rho^{\text{elec}} e = \sum_{i=1}^{N_{\text{occ}}} |\psi_i^{\text{elec}}|^2 e$$

Polarization

$$\mathbf{P} = \frac{1}{V_{\rm cell}} \int_{\rm cell} \mathbf{r}\,\rho(\mathbf{r})\,d^3r\,,$$

Charges separated,
polarized entities

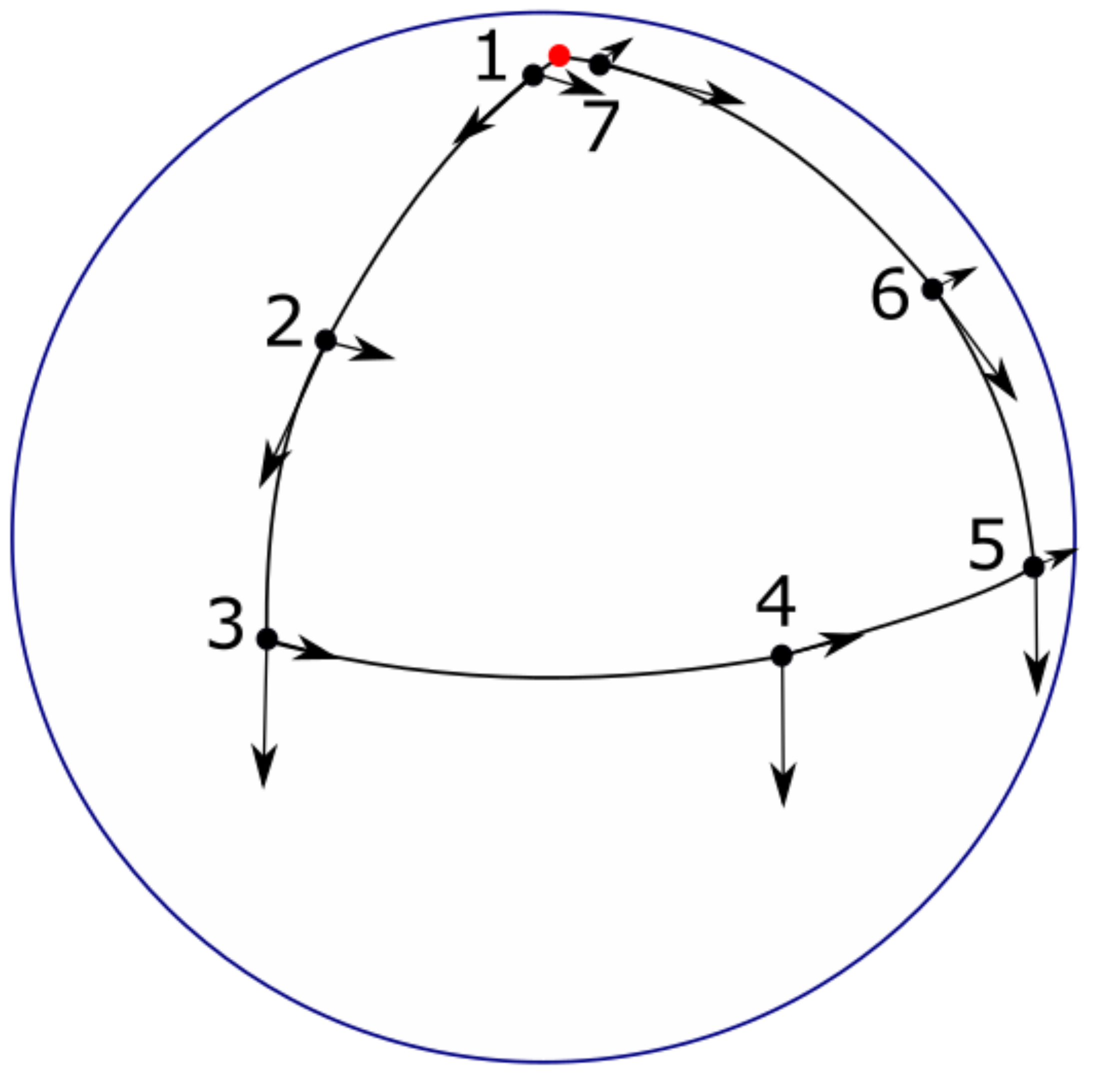




Charge-density
contour in a insulator

¿How to define a dipole per unit cell?

Modern theory of Polarization

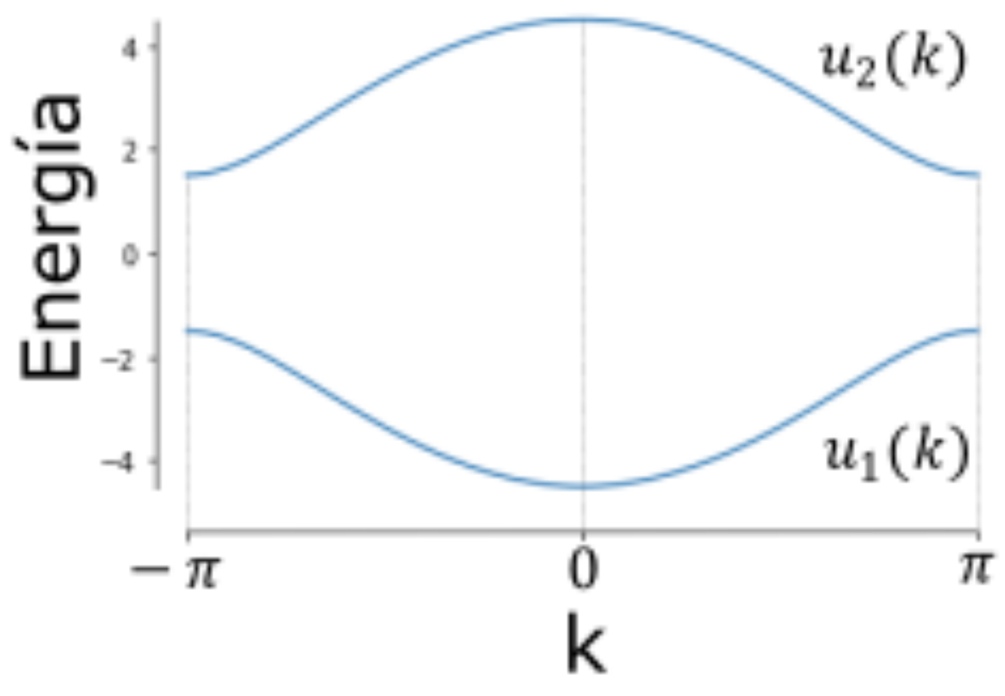


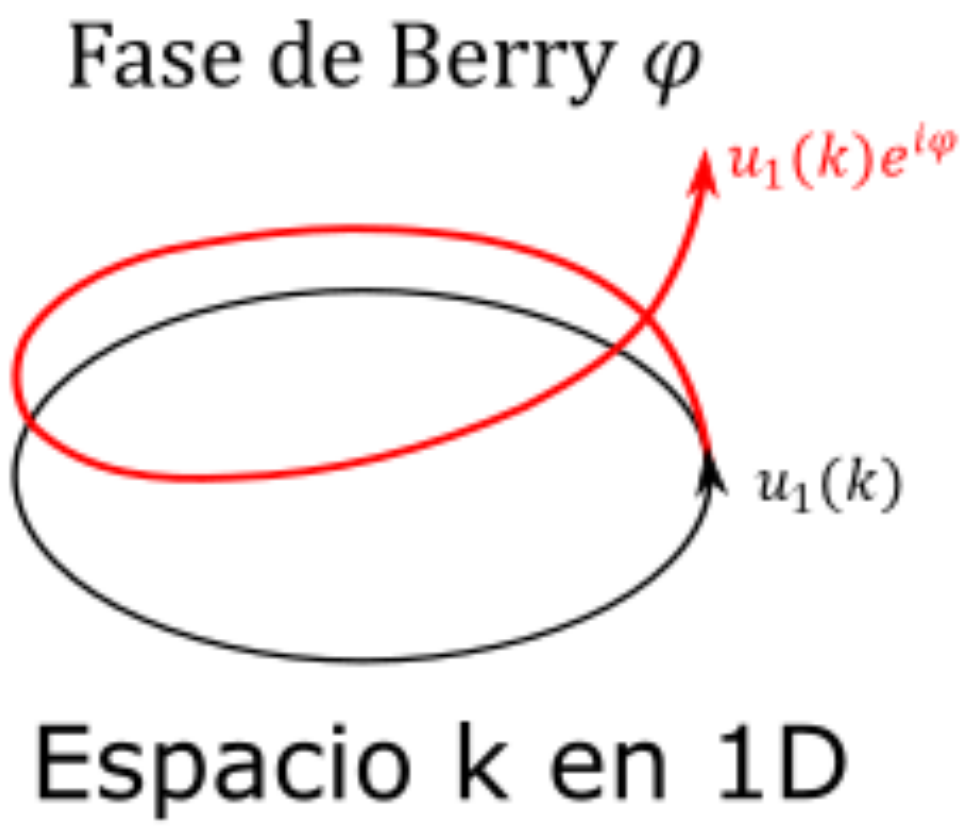
$$P_{elec} = \sum_{n}^{M} \varphi_n$$

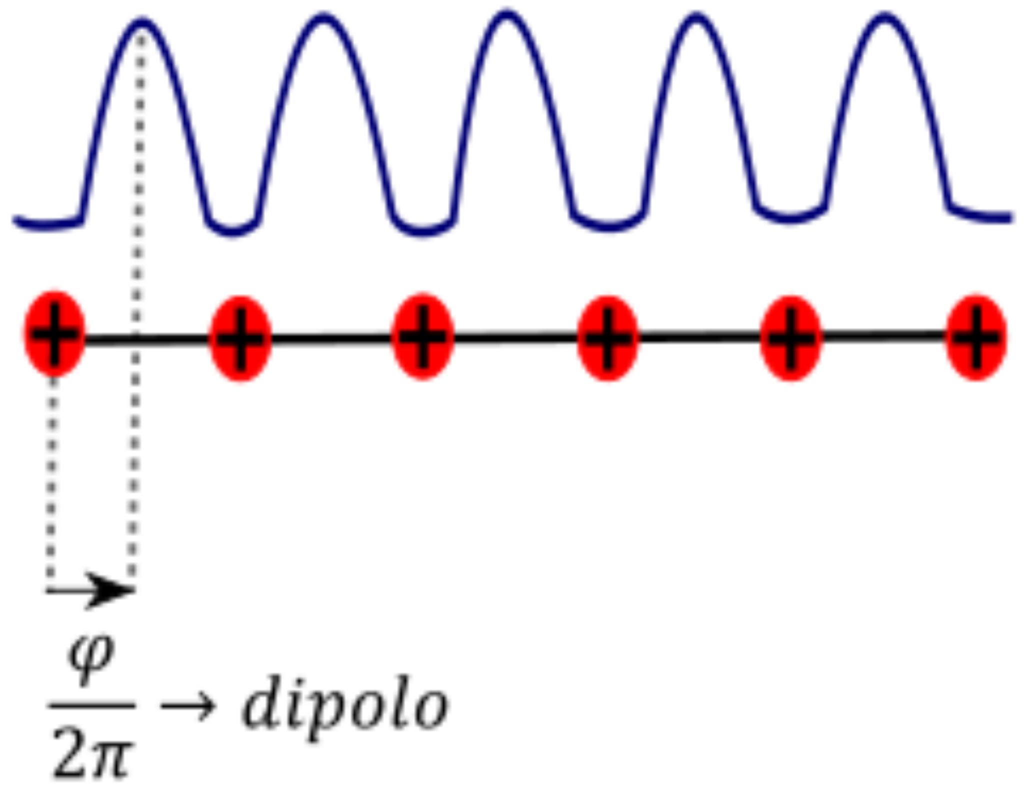
Reciprocal space
Berry phase

$$P_{elec} = \sum_{n}^{N} \bar{r}_n$$

Real space
Wannier center







Paquete de onda electrónica
(Centros de Wannier)

Wannier Functions

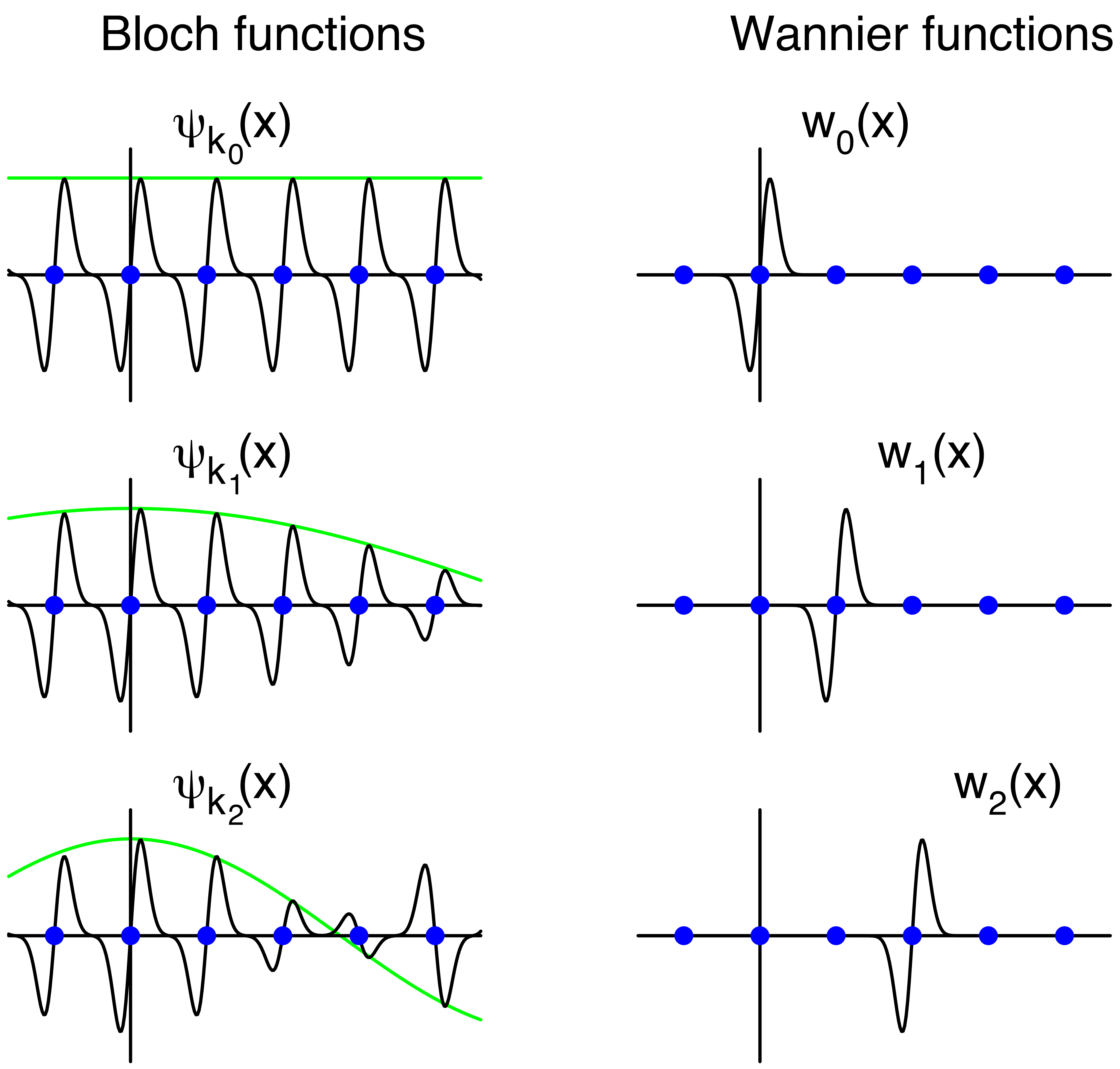
$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}.\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$ Bloch functions

$$W_n(\mathbf{r}-\mathbf{R}) = \frac{V}{(2\pi)^3}\int_{BZ} d^3\mathbf{k} e^{-i\mathbf{k}.\mathbf{R}} \psi_{n\mathbf{k}}(\mathbf{r})$$

Localized Wannier functions

$$\bar{\mathbf{r}}_n = \langle \mathbf{r}_n \rangle = \int W_n^*(\mathbf{r})\mathbf{r}W_n(\mathbf{r})d^3\mathbf{r}$$

Averaged electron position



10.1103/RevModPhys.84.1419 (2012)

Quantum-Mechanical Position Operator in Extended Systems
(R. Resta 1998)

$$\hat{X} = \sum_{i=1}^{N} x_i$$

Position operator

$$\langle X \rangle = \frac{L}{2\pi} \mathrm{Im}\ \ln \left\langle \psi_0 \left| e^{i \frac{2\pi}{L} \hat{X}} \right| \psi_0 \right\rangle$$

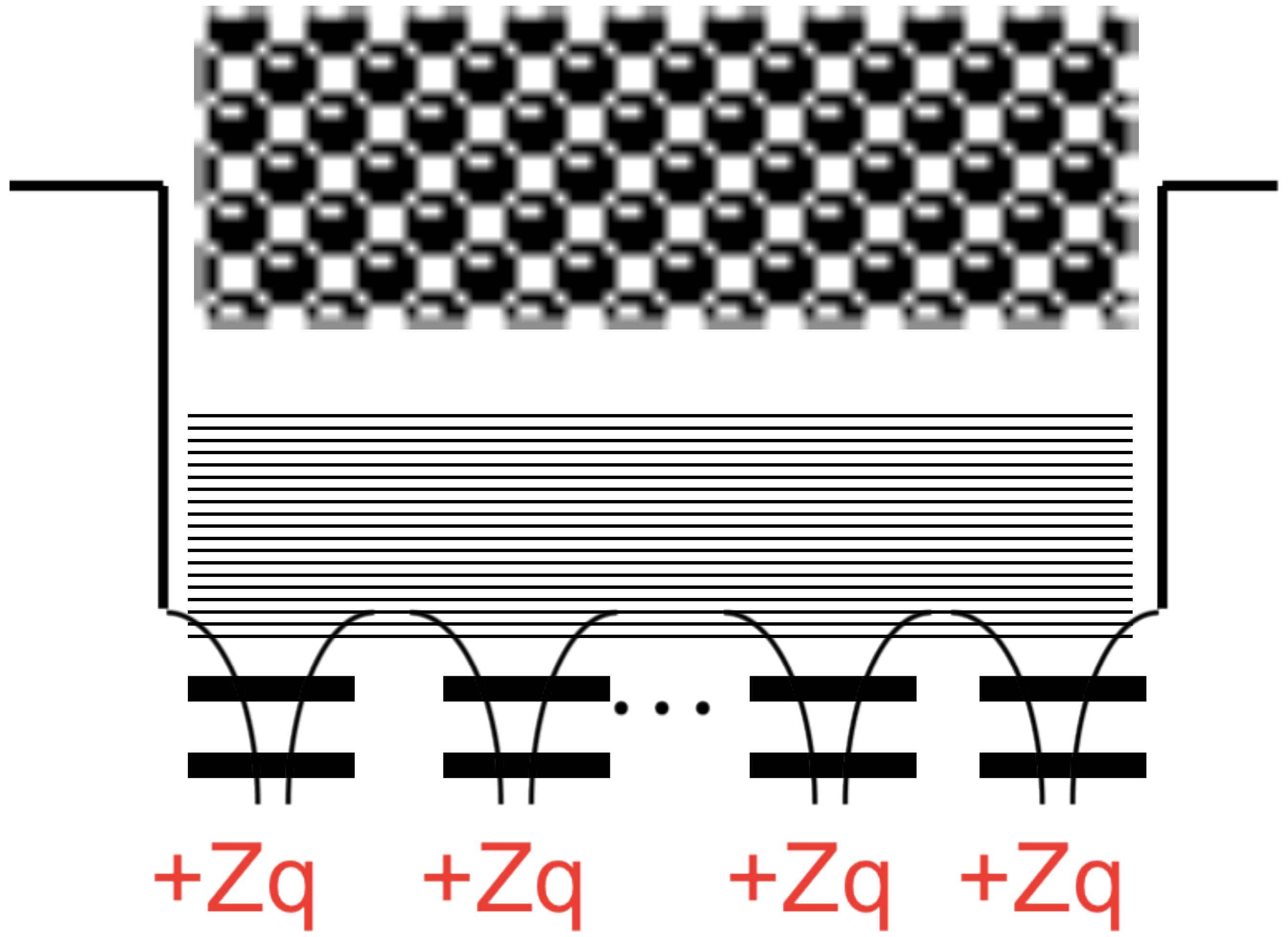
Many-body operator

$$e^{i \frac{2\pi}{L} 0} = e^{i \frac{2\pi}{L} L} = 1$$

$$P_{\mathrm{elec}} = \lim_{L \to \infty} \frac{e}{2\pi} \mathrm{Im}\ \ln \left\langle \psi_0 \left| e^{i \frac{2\pi}{L} \hat{X}} \right| \psi_0 \right\rangle$$

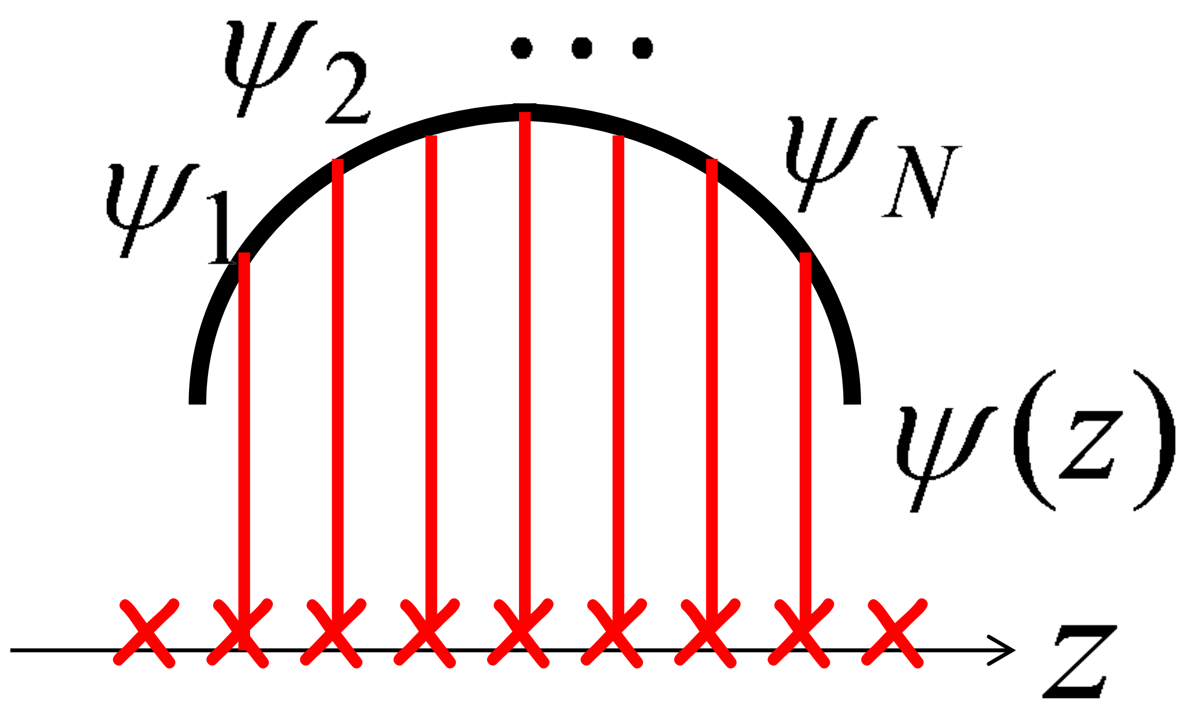
Wannier centers

Differential to Matrix



$$E\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)\psi(\vec{r})$$

Schrödinger Equation



N x N

$$E\,[S]\begin{Bmatrix}\psi_1\\ \psi_2\\ \cdots\\ \cdots\\ \psi_N\end{Bmatrix} = \begin{bmatrix}\cdots & \cdots & \cdots\\ \cdots & H & \cdots\\ \cdots & \cdots & \cdots\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\\ \cdots\\ \cdots\\ \psi_N\end{Bmatrix}$$

Matrix Schrödinger Equation

Differential to Matrix

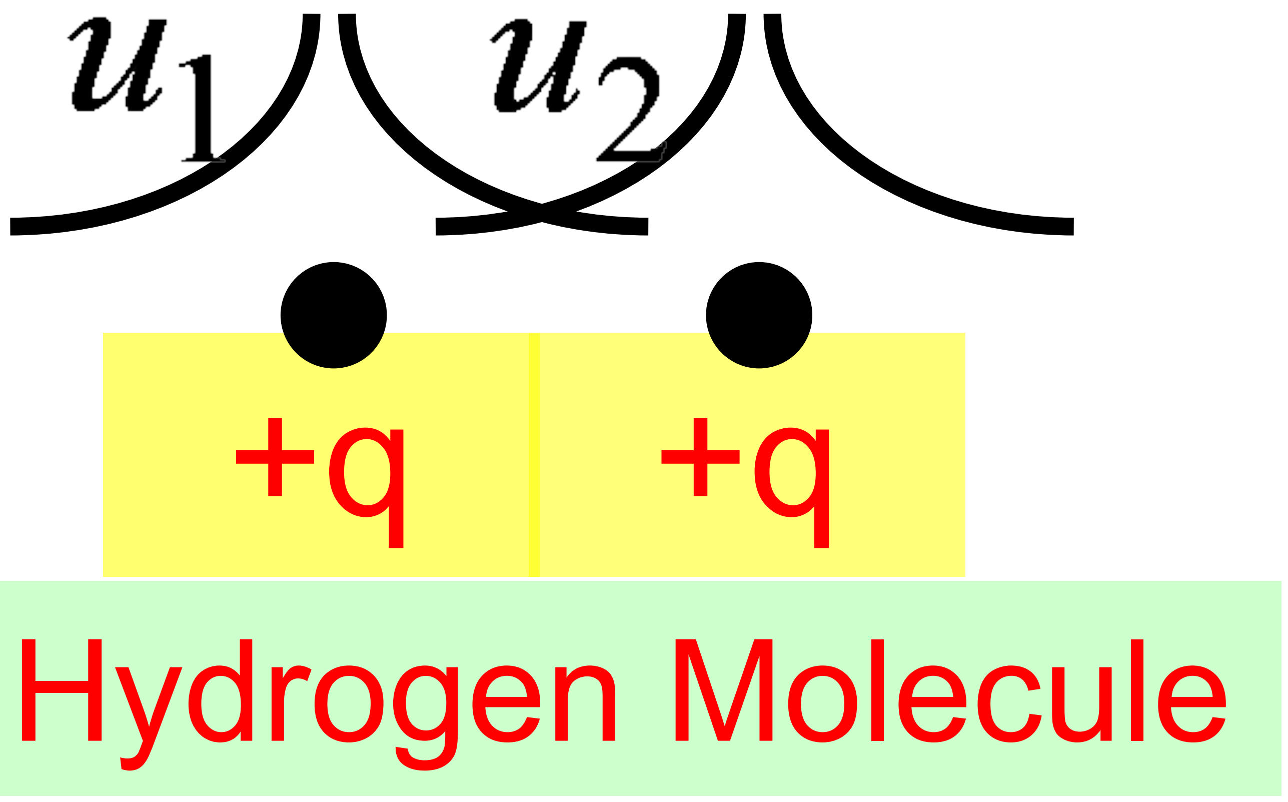
$$E[S]\{\psi\} = [H]\{\psi\}$$

$$E\psi(\vec{r}) = \underbrace{\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right)}_{H_{op}}\psi(\vec{r})$$

$$E\begin{bmatrix}1 & s\\ s & 1\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix} = \begin{bmatrix}\varepsilon & t\\ t & \varepsilon\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix}$$

$\varepsilon - t$

$\varepsilon + t$



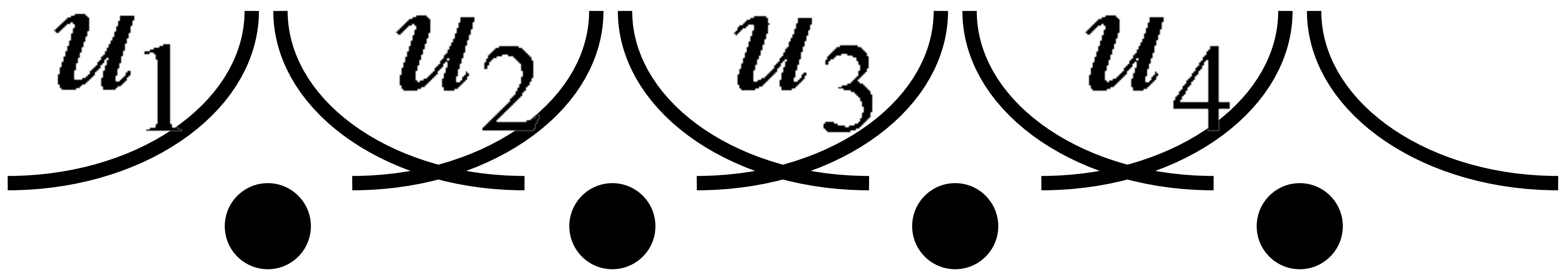
$$H_{mn} = \int dV\, u_m^*(\vec{r})\, H_{op}\, u_n(\vec{r})$$

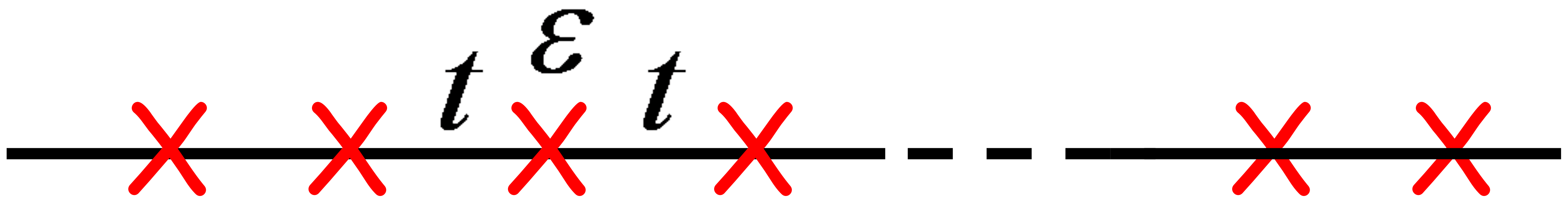
$$S_{mn} = \int dV\, u_m^*(\vec{r})\, u_n(\vec{r})$$

$$\psi(\vec{r}) = \sum_{m=1}^{N} \psi_m\, u_m(\vec{r})$$

N = number of “basis functions”

Models, models



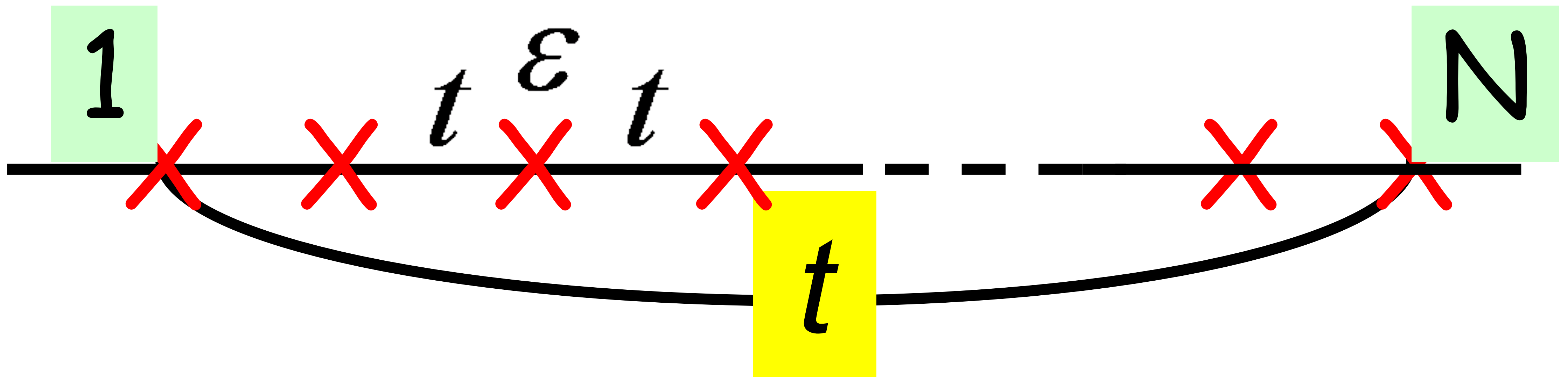


$$E\begin{Bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_{N-1}\\ \psi_N\end{Bmatrix} = \begin{bmatrix}\varepsilon & t & 0 & \cdots & & \\ t & \varepsilon & t & 0 & \cdots & \\ 0 & t & \varepsilon & t & 0 & \cdots \\ \vdots & \vdots & \vdots & & & \\ \cdots & \cdots & 0 & t & \varepsilon & \end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_{N-1}\\ \psi_N\end{Bmatrix}$$

Open boundary condition

$$E\psi_n = +t\,\psi_{n-1} + \varepsilon\,\psi_n + t\,\psi_{n+1}$$

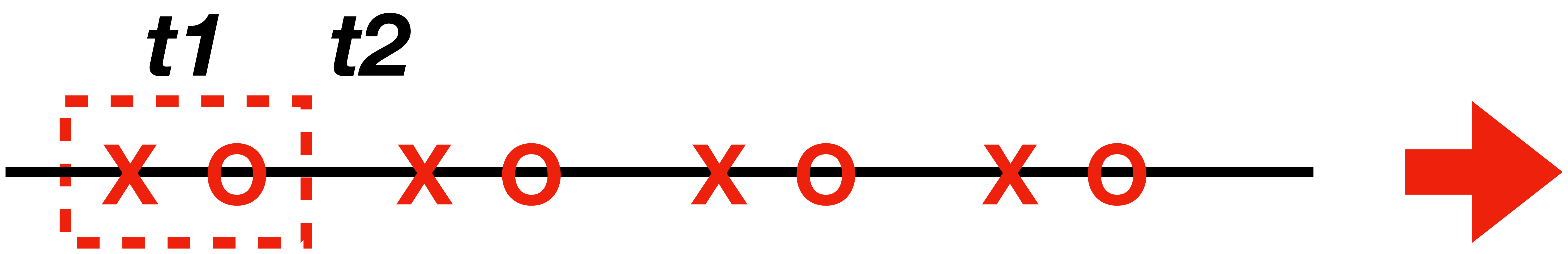
Models, models

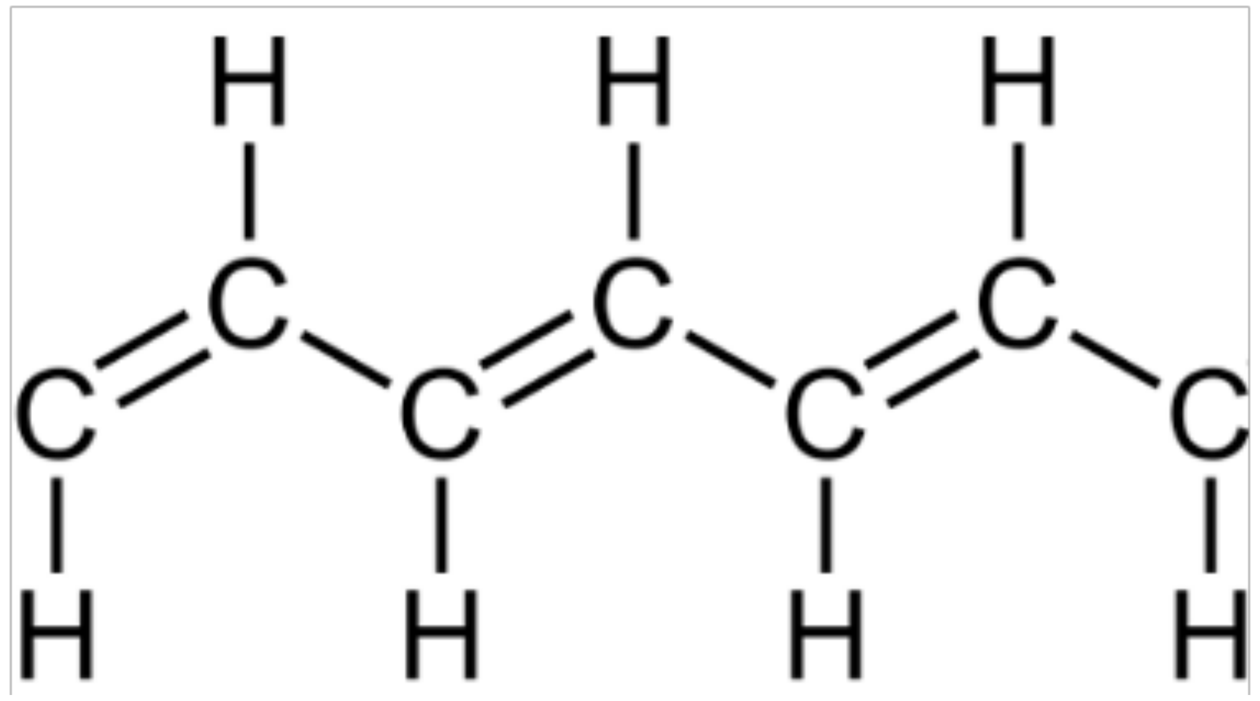


$$E\begin{Bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_{N-1}\\ \psi_N\end{Bmatrix}=\begin{bmatrix}\varepsilon & t & 0 & \cdots & & t\\ t & \varepsilon & t & 0 & \cdots & \\ 0 & t & \varepsilon & t & 0 & \cdots\\ & \vdots & \vdots & \vdots & & \\ t & & \cdots & 0 & t & \varepsilon\end{bmatrix}\begin{Bmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_{N-1}\\ \psi_N\end{Bmatrix}$$

Periodic boundary condition

Modelo SSH





Polyacetylene

$$H_{SSH} = \sum_{R=1}^{N} t_1(a_R^\dagger b_R + b_R^\dagger a_R) + t_2(b_R^\dagger a_{R+1} + a_{R+1}^\dagger b_R)$$

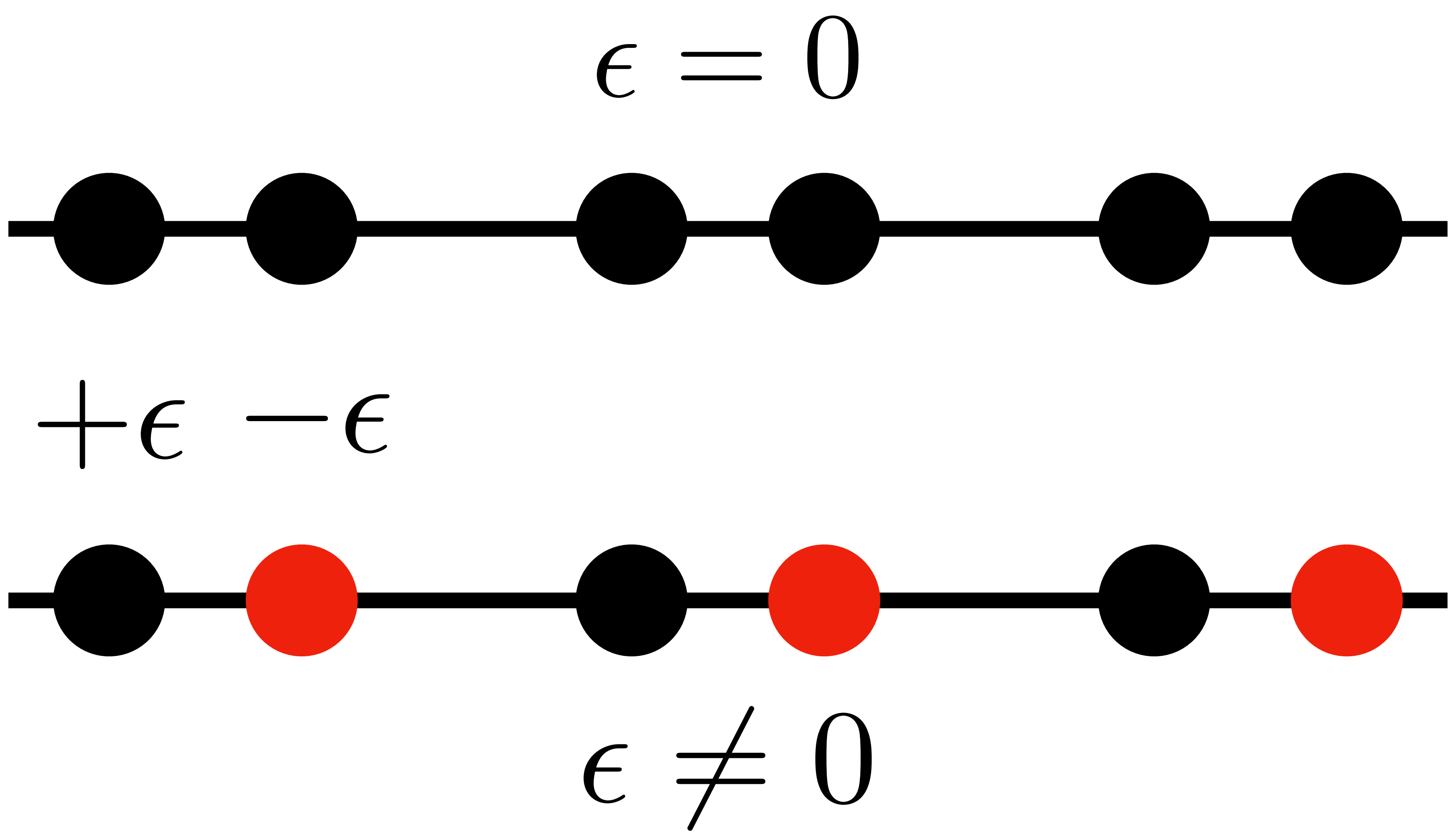
$$H_{SSH} = \begin{pmatrix} \epsilon & t_1 & 0 & 0 & \cdots & 0 \\ t_1^* & \epsilon & t_2 & 0 & 0 & \cdots \\ 0 & t_2^* & \epsilon & t_1 & 0 & 0 \\ 0 & 0 & t_1^* & \epsilon & t_2 & 0 \\ \cdots & 0 & 0 & t_2^* & \epsilon & \cdots \\ 0 & \cdots & 0 & 0 & t_1^* & \epsilon \end{pmatrix}$$

trivial phase t1 > t2

topological phase t1 < t2

Modelo SSH

$$H_{SSH} = \begin{pmatrix} \epsilon & t_1 & 0 & 0 & \cdots & t_2 \\ t_1^* & -\epsilon & t_2 & 0 & 0 & \cdots \\ 0 & t_2^* & \epsilon & t_1 & 0 & 0 \\ 0 & 0 & t_1^* & -\epsilon & t_2 & 0 \\ \cdots & 0 & 0 & t_2^* & \epsilon & \cdots \\ t_2^* & \cdots & 0 & 0 & t_1^* & -\epsilon \end{pmatrix}$$

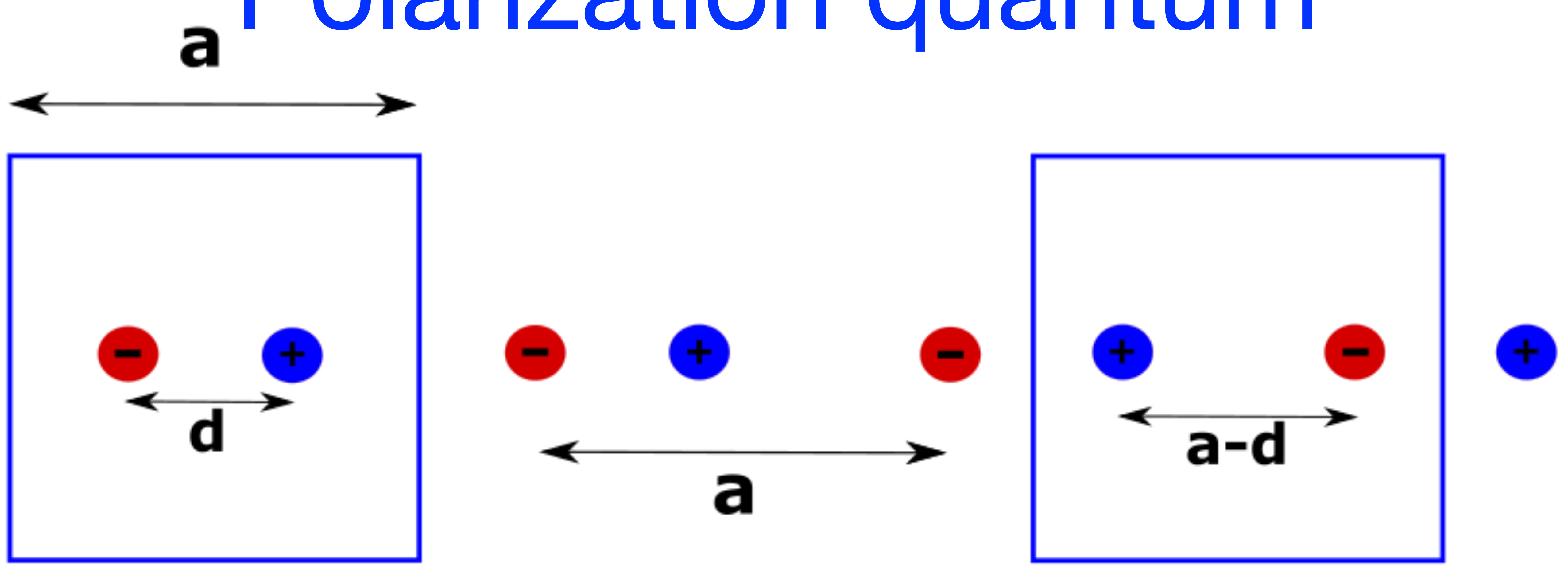


Broken inversion and chiral symmetry

$$H_{SSH} = \begin{pmatrix} \epsilon & t_1 & 0 & 0 & \cdots & t_2 \\ t_1^* & \epsilon & t_2 & 0 & 0 & \cdots \\ 0 & t_2^* & \epsilon & t_1 & 0 & 0 \\ 0 & 0 & t_1^* & \epsilon & t_2 & 0 \\ \cdots & 0 & 0 & t_2^* & \epsilon & \cdots \\ t_2^* & \cdots & 0 & 0 & t_1^* & \epsilon \end{pmatrix}$$

Periodic boundary condition

Polarization quantum



$$p = q^- d^- + q^+ d^+ = -e\frac{-1}{2} + e\frac{1}{2} = ed$$

Dipolar moment

$$P = \frac{ed}{V}$$

Polarization

$$p = q^+ d^+ + q^- d^- = +e\frac{a-d}{2} - e\frac{a-d}{2} = ed - ea$$

Dipolar moment

$$P = \frac{ed}{V} - \frac{ea}{V}$$

Polarization

$$\mathbf{P} = \frac{e\mathbf{d}}{V} + n\frac{e\mathbf{R}}{V}$$

Polarization quantum

Expected value of the position operator

$$U_x = \sum_{R=1}^{N} \sum_{\alpha=1}^{N_{\mathrm{orb}}} |R, \alpha\rangle \, e^{i \frac{2\pi}{N} R} \, \langle R, \alpha|$$

Position operator

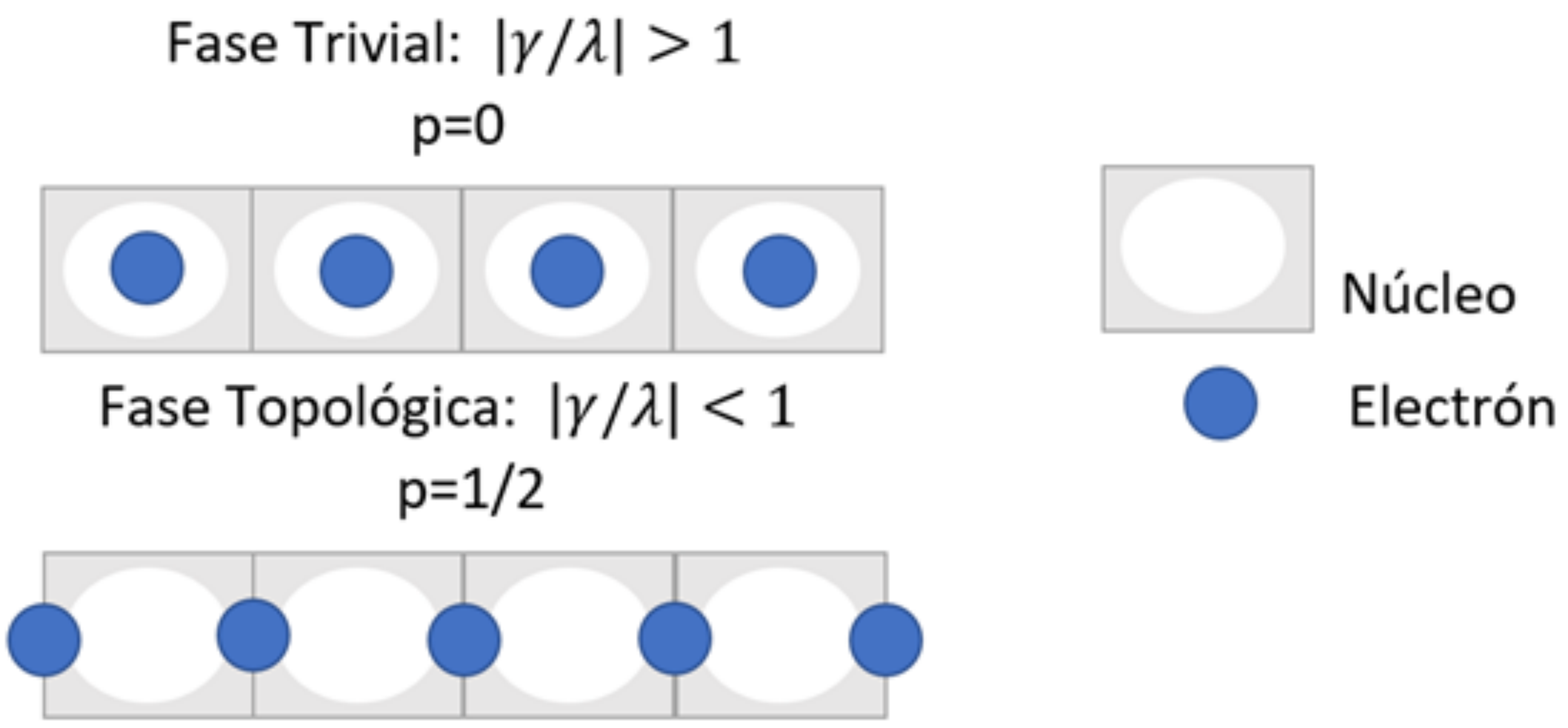
$$P_{\mathrm{occ}} = \sum_{n=1}^{N_{\mathrm{occ}}} \left|\psi_n^{\mathrm{elec}}\right\rangle \left\langle \psi_n^{\mathrm{elec}}\right|$$

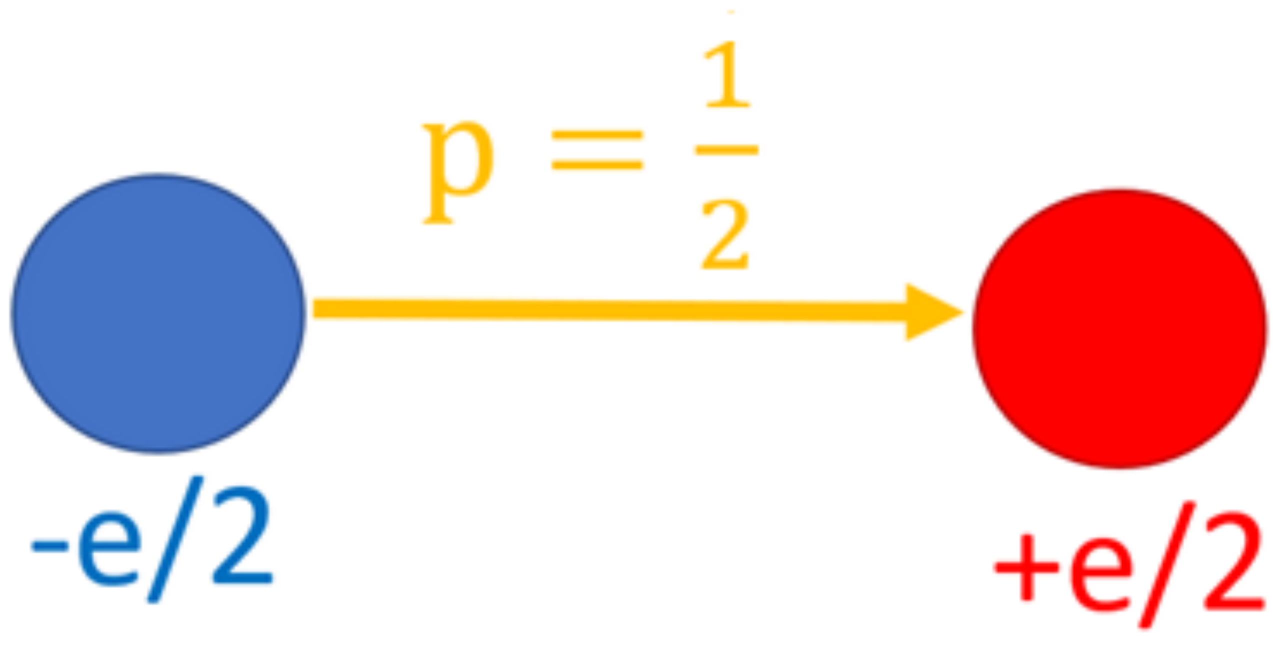
Projection operator on occupied states

$$\langle U_x \rangle = \langle P_{\mathrm{occ}} | U_x | P_{\mathrm{occ}} \rangle$$

Phase of eigenvalues → Electron positions

Electric dipole





$$p = q^- d^- + q^+ d^+ = \frac{-e}{2}\frac{-1}{2} + \frac{e}{2}\frac{1}{2} = \frac{1}{2}e$$

References

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GRACIAS