$$P_{\text{chain}} = \int_0^L dx\, x \left[\rho^{\text{ion}}(x) + \rho^{\text{el}}(x)\right] \tag{1}$$

$$\rho^{\text{ion}}(x) = \sum_j (+e)\delta(x - x_j^{\text{ion}}) \tag{2}$$

$$\rho^{\text{el}}(x) = -\frac{e}{L}\sum_j^{\text{occ}} |\psi_j(x)|^2 = -\frac{e}{L}\sum_j^{\text{occ}} |w_j(x)|^2, \qquad |w_j\rangle = \sum_i^{\text{occ}} |\psi_i\rangle U_{ij} \tag{3}$$

$$\hat{\mathbb{P}} = \sum_j^{\text{occ}} |\psi_j\rangle\langle\psi_j|, \qquad \hat{\mathbb{P}}\hat{x}\hat{\mathbb{P}}|w_j\rangle = x_j^{\text{WF}}|w_j\rangle, \qquad x_j^{\text{WF}} = \langle w_j|x|w_j\rangle \tag{4}$$

$$P_{\text{chain}} = \frac{1}{L}\sum_j \left[(+e)x_j^{\text{ion}} + (-e)x_j^{\text{WF}}\right] \tag{5}$$

$$P_{\text{chain}} = \frac{e}{a}\left(\tau^{\text{ion}} - \tau^{\text{WF}}\right) + e\left(N_{\text{head}}^{\text{ion}} - N_{\text{head}}^{\text{WF}}\right) = P_{\text{bulk}} + e \times (\text{integer}) \tag{6}$$

$$P_{\text{chain}} = \mathbf{Q}_{\mathbf{surf}}^{\mathbf{macro}} = \mathbf{P}_{\mathbf{bulk}}\ \textbf{modulo e} \tag{7}$$

$$|R\rangle = \frac{a}{2\pi}\int_0^{2\pi/a} dk\, e^{-ikR}|\psi_k\rangle, \qquad |\psi_k\rangle = \sum_R e^{ikR}|R\rangle \tag{8}$$

Continuum	Discrete
$\frac{a}{2\pi}\int dk$	$\frac{1}{N}\sum_k$
$\frac{2\pi}{a}\delta(k-k')$	$N\delta_{kk'}$

$$|R\rangle = \frac{1}{N}\sum_k e^{-ikR}|\psi_k\rangle, \qquad |\psi_k\rangle = \sum_R e^{ikR}|R\rangle \tag{9}$$

Bloch's theorem:

$$\psi_k(x+R) = e^{ikR}\psi_k(x), \quad \psi_k(x) \equiv e^{ikx}u_k(x) \;\Rightarrow\; u_k(x+R) = u_k(x) \tag{10}$$

Orthonormality:

$$\langle\psi_k|\psi_{k'}\rangle_{\text{all sp.}} = N\delta_{kk'} = (2\pi/a)\delta(k-k') \;\Rightarrow\; \langle R|R'\rangle_{\text{all sp.}} = \delta_{RR'} \tag{11}$$

$$\text{Periodic gauge: } \psi_{k+2\pi/a} = \psi_k \;\Rightarrow\; u_{k+2\pi/a} = e^{-i(2\pi/a)x}u_k \tag{12}$$

$$\tau^{\rm WF} \equiv \langle 0|\hat{x}|0\rangle_{\text{all sp.}} = \frac{a}{2\pi}\int_0^{2\pi/a} dk\,\langle u_k|i\partial_k u_k\rangle_{\rm cell} \equiv \frac{\phi}{2\pi}a \quad \text{Berry phase} \tag{13}$$

$$P_{\rm bulk} = e\left(\frac{\tau^{\rm ion}}{a} - \frac{\tau^{\rm WF}}{a}\right) = e\left(\frac{\tau^{\rm ion}}{a} - \frac{\phi}{2\pi}\right) \tag{14}$$

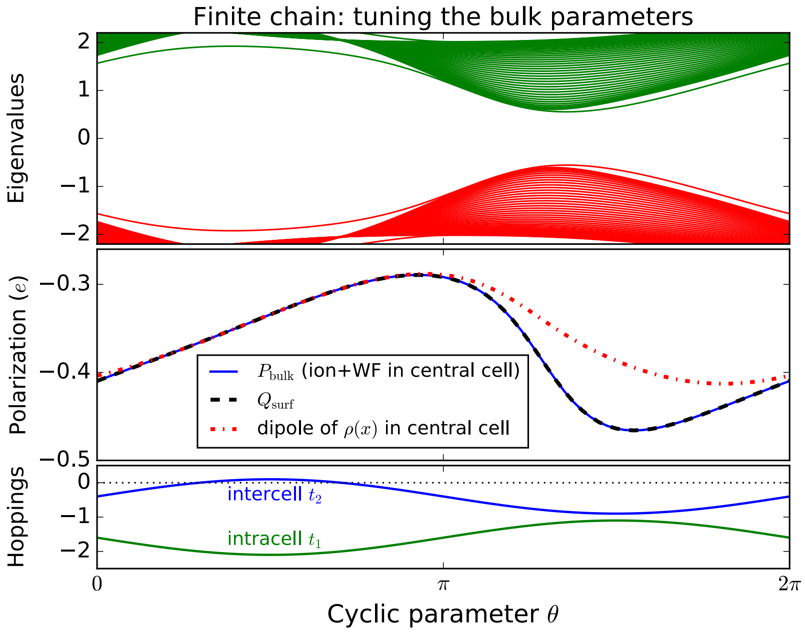
Gauge freedom:

$$|\widetilde{\psi}_k\rangle = e^{-i[\beta_{\rm per}(k)+nka]}|\psi_k\rangle \quad \Rightarrow \quad \begin{aligned} \widetilde{\phi} &= \phi + 2\pi n \\ \widetilde{\tau}^{\rm WF} &= \tau^{\rm WF} + na \\ \widetilde{\mathbf{P}}_{\mathbf{bulk}} &= \mathbf{P}_{\mathbf{bulk}} - \mathbf{ne} \end{aligned} \tag{15}$$

$$\phi \cong -{\rm Im}\ln\prod_{j=0}^{N-1}\langle u_{k_j}|u_{k_{j+1}}\rangle, \qquad k_j = \frac{2\pi}{a}\frac{j}{N}, \qquad |u_{\frac{2\pi}{a}}\rangle = e^{-i(2\pi/a)x}|u_0\rangle \tag{16}$$

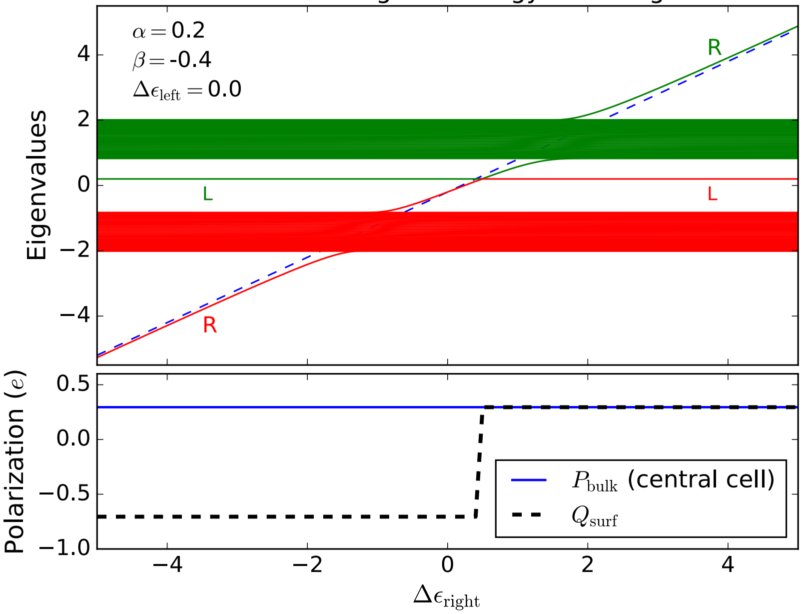
$$\Delta P_{\rm bulk}^{(\text{cycle})} \equiv \int_0^{2\pi}(\partial P_{\rm bulk}/\partial\theta)\,d\theta = eC$$

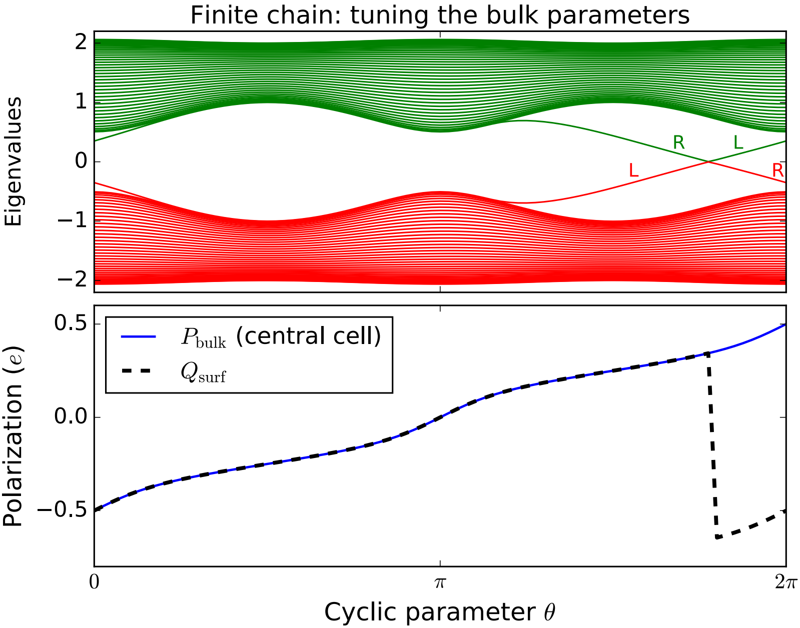
$$C = \frac{1}{2\pi}\int_0^{2\pi}d\theta\int_0^{2\pi/a}dk\,\overbrace{[-2{\rm Im}\langle\partial_k u|\partial_\theta u\rangle]}^{\text{Berry curv. } F_{k\theta}} = \text{integer} \tag{17}$$



Finite chain: tuning the bulk parameters
Eigenvalues
2
1
0
−1
−2
Polarization (e)
−0.3
−0.4
−0.5
P_{bulk} (ion+WF in central cell)
Q_{surf}
dipole of $\rho(x)$ in central cell
Hoppings
0
−1
−2
intercell t_2
intracell t_1
0
π
2π
Cyclic parameter θ

Finite chain: tuning site energy at the right end




Finite chain: tuning the bulk parameters
Eigenvalues
2
1
0
−1
−2
R
L
L
R
Polarization (e)
0.5
0.0
−0.5
P_{bulk} (central cell)
Q_{surf}
0
π
2π
Cyclic parameter θ

periodic chain: Berry phases