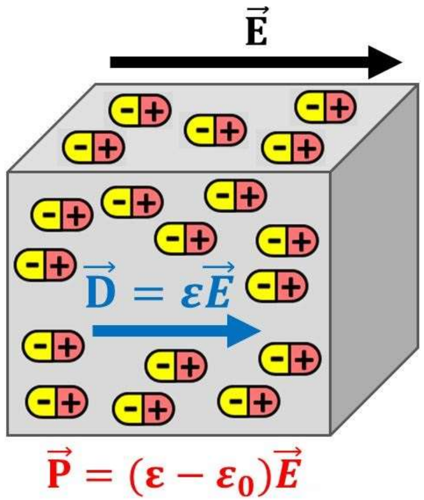
Modern theory of charge polarization

Electric polarization $$\vec{P} = \frac{1}{V}\int d^3r\, \vec{r}\,\rho(\vec{r})$$



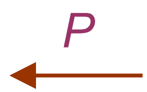
- well defined for finite system (sensitive to boundary)
- for crystal with localized dipoles

  P = dipole moments/volume

  (Claussius-Mossotti theory)

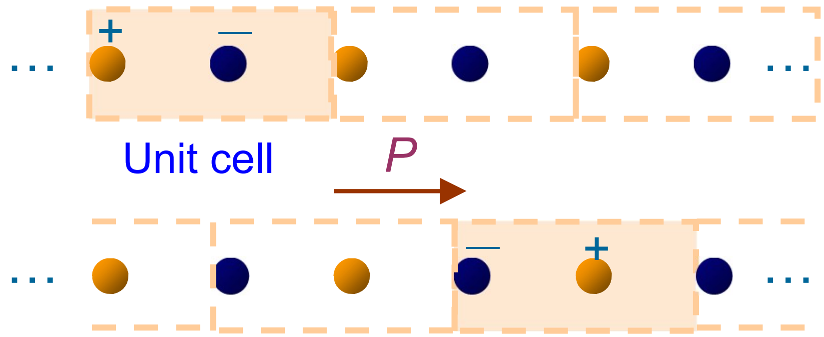
- *P* is **not** well defined for infinite system with non-localized dipoles

One-dimensional crystal

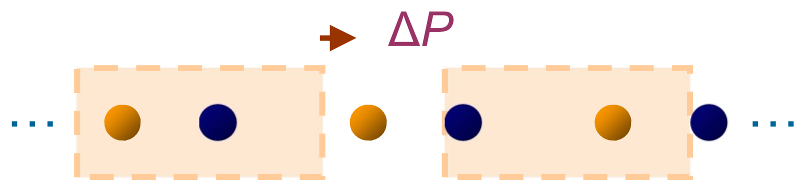


Choice 1

Choice 2



- However, the change of *P* is well-defined



Modern theory of charge polarization (King-Smith and Vanderbilt, PRB 1993)

Consider a one-dimensional crystal (λ=atomic displacement in a unit cell)

- Bloch basis

$$P = \frac{q}{L}\sum_{nk}\left\langle \psi_{nk}^{\lambda}\middle| r \middle|\psi_{nk}^{\lambda}\right\rangle \qquad \psi_{nk}^{\lambda}(r) = e^{ikr}u_{nk}^{\lambda}(r)$$

ill-defined

- Wannier basis (ΔP from the shift of the charge center of Wannier function)

$$P = q \sum_{\text{filled } n} \langle n0|x|n0\rangle, \; q = -e$$

$$\Rightarrow P(\lambda) = qa\sum_{n}\int_{BZ}\frac{dk}{2\pi}\left\langle u_{nk}^{\lambda}\middle| i\frac{\partial}{\partial k}\middle| u_{nk}^{\lambda}\right\rangle$$ Berry connection

$$= qa\sum_{n}\frac{\gamma_n}{2\pi}$$

- Zak phase (PRL, 1989), Berry phase in one-dimension

$$\gamma_n \equiv \int_{BZ} dk\, A_{nk}$$

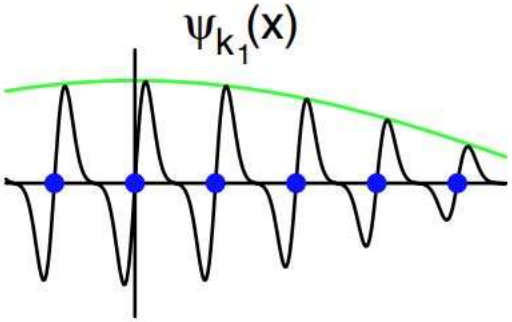
Similar formulation in 3-dim using Kohn-Sham orbitals

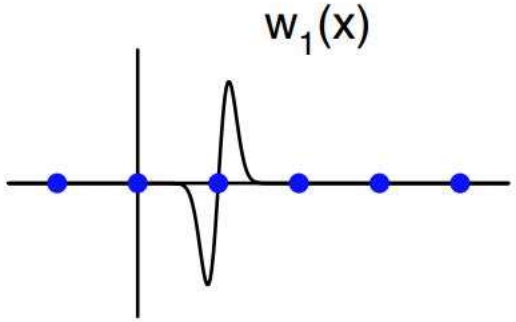
Bloch functions

$$\psi_{nk}(x) = e^{ikx} u_{nk}(x)$$

Wannier functions (localized)

$$|nR_\ell\rangle = \frac{1}{\sqrt{N}} \sum_{k=-\pi/a}^{\pi/a} e^{-ikR_\ell} |\psi_{nk}\rangle$$





Rubel's ppt

- Both sets are complete and orthonormal bases

$$\langle \psi_{n'k'} | \psi_{nk} \rangle = \delta_{nn'} \delta_{kk'} \qquad \langle n'R' | nR \rangle = \delta_{nn'} \delta_{RR'}$$

Note: atomic orbitals are also localized, but they are not orthonormal basis

Polarization from the shift of charge center

$$P = q \sum_{\text{filled } n} \langle n0|x|n0\rangle, \; q = -e$$
$$= \frac{q}{N} \sum_n \sum_{kk'} \langle u_{nk'}|e^{-ik'x} \frac{1}{i}\frac{\partial}{\partial k}\left(e^{ikx}\right)|u_{nk}\rangle$$
$$= \frac{q}{N} \sum_n \sum_{kk'} \langle u_{nk'}|e^{i(k-k')x} i\frac{\partial}{\partial k}|u_{nk}\rangle.$$

$$\Rightarrow P = \frac{q}{N} \sum_n \sum_k \langle u_{nk}|i\frac{\partial}{\partial k}|u_{nk}\rangle$$
$$= qa \sum_n \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} A_n(k).$$

$$\langle u_{nk'}|e^{i(k-k')x} i\frac{\partial}{\partial k}|u_{nk}\rangle = N\delta_{k,k'}\langle u_{nk}|i\frac{\partial}{\partial k}|u_{nk}\rangle_{cell}$$
$$= \delta_{k,k'}\langle u_{nk}|i\frac{\partial}{\partial k}|u_{nk}\rangle,$$

- Gauge transformation

$$|u'_{nk}\rangle = e^{i\chi_{nk}}|u_{nk}\rangle$$

$$\Rightarrow P'_n = P_n - qa\frac{\chi_{n\pi/a} - \chi_{n-\pi/a}}{2\pi} \qquad \chi_{nk+2\pi/a} = \chi_{nk} + 2\pi m a$$

$$\Rightarrow P'_n = P_n - qma$$ same ΔP

Inversion symmetry

With inversion symmetry $A_n(-k) = -A_n(k)$

$$\Rightarrow \quad P_n \to P'_n = qa \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} A_n(-k) = -P_n$$

$$\begin{aligned} P_n &= -P_n \quad \mod qa \\ \to P_n &= 0 \;\text{ or }\; q\frac{a}{2} \quad \mod qa \end{aligned}$$

- For a one-dimensional lattice **with** *inversion* symmetry

(*if* the origin is a symmetric point)

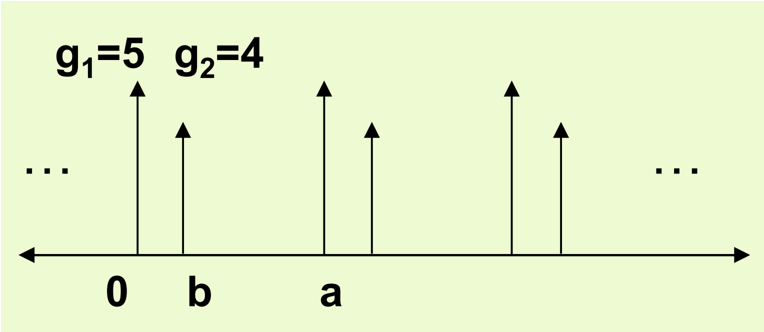
$$\gamma_n = 0 \;\text{ or }\; \pi$$ (Zak, PRL 1989)

- Other values are possible **without** inversion symmetry

Review: Resta, J. Phys.: Condens. Matter 12, R107 (2000)

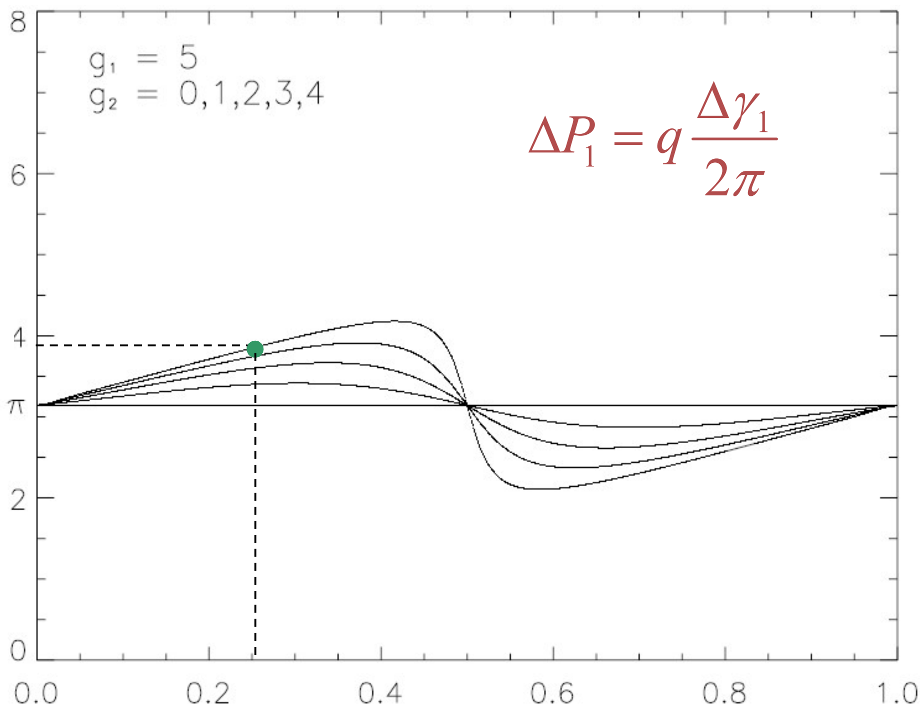
Berry phase and electric polarization

Dirac comb model:



Rave and Kerr, EPJ B 2005

Lowest energy band: γ_1

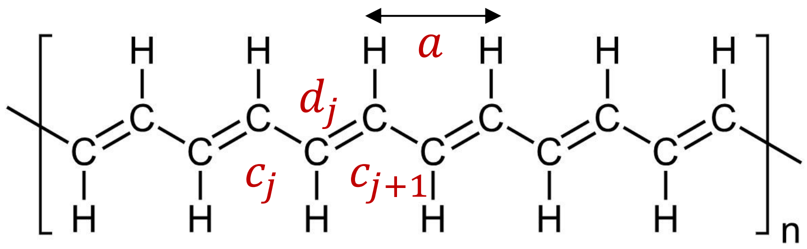


← g_2=0

γ_1=π

r =b/a

Su-Schrieffer-Heeger (SSH) model, a model of polyacetylene (PRL 1979)



- Tight-binding formulation (for spinless electrons)

$$H = \sum_{j=1}^{N} t_- \left(c_j^\dagger d_j + h.c. \right) + \\ + \sum_{j=1}^{N} t_+ \left(c_{j+1}^\dagger d_j + h.c. \right)$$

Fourier transform

$$c_j = \frac{1}{\sqrt{N}} \sum_k e^{ijak} c_k$$

$$d_j = \frac{1}{\sqrt{N}} \sum_k e^{ijak} d_k$$

$$\Rightarrow \quad H = \sum_k (c_k^\dagger, d_k^\dagger) \begin{pmatrix} 0 & t_- + t_+ e^{-iak} \\ t_- + t_+ e^{+iak} & 0 \end{pmatrix} \begin{pmatrix} c_k \\ d_k \end{pmatrix}$$

$$= \sum_k (c_k^\dagger, d_k^\dagger) \mathsf{H}(k) \begin{pmatrix} c_k \\ d_k \end{pmatrix}.$$

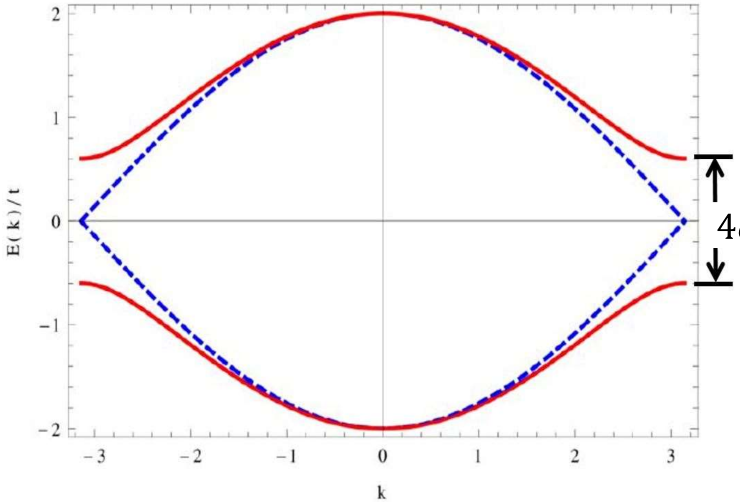
$$\mathrm{H}(k) = \mathbf{h}(k) \cdot \boldsymbol{\sigma}$$

$$\mathbf{h}(k) = (t_- + t_+ \cos ka, t_+ \sin ka,\ 0\,)$$

$$\Rightarrow \quad \varepsilon_\pm = \pm\sqrt{\{(t_- + t_+\cos ka)^2 + (t_+\sin ka)^2\}}$$

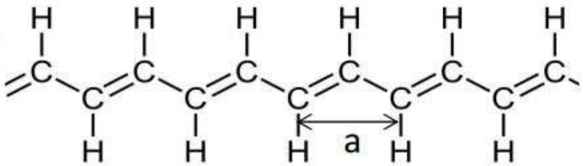
$$(t_\pm = t \pm \delta)$$

It's gapped when $\delta \neq 0$



A phase

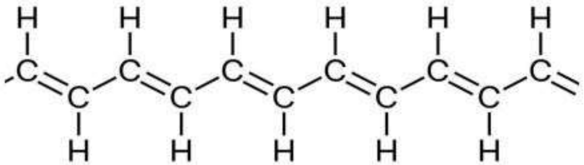
$\delta > 0$



B phase

i=1

$\delta < 0$

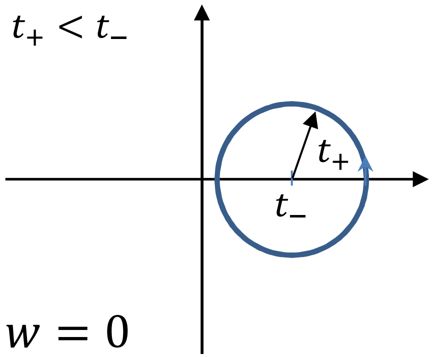


i=1

Winding number of $\boldsymbol{h}(k)$

B phase

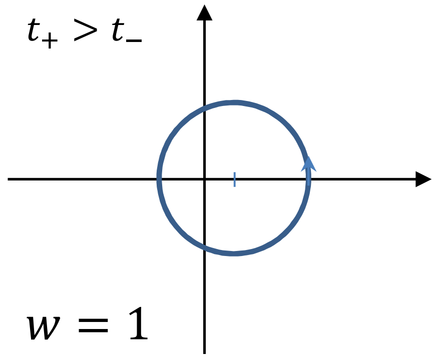
$t_+ < t_-$



$w = 0$

A phase

$t_+ > t_-$



$w = 1$

Note: $$w = \frac{1}{2\pi}\int_{BZ} dk\ \frac{1}{h^2}\hat{\mathbf{z}} \cdot \mathbf{h} \times \frac{d\mathbf{h}}{dk}$$

Zak phase $\gamma = \int_{-\pi}^{\pi} dk\, A(k)$ = solid angle of the ***h***(k) loop w.r.t. the origin

- A phase $t_+ > t_-$ (w=1): $\gamma = \pi$
- B phase $t_+ < t_-$ (w=0): $\gamma = 0$

measurement of Zak phase using optical lattice: Atala et al, Nat Phys 2013

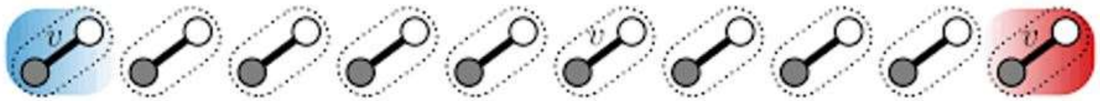
Edge state, bulk-edge correspondence

- A: $t_+ > t_-, w = 1, \gamma = \pi$

Edge state

Edge state

- B: $t_+ < t_-, w = 0, \gamma = 0$

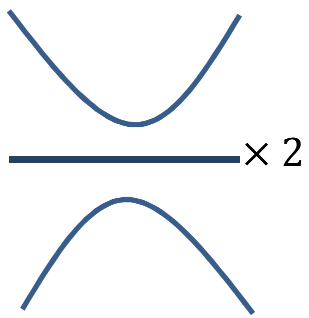


1. Edge states are located at zero energy

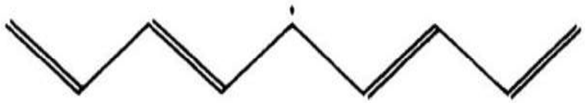
2. There is one electron per dimer (for spinless case)

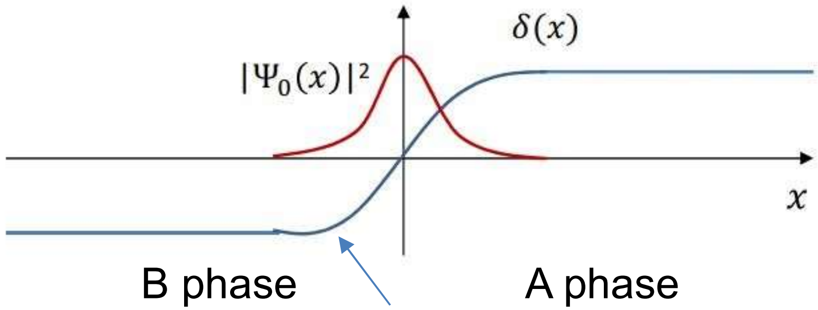
When an electron fills the right end, it has charge $q/2$,

while the left end is $-q/2$ (w.r.t. to the trivial case)



Localized state near a domain wall





Called a kink, or a soliton

- Low-energy continuum theory

Requantization: $k \to \frac{\pi}{a} + q$; $\boxed{q \to -i\partial_x}$

valid when the environment varies slowly (Slater, Phys Rev 1949)

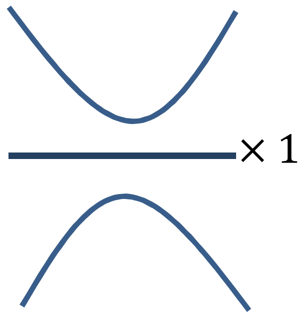
$$\text{H} \simeq \begin{pmatrix} 0 & -\delta + it_+ q\frac{a}{2} \\ -\delta - it_+ q\frac{a}{2} & 0 \end{pmatrix} = -\delta(x)\,\sigma_x - t_+(x) q \frac{a}{2}\,\sigma_y$$

~ Jackiw-Rebbi model (1976)

$$\begin{pmatrix} 0 & -\delta + t_+ \frac{a}{2}\frac{d}{dx} \\ -\delta - t_+ \frac{a}{2}\frac{d}{dx} & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

Zero-energy solution (domain-wall state)

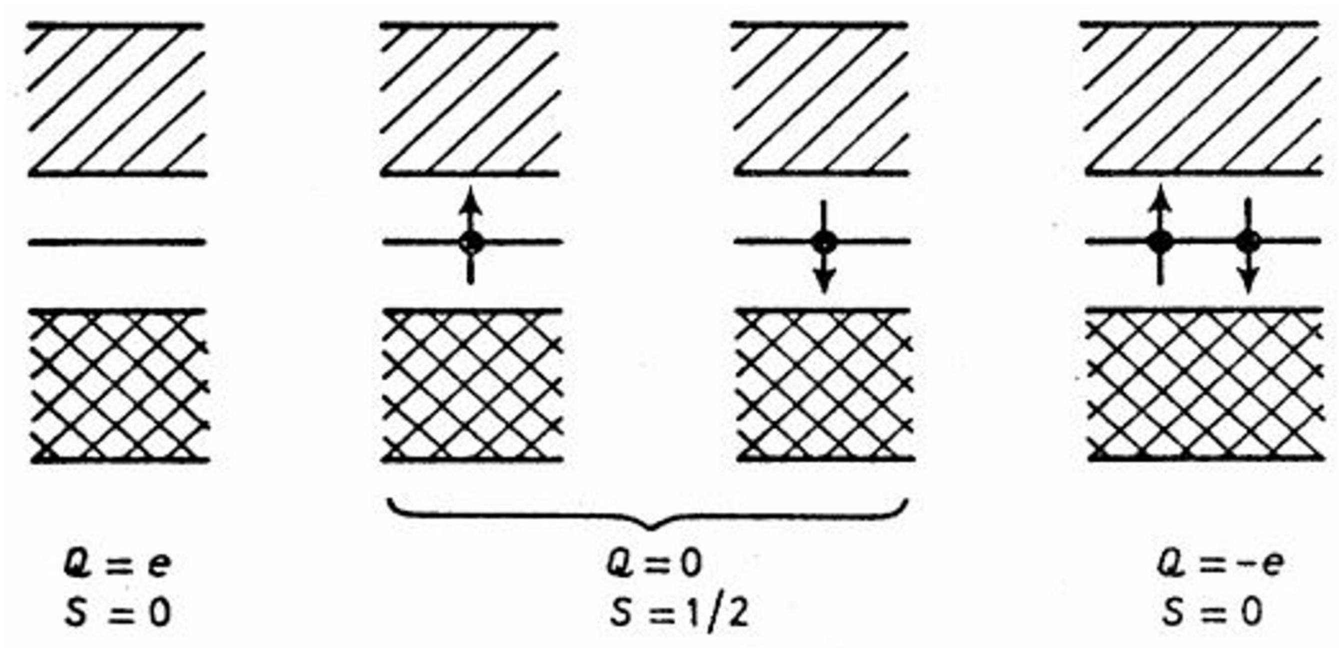
$$\Psi_0(x) = e^{-\int_0^x dx' \frac{2}{t_+(x')a}\delta(x')} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$



If filled (empty), its charge is –e/2 (e/2)

But electrons have spins

Electron with spin



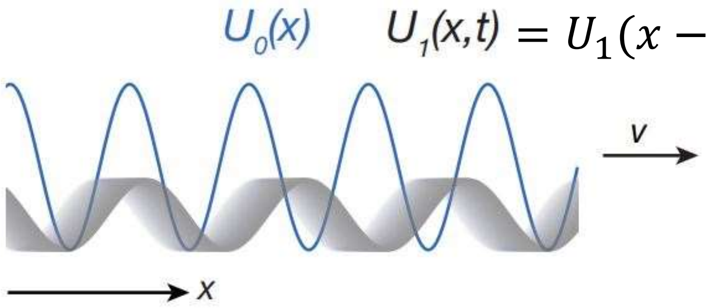
Exp’t
Ikehata et al,PRL 1980

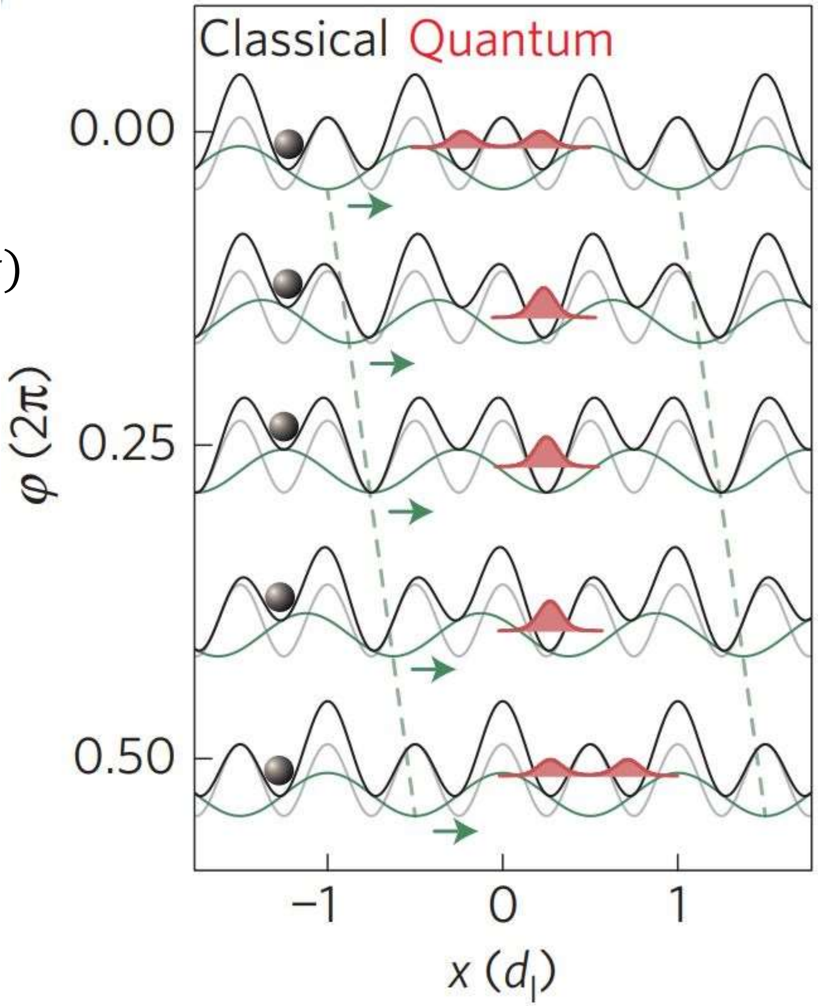
Goldberg et al, J Chem Phys 1979

Quantized charge pump (Thouless, 1983)

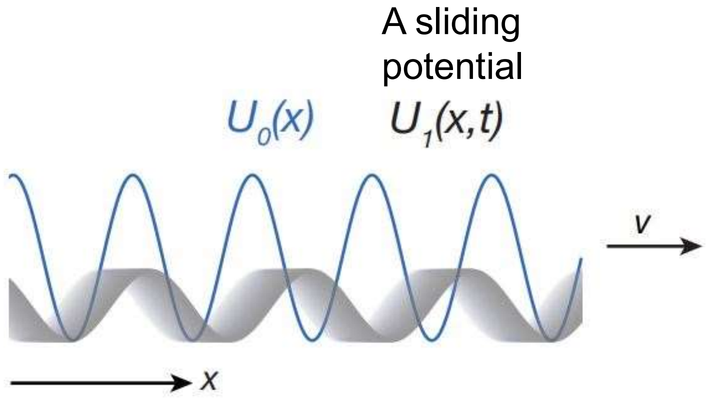
A sliding potential

$U_1(x,t) = U_1(x - vt)$



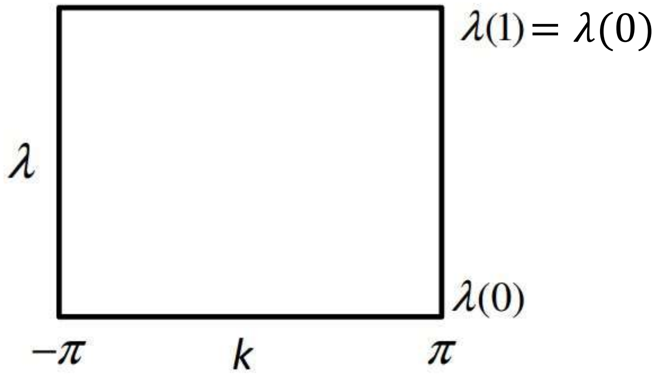


Quantized charge pump (coherence, filled band)



$$P(\lambda_2) - P(\lambda_1) = qa \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} \left[A(k,\lambda_2) - A(k,\lambda_1)\right]$$

Demand $\langle u_{nk}|\frac{\partial}{\partial\lambda}|u_{nk}\rangle = 0$



➡ $$\Delta P = -\frac{qa}{2\pi}\oint d\mathbf{k}\cdot\mathbf{A}(\mathbf{k}), \quad \mathbf{k} \equiv (k,\lambda)$$
$$= -\frac{qa}{2\pi}\int d^2k F_z(\mathbf{k}),$$

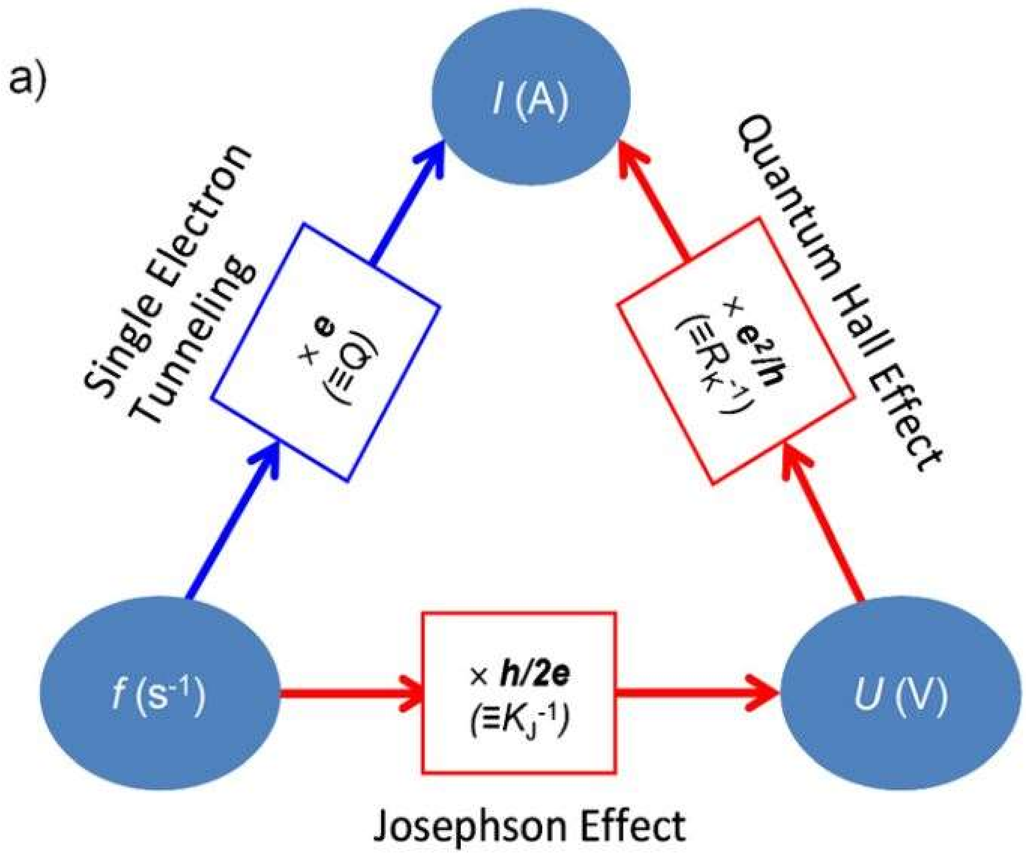
where $F_z(\mathbf{k}) = \partial_k A_\lambda - \partial_\lambda A_k$, and $A_\lambda = i\langle u_{\mathbf{k}}|\partial_\lambda|u_{\mathbf{k}}\rangle$.

(1D space +1D time ~ 2D quantum Hall)

➡ $\Delta P = qaC_1$

Citro and Aidelsburger, Nat Rev Phys 2023

Quantum metrology triangle



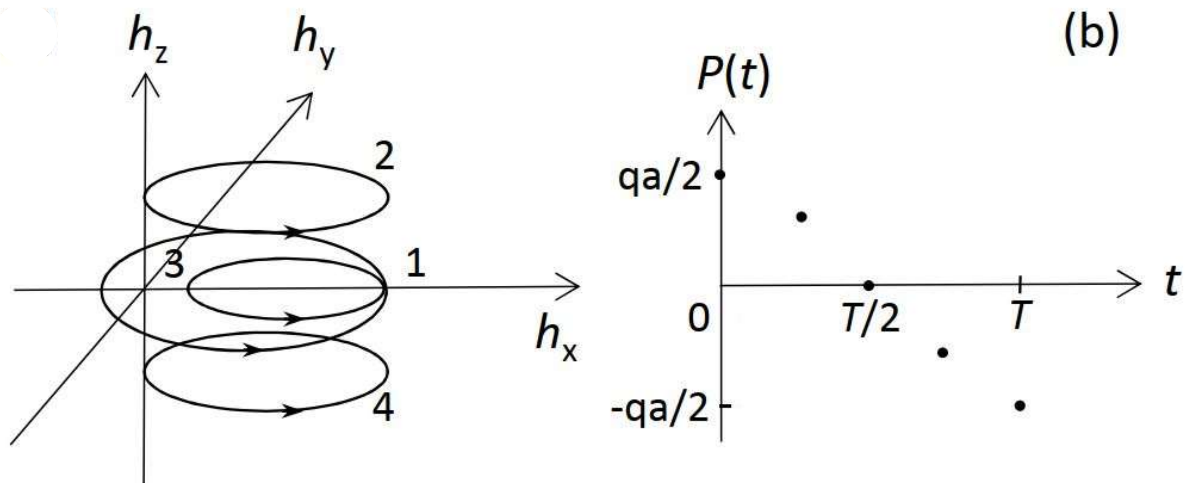
Rice-Mele model, a generalization of the SSH model

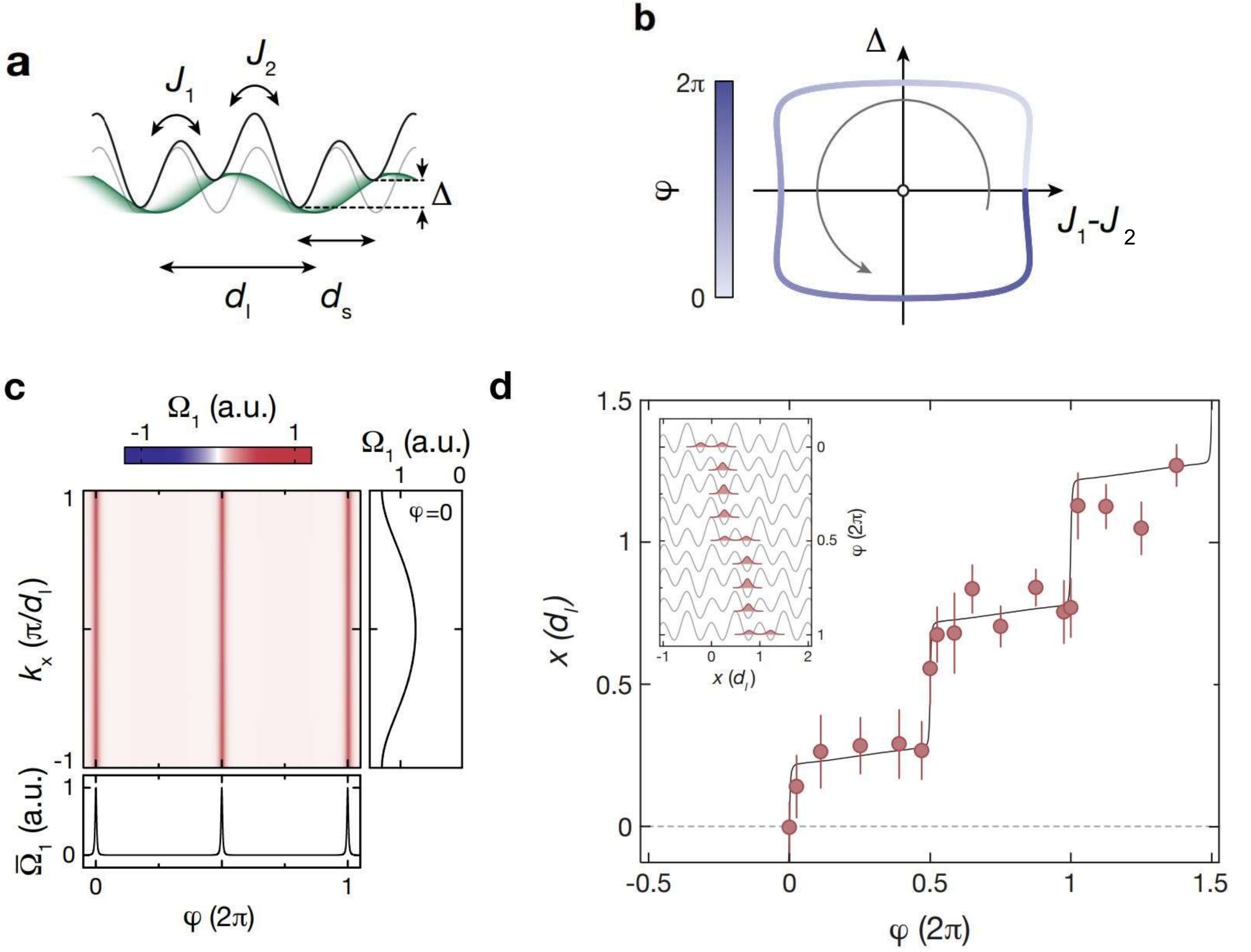
$$H = H_{SSH} + \sum_{j=1}^{N} \Delta c_j^\dagger c_j - \sum_{j=1}^{N} \Delta d_j^\dagger d_j$$

$$H = \sum_k (c_k^\dagger, d_k^\dagger) \begin{pmatrix} \Delta & t_- + t_+ e^{-iak} \\ t_- + t_+ e^{+iak} & -\Delta \end{pmatrix} \begin{pmatrix} c_k \\ d_k \end{pmatrix}$$

$$= \mathbf{h}(k) \cdot \boldsymbol{\sigma} \qquad \mathbf{h}(k) = (t_- + t_+ \cos ka, t_+ \sin ka, \Delta)$$

$$(\delta(t), \Delta(t)) = \left(\delta_0 \cos 2\pi \frac{t}{T}, \Delta_0 \sin 2\pi \frac{t}{T} \right)$$





Citro and Aidelsburger, Nat Rev Phys 2023

Term report

1. A reading report with 4 to 6 pages
2. At least 5 references
3. Level: 1st year graduate student
4. Some topic related to what we have learned this semester
5. You can turn it in anytime, starting from today till the last day of the class