HUNGARIAN ACADEMY OF SCIENCES
WIGNER RESEARCH CENTRE FOR PHYSICS

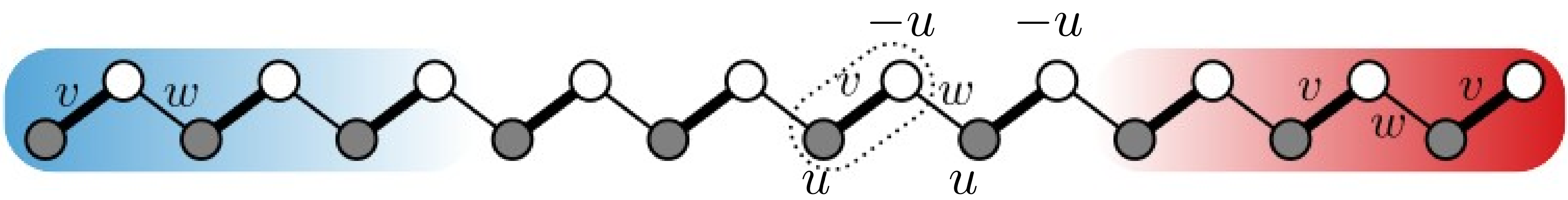
MŰEGYETEM 1782

Topological insulators

3. Thouless (Adiabatic) charge pump
+ Polarization, Wannier states, Rice-Mele model

Budapest, 2019 October 1

Rice-Mele model: SSH model+sublattice potential. Breaks chiral & inversion symmetry → ...charge pumping

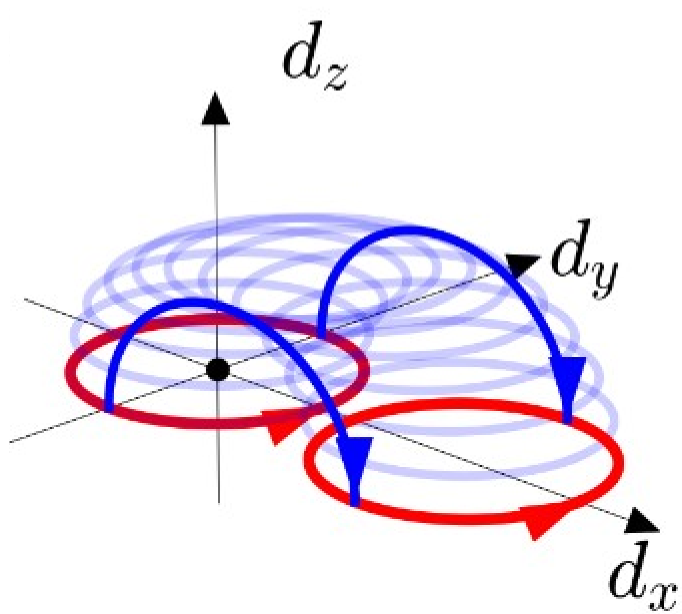


$$\hat{H} = v \sum_{m=1}^{N} |m, A\rangle\langle m, B| + h.c. + w \sum_{m=1}^{N-1} |m+1, B\rangle\langle m, A| + h.c.$$

$$+u \sum_{m=1}^{N} |m, A\rangle\langle m, A| - |m, B\rangle\langle m, B|$$

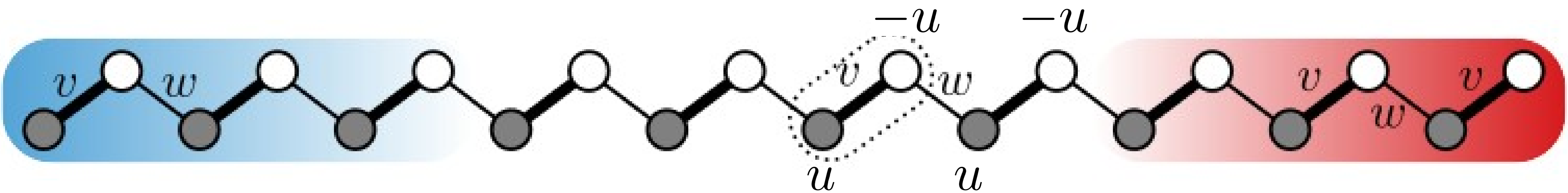
$$H(k) = \begin{pmatrix} u & v + we^{-ik} \\ v + we^{ik} & -u \end{pmatrix}$$

$$= u\sigma_z + (v + w\cos k)\sigma_x + w \sin k \sigma_y$$



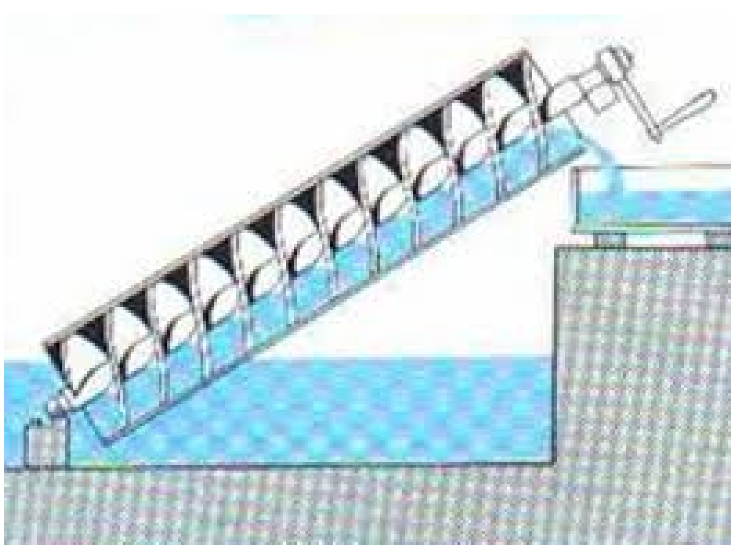
Used in Chapter 1 to break chiral symmetry

Run a charge pump by making Rice-Mele parameters time-dependent (periodically)



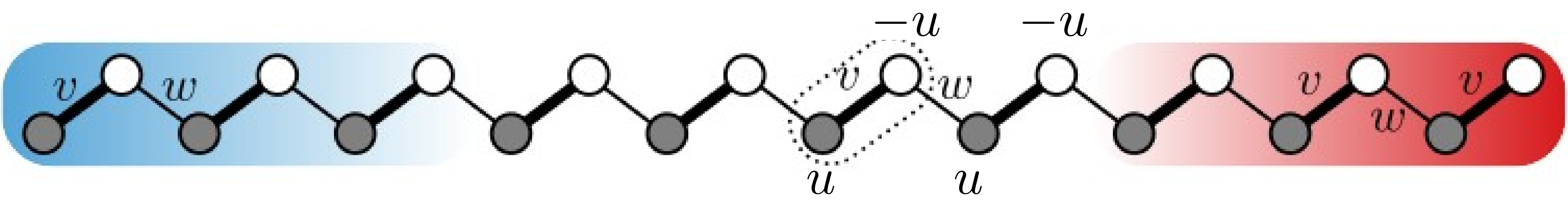
$$\hat{H} = v\sum_{m=1}^{N} |m,A\rangle\langle m,B| + h.c. + w\sum_{m=1}^{N-1} |m+1,B\rangle\langle m,A| + h.c. + u\sum_{m=1}^{N} |m,A\rangle\langle m,A| - |m,B\rangle\langle m,B|$$

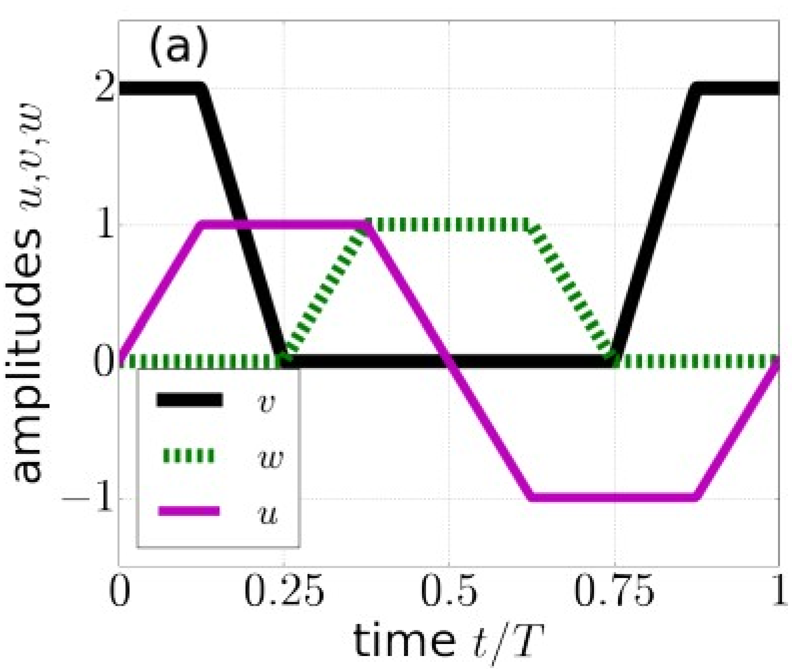
Make hoppings v(t), w(t), onsite energies u(t) periodically time-dependent



1. Charge pumping in control freak
2. Notice topological pumping at edge
3. More general than control freak
4. Apply to general case

1. Charge pumping as a “control freak” means we always we know which dimer an electron is on





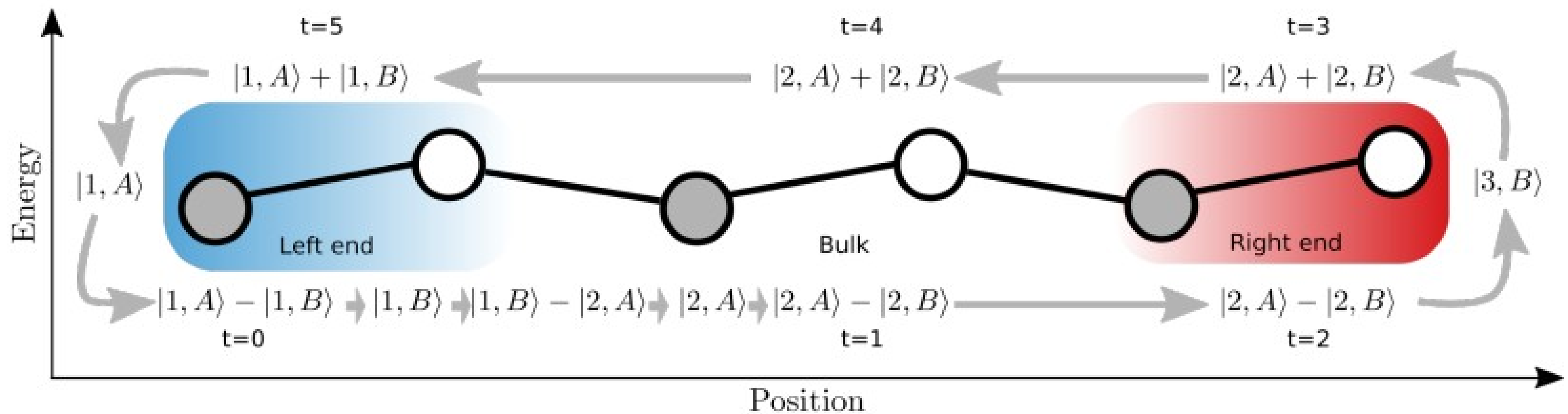
Control freak:

no hopping between dimers:
v(t)=0 or w(t)=0, always.

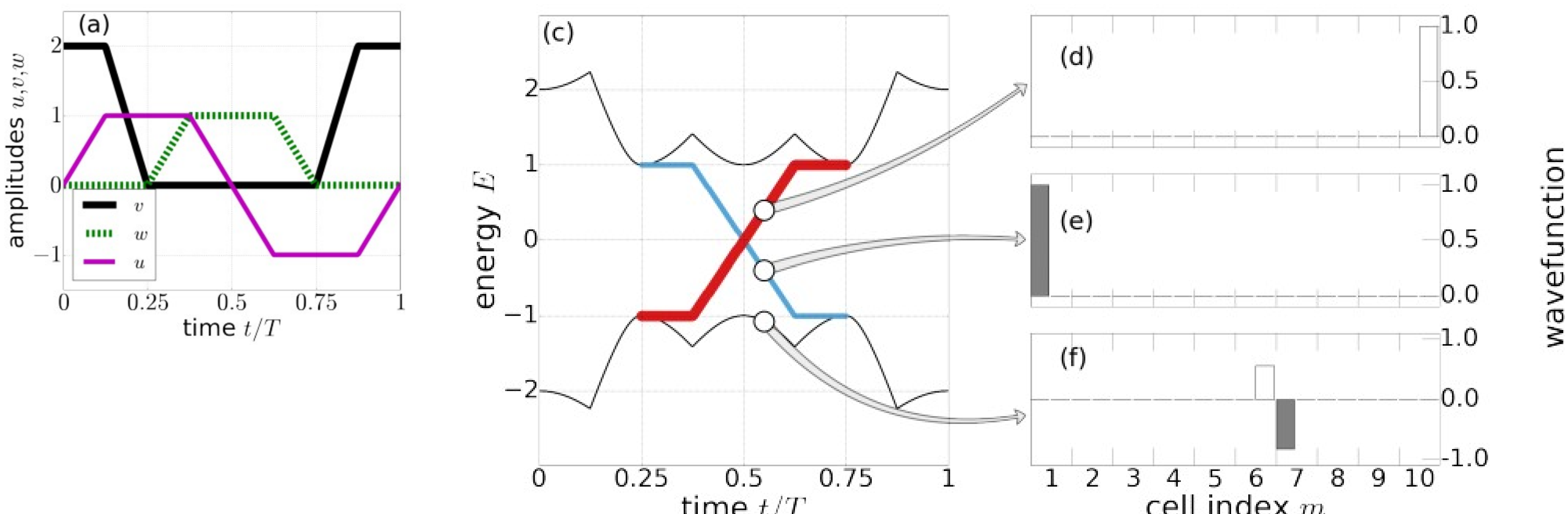
→ Know where electron is

→ “Bucket brigade” for electrons

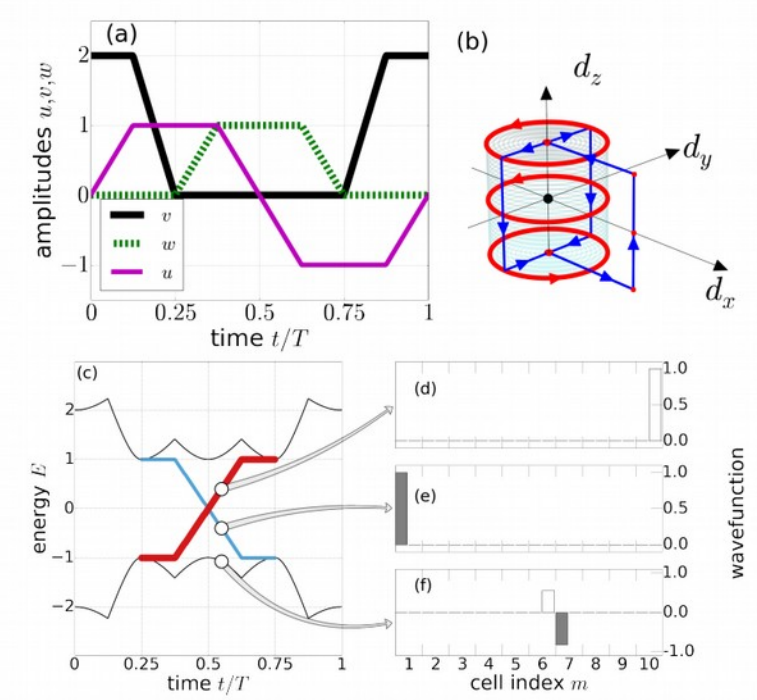
2. Shifting position in bulk → must shift energy at edge → topological dispersion relation branches at edge

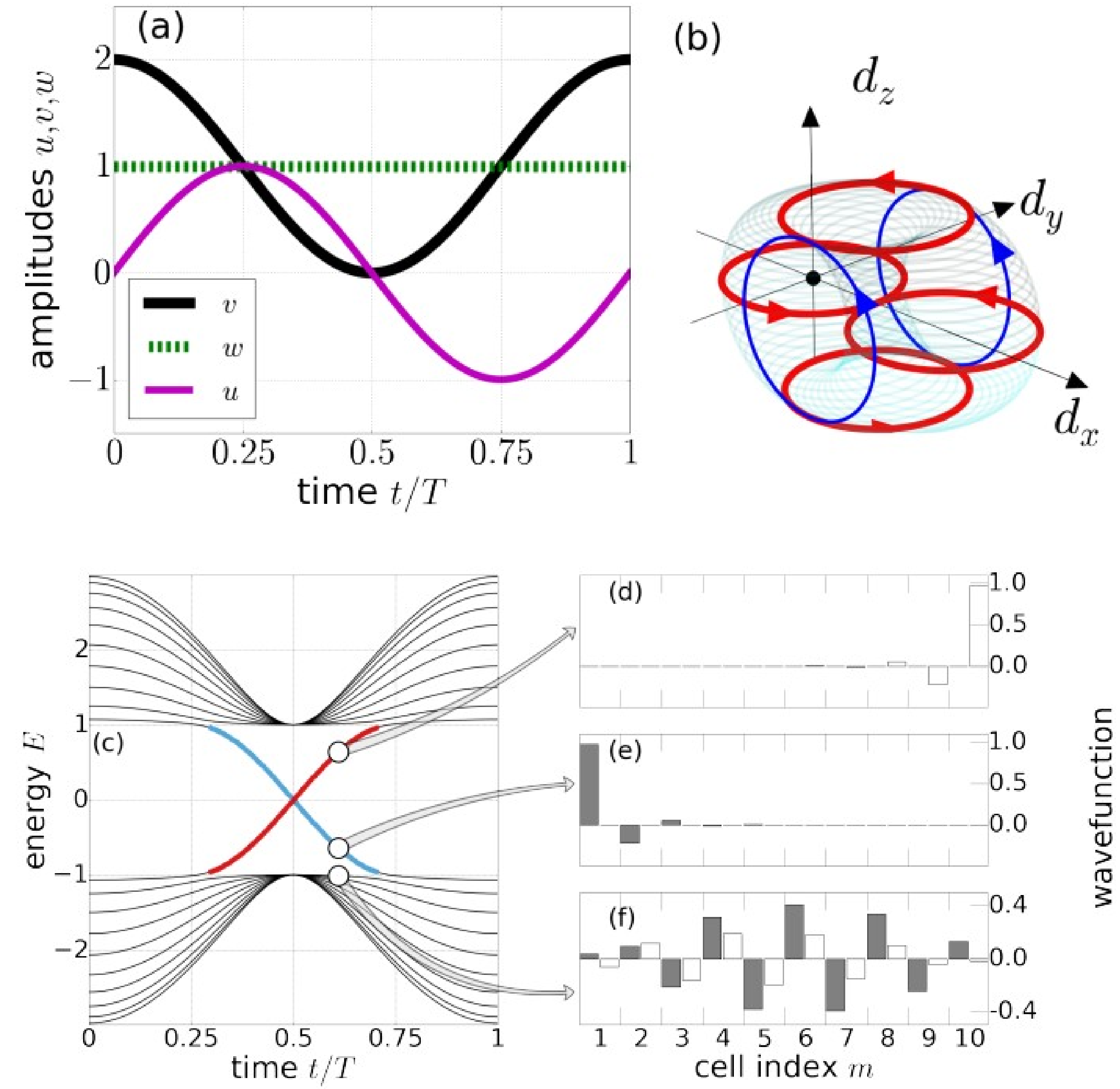


$$\hat{H} = v\sum_{m=1}^{N} |m,A\rangle\langle m,B| + h.c. + w\sum_{m=1}^{N-1} |m+1,B\rangle\langle m,A| + h.c. \; + u\sum_{m=1}^{N} |m,A\rangle\langle m,A| - |m,B\rangle\langle m,B|$$



3. If this pump effect is topological, it must persist even if we don’t keep track of electrons (not control freak)



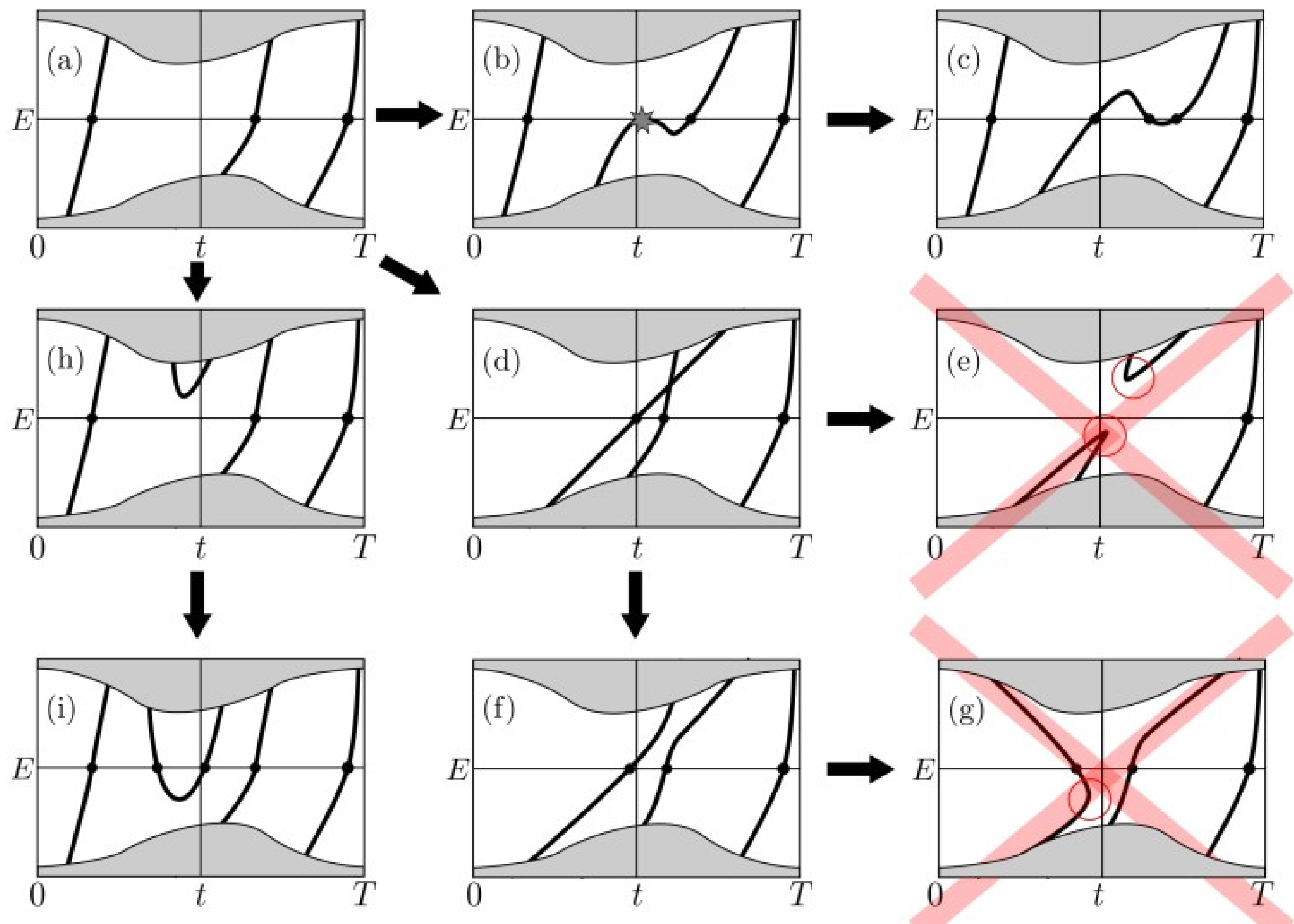


4. State transfer between bulk bands takes place at edge. Net no. of states transferred = Q topological invariant

$$N_+ = \text{number of times } E = \varepsilon \text{ is crossed from } E < \varepsilon \text{ to } E > \varepsilon; \tag{4.10}$$

$$N_- = \text{number of times } E = \varepsilon \text{ is crossed from } E > \varepsilon \text{ to } E < \varepsilon; \tag{4.11}$$

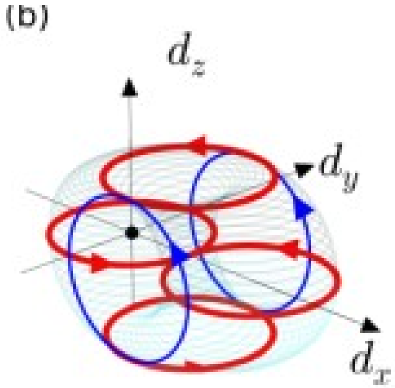
$$Q = N_+ - N_- = \text{net number of edge states pumped up in energy}\ . \tag{4.12}$$



Bulk topological invariant in charge pumping is Chern number

- Proof 1: track "electron positions" using Wannier states (today)

$$\Delta x_{0,t} = \frac{1}{2\pi} \oint_{-\pi}^{\pi} B^{(n)} dk dt.$$



- Proof 2: integrate adiabatic current over timestep (next week)

$$\mathscr{Q} = -i \frac{1}{2\pi} \int_0^T dt \int_{-\pi}^{\pi} dk \left(\partial_k \langle u_1(k,t) | \partial_t u_1(k,t) \rangle - \partial_t \langle u_1(k,t) | \partial_k u_1(k,t) \rangle \right). \quad (5.4)$$

Polarization, Berry phase, Wannier states, charge pumping

needed to prove charge pumping

great tool for visualizing bulk processes

Main result:

Wannier center = Berry phase, gauge independent mod 2pi

$$\langle w(j)|\hat{x}|w(j)\rangle = \frac{i}{2\pi}\int_{-\pi}^{\pi} dk\,\langle u(k)\,|\,\partial_k u(k)\rangle + j$$

Interpret as Bulk Electric Polarization

$$P_{\text{electric}} = \frac{i}{2\pi}\int_{-\pi}^{\pi} dk\langle u(k)|\partial_k|u(k)\rangle$$

+ Inversion symmetry quantizes polarization
+ Chiral symmetry quantizes polarization

Don't confuse plane wave eigenstates $|\Psi_n(k)\rangle$ with internal space states $|u_n(k)\rangle$

Eigenstates of bulk Hamiltonian: plane waves delocalized over whole lattice

$$|\Psi_n(k)\rangle = |k\rangle \otimes |u_n(k)\rangle \qquad \langle \Psi_n(k')|\Psi_n(k)\rangle = \delta_{k',k}$$

Fourier transform,
unit cell single coordinate $\quad |k\rangle = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{imk} |m\rangle$

amplitude of plane wave: $\big|u_n(k)\big\rangle \qquad \langle u_n(k')|u_n(k)\rangle \neq \delta_{k',k}$

Example, Rice-Mele:

$$\hat{H}(k) = u\hat{\sigma}_z + (v + w\cos k)\hat{\sigma}_x + w\sin k\hat{\sigma}_y$$

$$\hat{H}(k)|u_n(k)\rangle = E_n(k)|u_n(k)\rangle$$

Wannier states are a set of tightly localized basis states that span the occupied band

$$\hat{P} = \sum_k |\Psi(k)\rangle\langle\Psi(k)|$$

projector to occupied subspace

$$\langle w(j') \,|\, w(j)\rangle = \delta_{j'j} \qquad \text{Orthonormal set} \qquad (3.8a)$$

$$\sum_{j=1}^{N} |w(j)\rangle\langle w(j)| = \hat{P} \qquad \text{Span the occupied subspace} \qquad (3.8b)$$

$$\langle m+1 \,|\, w(j+1)\rangle = \langle m \,|\, w(j)\rangle \qquad \text{Related by translation} \qquad (3.8c)$$

$$\lim_{N\to\infty} \langle w(N/2)|\,(\hat{x}-N/2)^2\,|w(N/2)\rangle < \infty \qquad \text{Localization} \qquad (3.8d)$$

$$|w(j)\rangle = \frac{1}{\sqrt{N}} \sum_{k=\delta_k}^{N\delta_k} e^{-ijk} e^{i\alpha(k)} |\Psi(k)\rangle$$

Wannier states are obtained by Fourier transform, with arbitrary gauge function α(k)

$$|w(j)\rangle = \frac{1}{\sqrt{N}} \sum_{k=\delta_k}^{N\delta_k} e^{-ijk} e^{i\alpha(k)} |\Psi(k)\rangle$$

gauge function α(k) can be used to make
Wannier function tightly localized
(1D: can be exponentially localized)

Wannier center $\langle w(j)|\,\hat{x}\,|w(j)\rangle$ ≈position of charge = Berry phase of $|u(k)\rangle$

$$\langle w(j)|\,\hat{x}\,|w(j)\rangle = \frac{i}{2\pi}\int_{-\pi}^{\pi} dk\,\langle u(k)|\,\partial_k u(k)\rangle + j$$

obtained by partial integration
j∈ℤ gauge dependent (bulk polarization defined mod 1)
Agrees with intuitive result

$$P_{\text{electric}} = \frac{i}{2\pi}\int_{-\pi}^{\pi} dk\langle u(k)|\partial_k|u(k)\rangle$$

Useful numerical tool to calculate Wannier centers is Resta's unitary position operator $\hat{X} = e^{i\delta_k \hat{x}}$.

Definition: $$\hat{X} = e^{i\delta_k \hat{x}}.$$

Respects periodic boundary condition
Unitary operator that shifts momentum

Connection to position:

$$\langle x \rangle = \frac{N}{2\pi} \log \langle \Psi | \hat{X} | \Psi \rangle$$

(see discussion in quantum optics on "phase operator")

Eigenvalues of the projected unitary position operator give the Wannier centers

$$\hat{X} = e^{i\delta_k \hat{x}}. \qquad \hat{P} = \sum_k |\Psi(k)\rangle\langle\Psi(k)|$$

$$\hat{X}_P = \hat{P}\hat{X}\hat{P}$$

projection kills unitarity, → eigenstates not orthogonal, except N→ ∞

$$\hat{X}_P^N = \underbrace{\langle u(2\pi)|u(2\pi-\delta_k)\rangle \cdot \ldots \cdot \langle u(2\delta_k)|u(\delta_k)\rangle\langle u(\delta_k)|u(2\pi)\rangle}_{W=|W|e^{i\phi}} \hat{P}$$

W Wilson loop, Φ is Berry phase

eigenvalues λ of X_p give Wannier centers

$$\lambda_n = e^{in\delta_k + \log(W)/N} = |W|^{1/N} e^{i(\phi+n\delta_k)/N}$$

Chiral symmetry quantizes bulk polarization

$$\hat{H}(k)|u(k)\rangle = -E(k)|u(k)\rangle$$

$$\hat{H}(k)|v(k)\rangle = E(k)|v(k)\rangle$$

$$|v(k)\rangle = e^{i\phi_k}\hat{\Gamma}|u(k)\rangle$$

Berry phase of lower band = Berry phase of upper band:

Chiral symmetry quantizes bulk polarization

$$\hat{H}(k)|u(k)\rangle = -E(k)|u(k)\rangle \qquad \hat{H}(k)|v(k)\rangle = E(k)|v(k)\rangle$$

$$|v(k)\rangle = e^{i\phi_k}\hat{\Gamma}|u(k)\rangle$$

Berry phase of lower band = Berry phase of upper band:

$$\begin{aligned}
|W|\, e^{i\phi_-} &= \langle u(2)|u(1)\rangle\langle u(1)|u(0)\rangle\langle u(0)|u(-1)\rangle\langle u(-1)|u(2)\rangle \\
&= \langle u(2)|\hat{\Gamma}\hat{\Gamma}|u(1)\rangle\langle u(1)|\hat{\Gamma}\hat{\Gamma}|u(0)\rangle \ldots \langle u(-1)|\hat{\Gamma}\hat{\Gamma}|u(2)\rangle \\
&= \langle v(2)|v(1)\rangle\langle v(1)|v(0)\rangle\langle v(0)|v(-1)\rangle\langle v(-1)|v(2)\rangle = |W|\, e^{i\phi_+}
\end{aligned}$$

Elementary properties of Berry phase: $e^{i\phi_+}e^{i\phi_-} = 1$

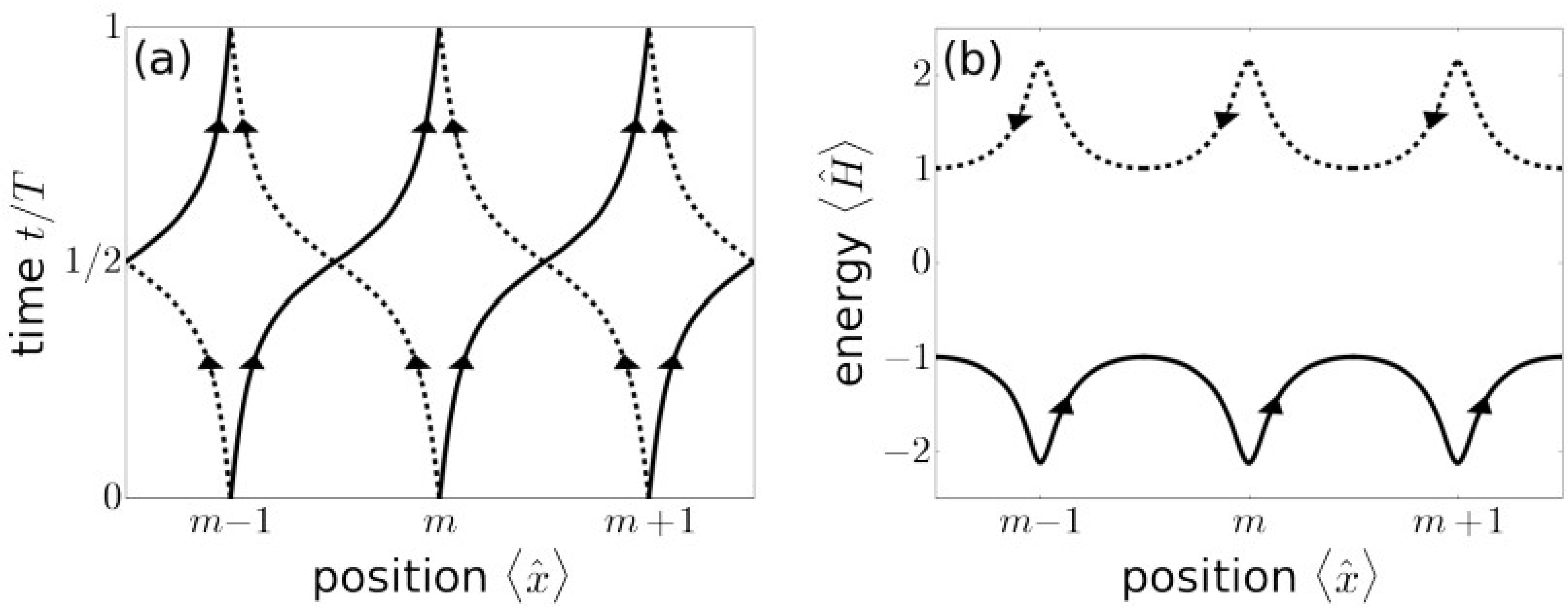
Two options: bulk polarization 0 or ½

Bulk topological invariant in charge pumping using Wannier states

Fully occupied band
 = Slater determinant of plane waves
 = Slater det'nt of localized, equidistant Wannier states

Wannier states gauge dependent,
Wannier state center = Berry phase, only up to n2pi

$$\langle w(j)|\hat{x}|w(j)\rangle = \frac{i}{2\pi}\int_{-\pi}^{\pi} dk\, \langle u(k)\,|\,\partial_k u(k)\rangle + j.$$



Using locally smooth gauge, calculate Wannier charge pumping via Stokes theorem → Chern number

Peer instruction questions

Wannier states

The Wannier state from the n_{th} band centered around site j is denoted by $|w_{(n)}(j)\rangle$.

Consider the Wannier states from different bands, $n' \neq n$, and for different positions, $j' \neq j$, i.e., $|w_{(n')}(j)\rangle$, $|w_{(n)}(j')\rangle$.

Which of the overlaps is guaranteed to be zero by construction, the one between different bands, or the one between different positions?

$$\left|\langle w^{(n')}(j)|w^{(n)}(j)\rangle\right| = 0? \qquad \left|\langle w^{(n)}(j')|w^{(n)}(j)\rangle\right| = 0?$$

a) Only the first

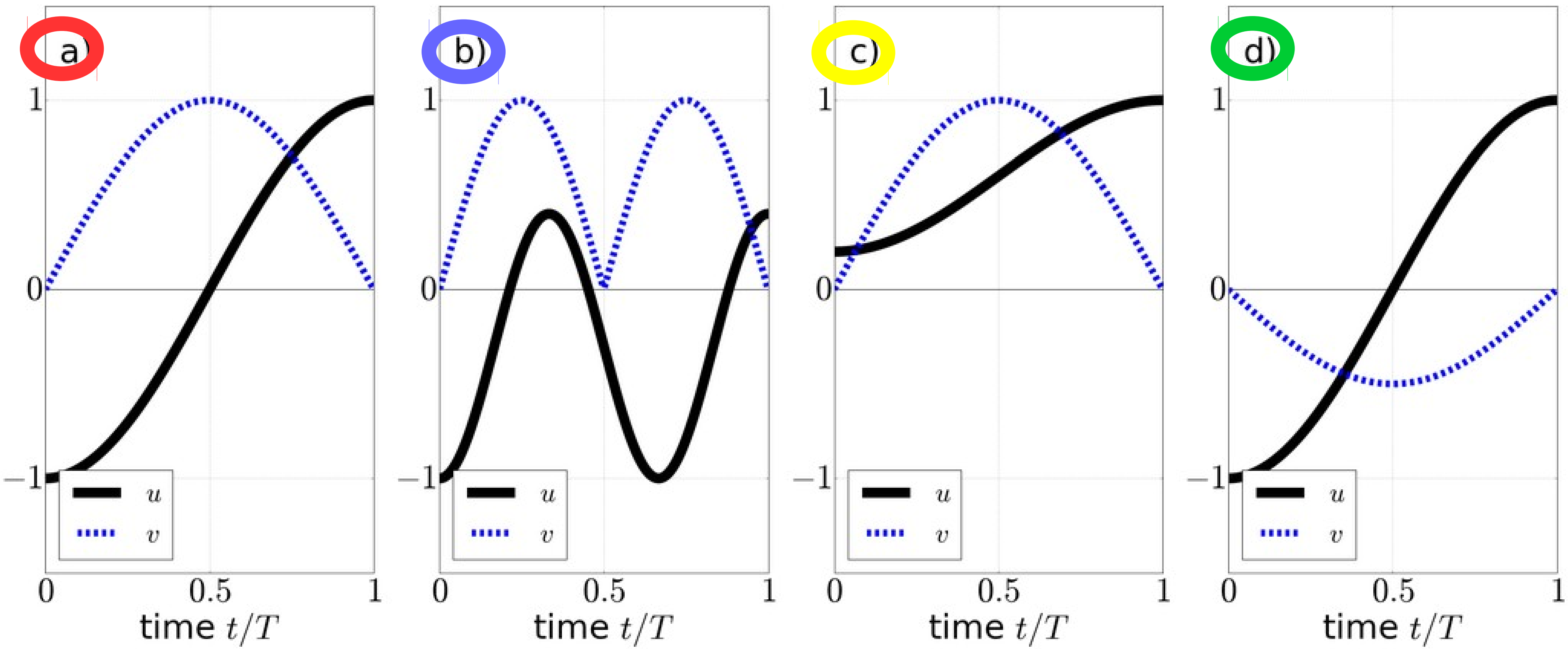
b) Only the second

c) Neither the one nor the second

d) Both

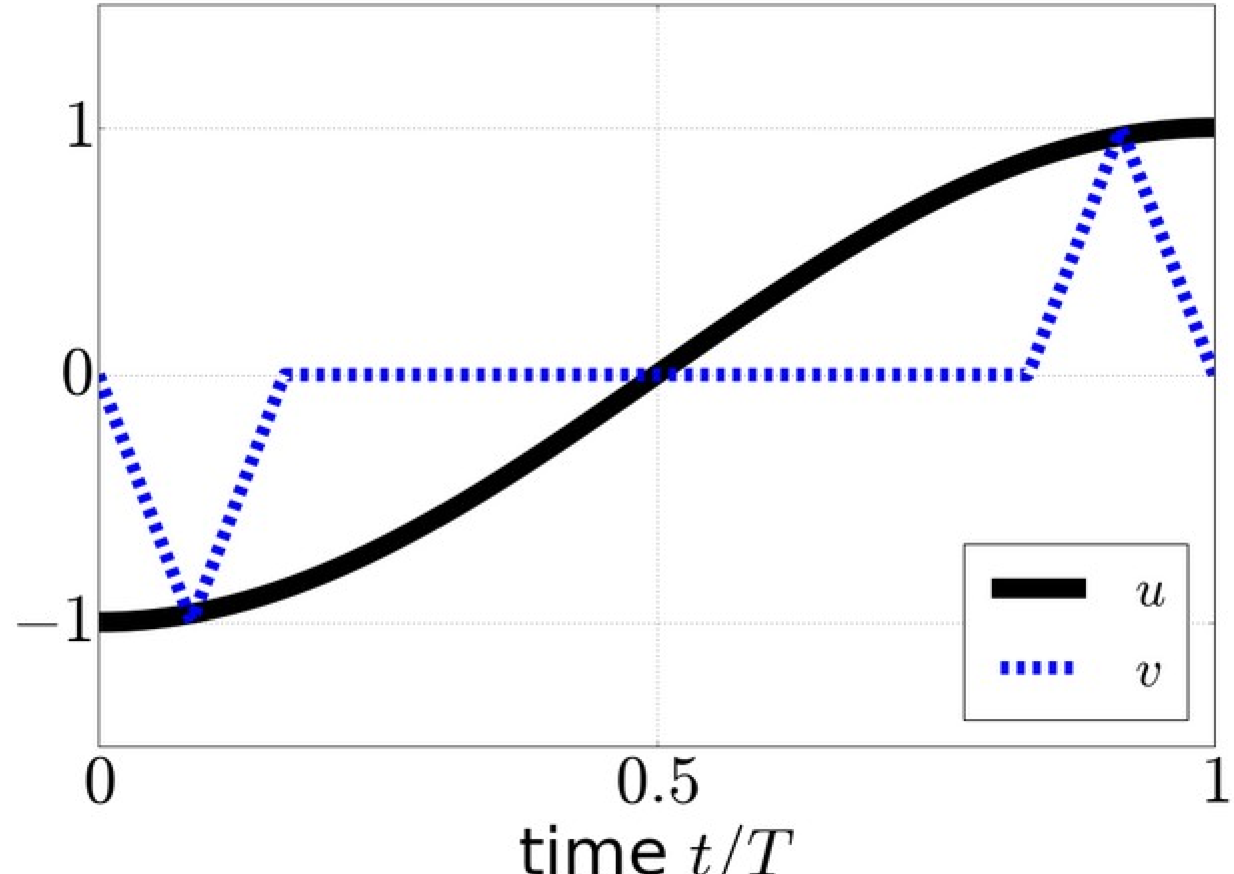
Pumping on a single dimer I.

Consider the very slow pump protocol, where $H = v(t)\sigma_x + u(t)\sigma_z$. The initial state is the ground state at $t = 0$, that is, $\psi_i = (1, 0)$. Which protocol does not shift the charge?



Pumping on a single dimer II.

Consider the very slow pump protocol, where $H = v(t)\sigma_x + u(t)\sigma_z$ The initial state is the ground state at $t = 0$, that is, $\psi_i = (1, 0)$. What is the final state and why?



a $(1, 0)$

b $\frac{(1,1)}{\sqrt{2}}$

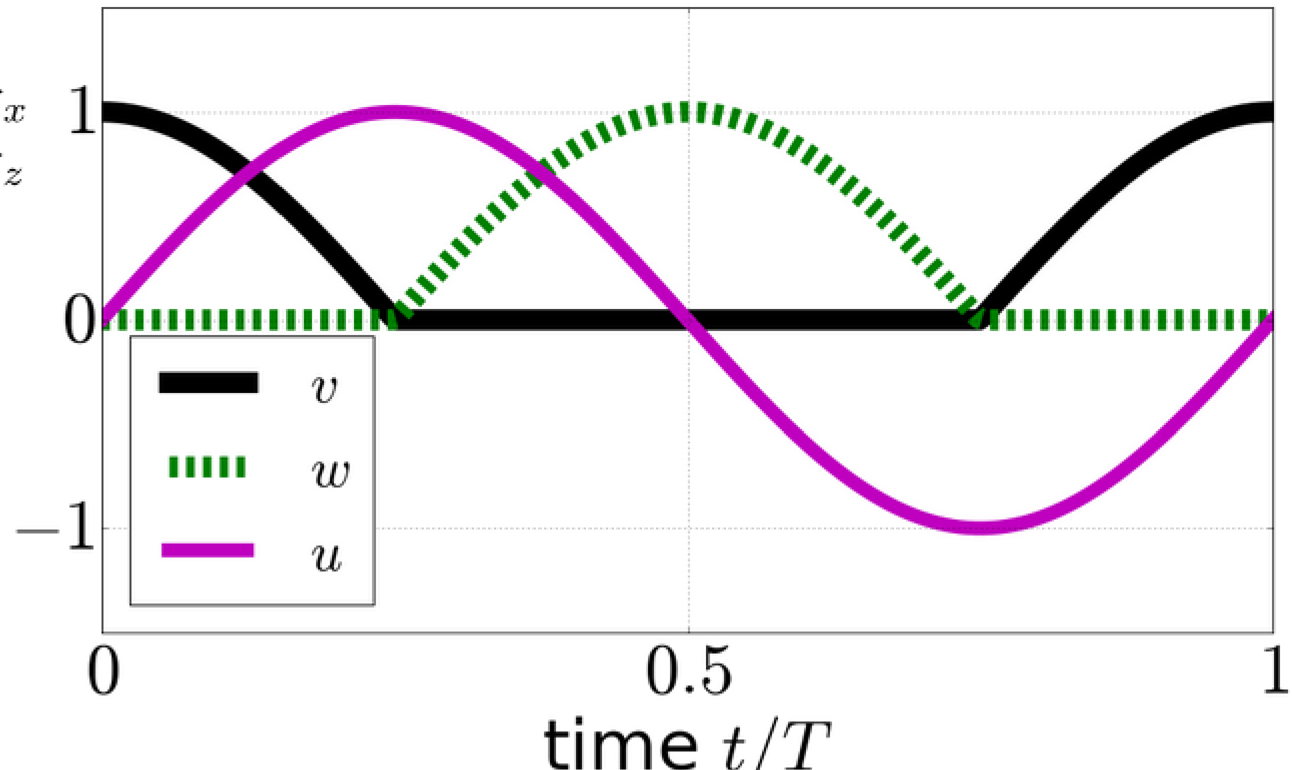
c $(0, 1)$

d the question does not make sense, the energy splitting is zero at t=T/2!

Control-freak pumping II.

Consider adiabatic pumping in the Rice-Mele model with the depicted time dependence of the parameters. Is this a control-freak pump?

$$\mathbf{d}(k,t)\hat{\sigma} = [v(t) + w(t)\cos(k)]\sigma_x + w(t)\sin(k)\sigma_y + u(t)\sigma_z$$



a) it is not a control-freak cycle as the graph is not assembled from straight lines

b) it is not even adiabatic as the gap closes during the cycle

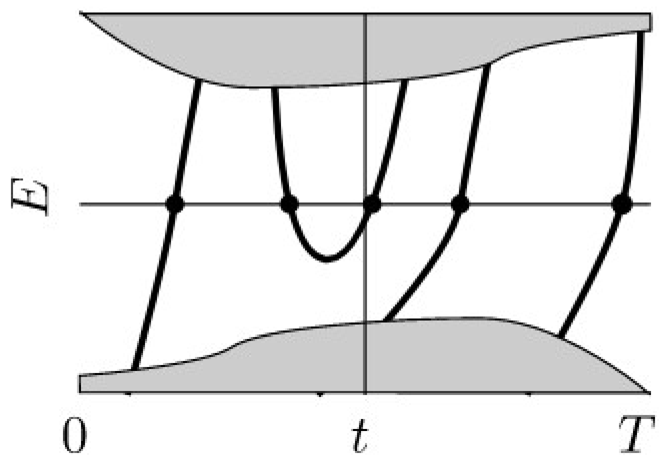
c) it is a control-freak cycle because the corresponding $\mathbf{d}(k,t)$ surface is a torus

d) it is a control-freak cycle because the energy eigenstates can be chosen to be localized to dimers

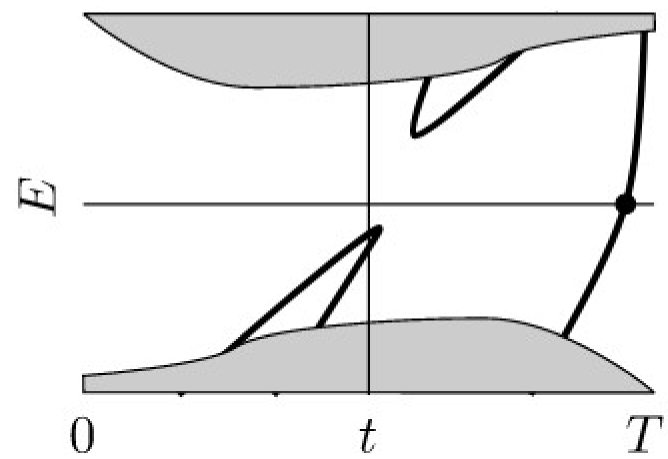
Edge states

Which of the figures below could represent the edge states at a certain edge in a pumping process?

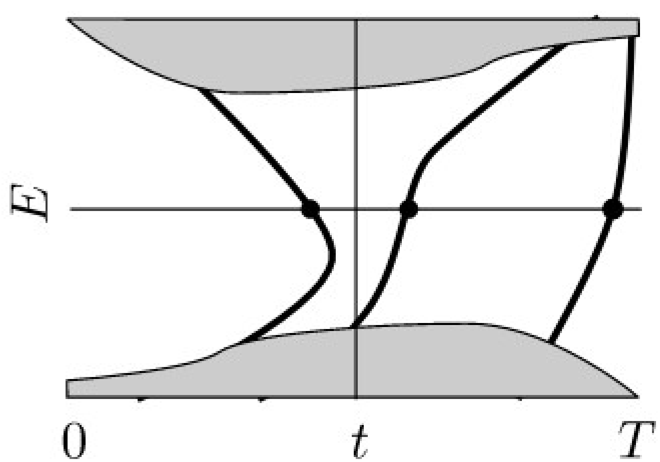
a)



b)



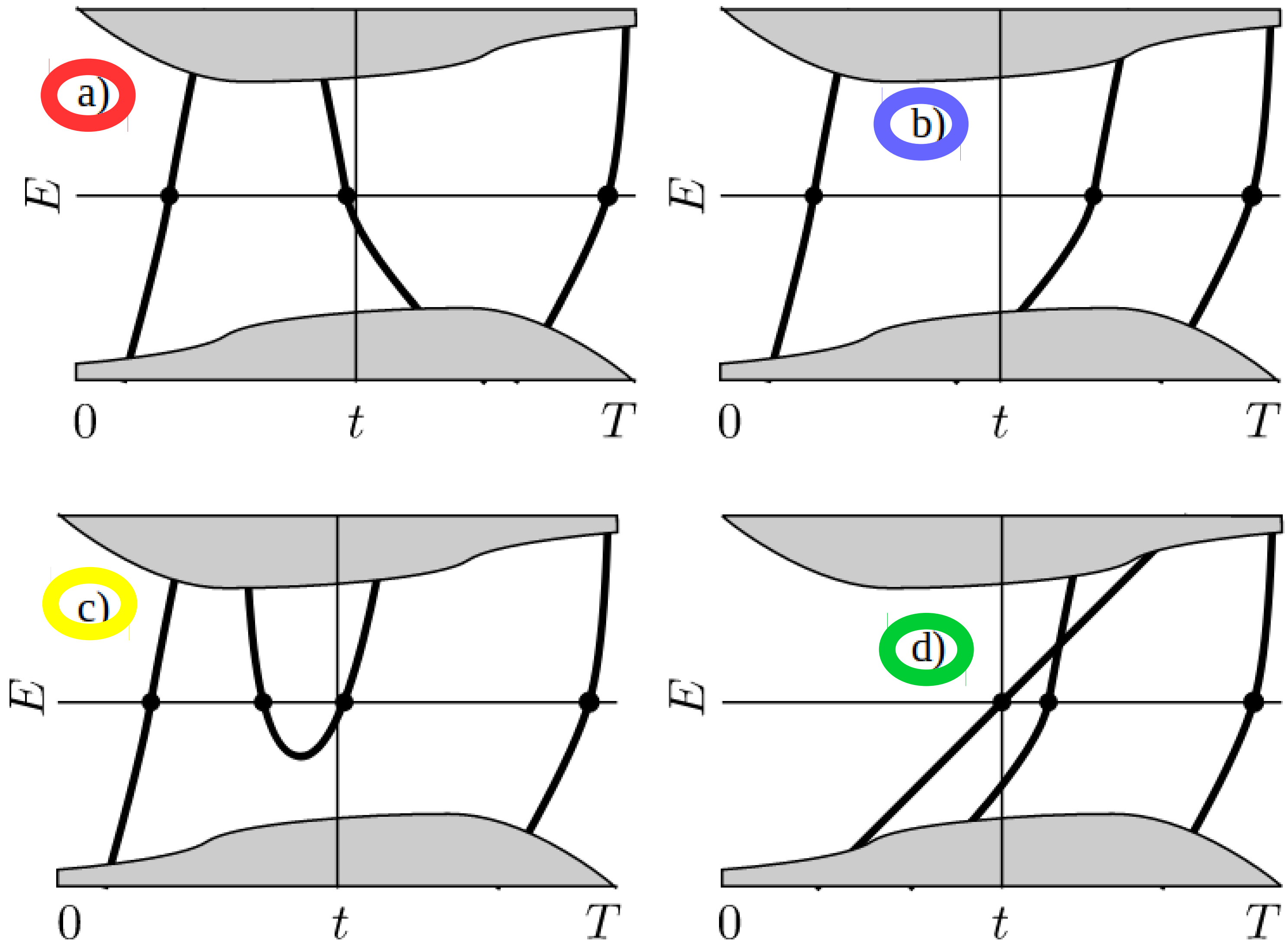
c)



d) None of the above

Edge states and Chern number

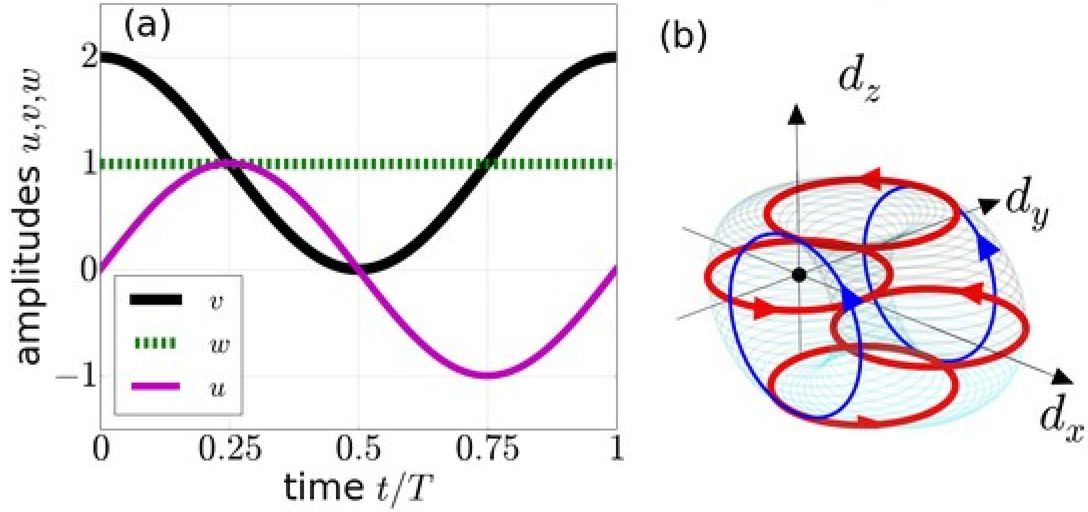
Which of the figures below could represent the edge states of a pump sequence with Chern number 2?



Adiabatic pumping in a finite chain I.

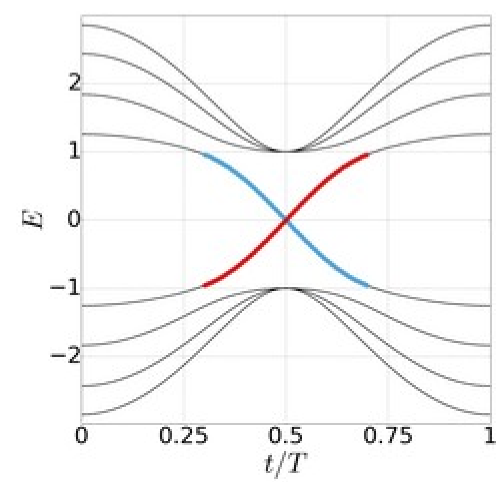
The figures represent the $\bar{v} = 1$ case of the pump sequence defined by

$$\begin{aligned} u(t) &= \sin(2\pi t/T), \\ v(t) &= \bar{v} + \cos(2\pi t/T), \\ w(t) &= 1, \end{aligned}$$



in the finite-sized Rice-Mele model with N=4 unit cells.

Assume that initially the electronic system is in its ground state: the four electrons occupy the negative-energy states. At least how many cycles should be completed to arrive to this ground state again?

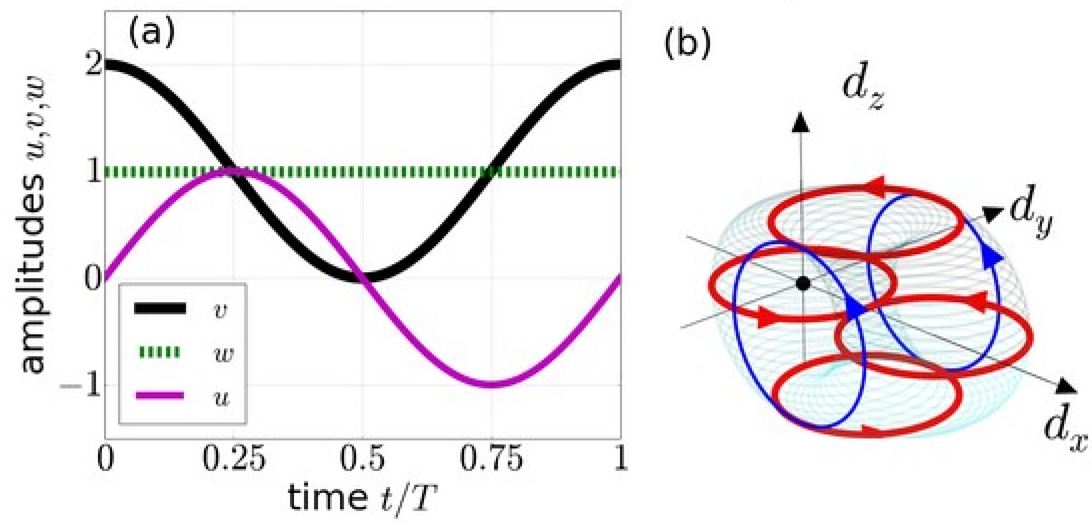


a) 1
b) 2
c) 4
d) 8

Smooth pumping sequence

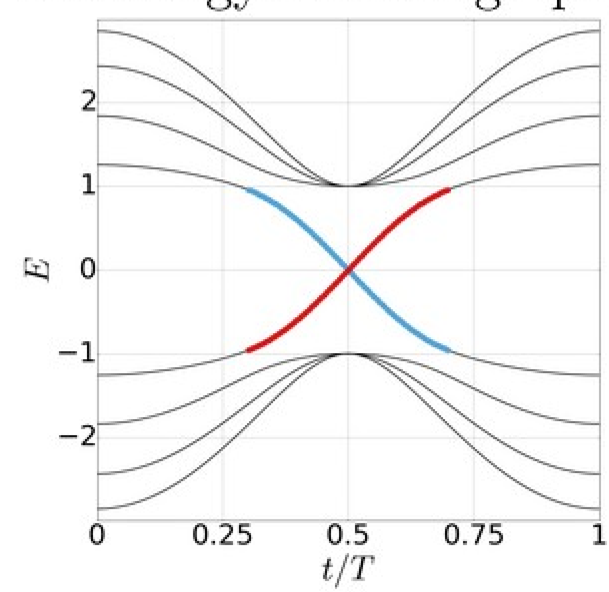
The figures represent the $\bar{v} = 1$ case of the pump sequence defined by

$$\begin{aligned} u(t) &= \sin(2\pi t/T), \\ v(t) &= \bar{v} + \cos(2\pi t/T), \\ w(t) &= 1, \end{aligned}$$



in the finite-sized Rice-Mele model with N=4 unit cells.

Do you expect to see any qualitative difference in the energy-vs-time graph, if $\bar{v} = 1$ is changed to $\bar{v} = 1.5$?



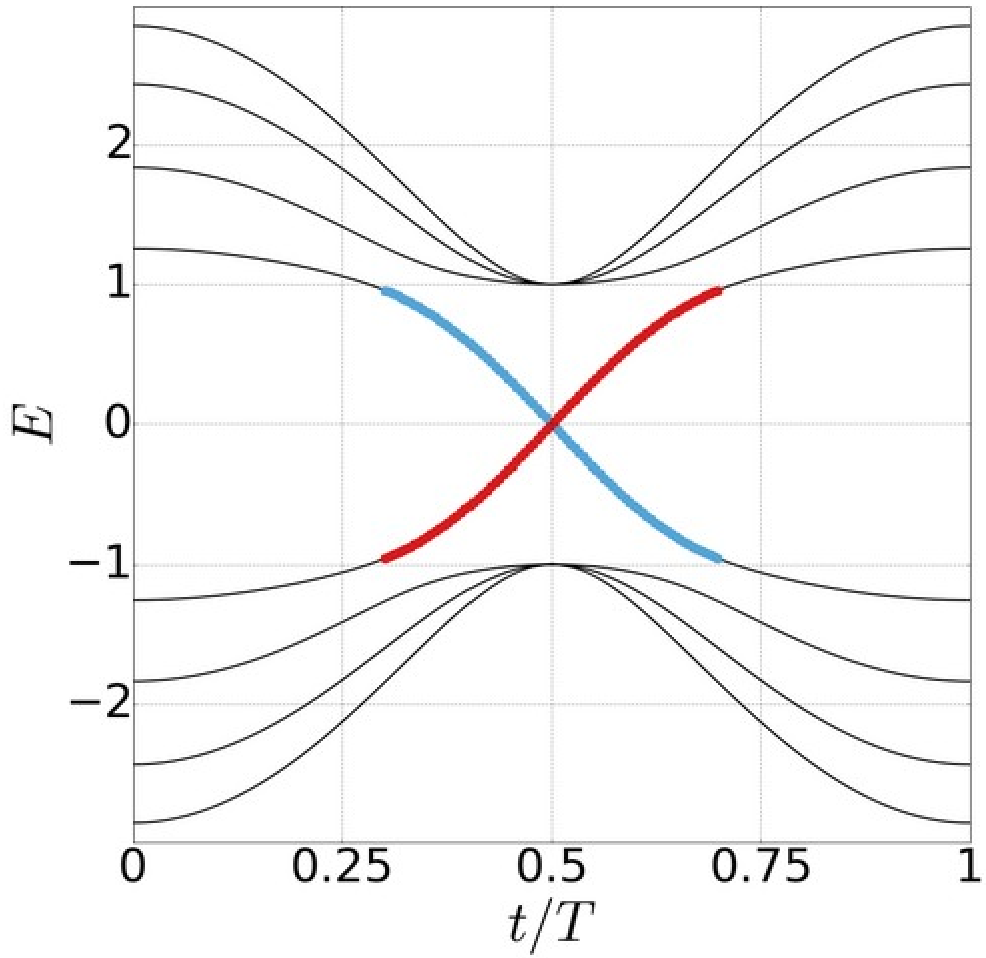
a) No

b) Yes: bulk states become degenerate

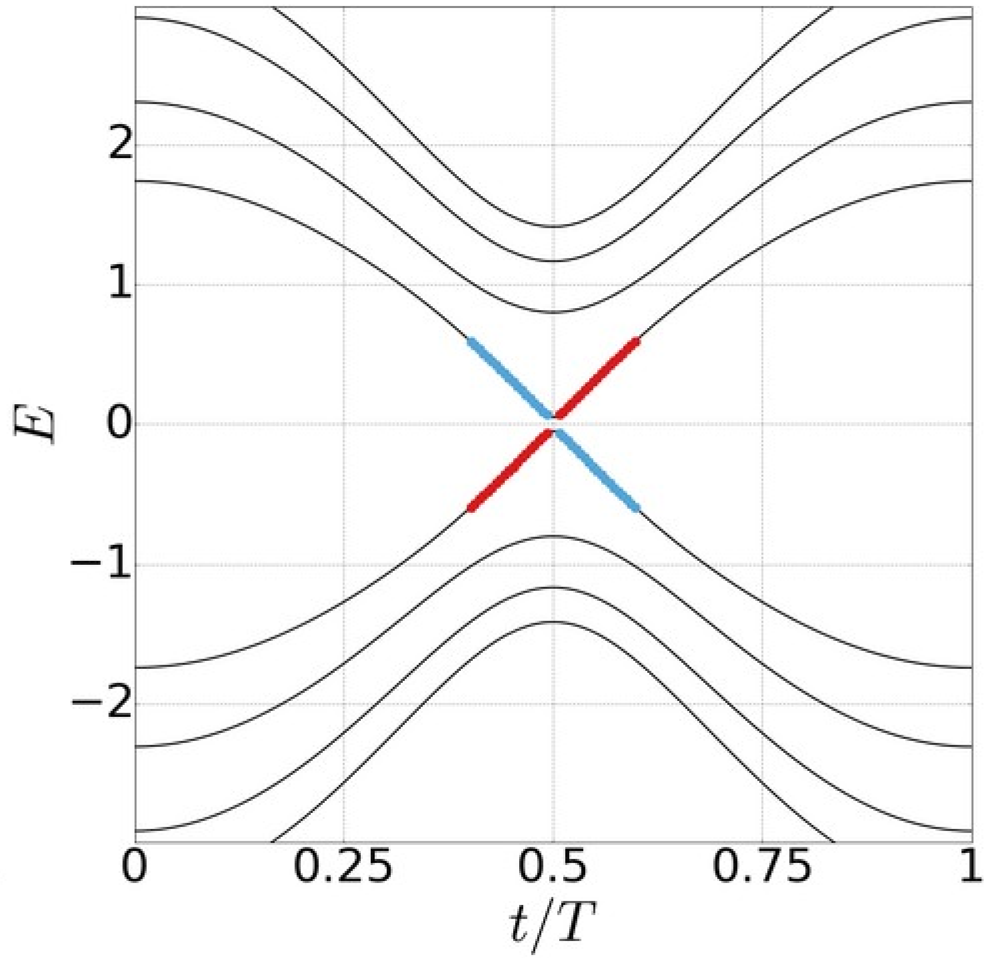
c) Yes: all degeneracies are lifted at t=0.5 T

d) Yes: two edge states appear on both edges

What really happens



$\bar{v} = 1$



$\bar{v} = 1.5$

Adiabatic pumping in a finite chain II.

The figure represent the $\bar{v} = 1.5$ case of the pump sequence defined by

$$\begin{aligned} u(t) &= \sin(2\pi t/T), \\ v(t) &= \bar{v} + \cos(2\pi t/T), \\ w(t) &= 1, \end{aligned}$$

in the finite-sized Rice-Mele model with N=4 unit cells.

Assume that initially the electronic system is in its ground state: the four electrons occupy the negative-energy states. At least how many cycles should be completed to arrive to this ground state again?

a) 1
b) 2
c) 4
d) 8