Spatial embedding of orbitals & 1D topological insulators

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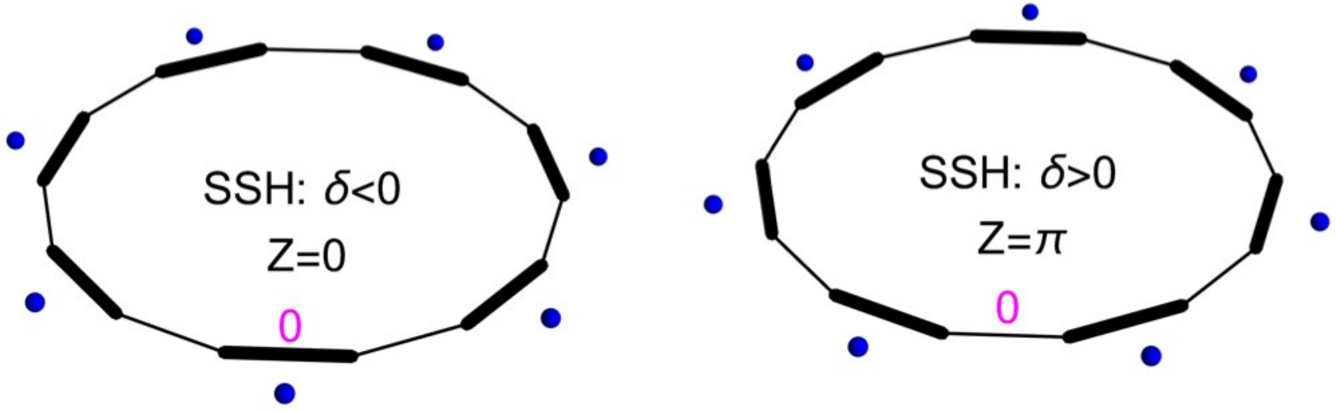
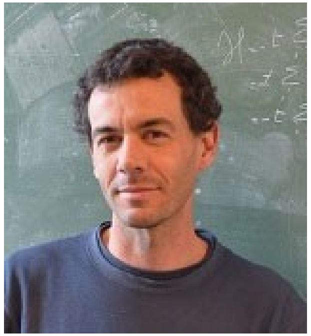


With F. Piéchon, "Orbital embedding and topology of one-dimensional insulators'',
Phys. Rev. B. **104**, 235428 (2021), arXiv:2106.03595

30'+10'

Benasque, 23/02/2022

String-nets in Paris (Jussieu)



Anna Ritz-Zwilling: poster on
Wegner-Wilson loops in string nets

Julien Vidal: talk (next week) on
Partition function of Levin-Wen model
(slides)

This talk : topological band insulators not topological order

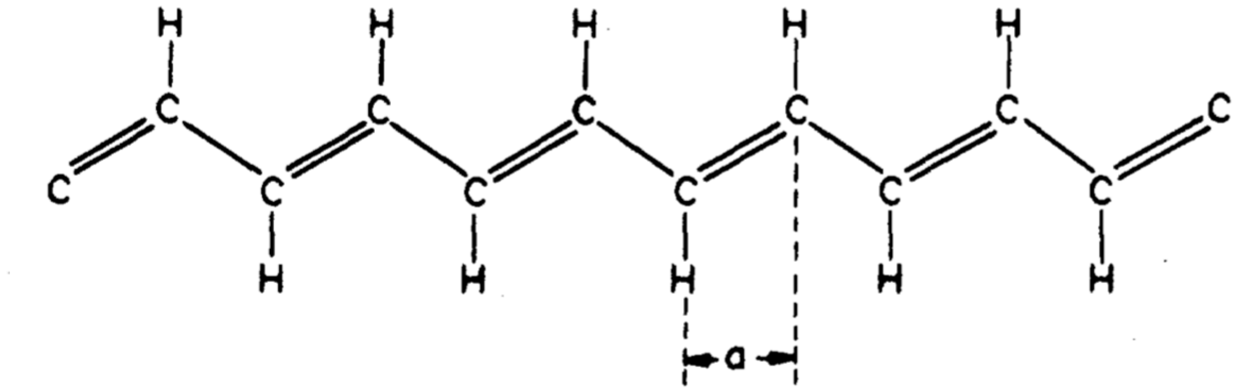
On the simplest example: SSH

1980’s: Su-Schrieffer-Heeger model to explain electric conduction of polyacetylene (a 1D “band-insulating” polymer).

2010’s: SSH as a chiral insulator with a phase transition between trivial and topological insulator (textbook example). Invariant = winding number (protected by sublattice symmetry, SPT).

This talk: no topological phase transition in SSH. A single trivial phase with vanishing electric polarization. Invariant = quantized polarization (protected by inversion symmetry, TCI).

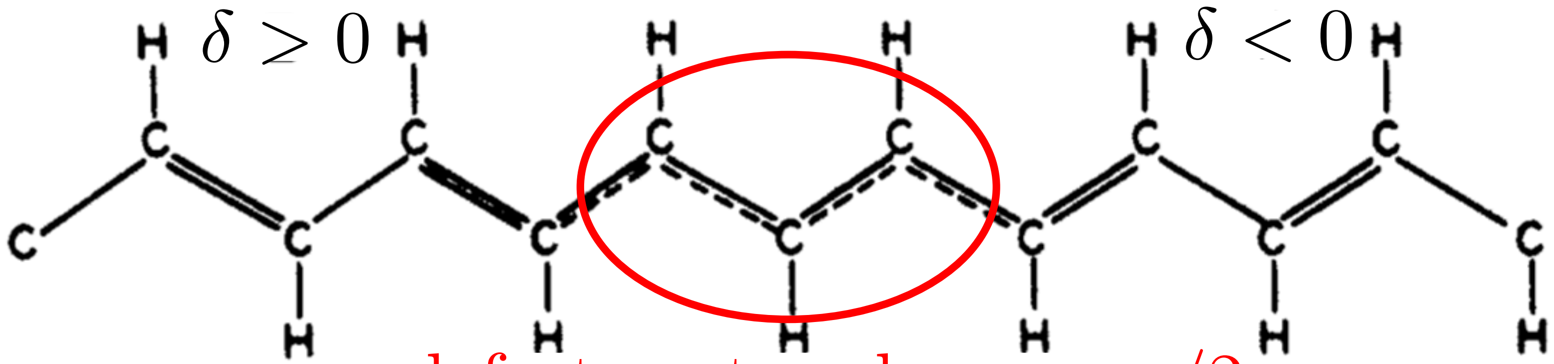
1) Trans-polyacetylene: SSH model



Dimerized chain due to Peierls instability ($\mathbb{Z}_2$ SSB)
Turns metal into band insulator
Conducting due to charged solitons

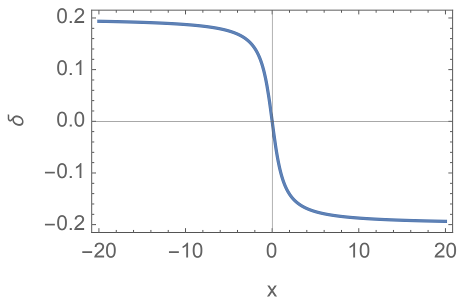
Su, Schrieffer & Heeger 1979

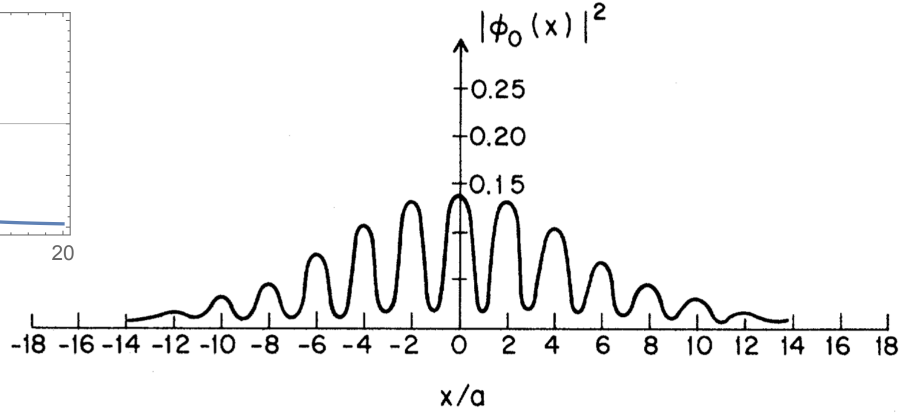
Topological defects trap mid-gap states

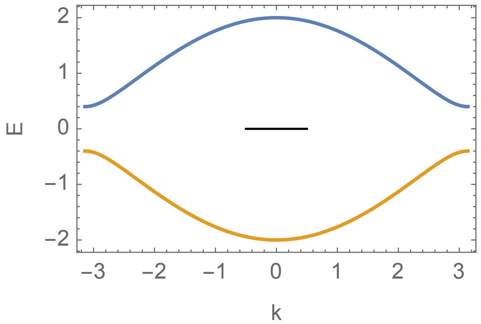


defect: extra charge $-e/2$

Intuition: space-dependent gap vanishes near the defect







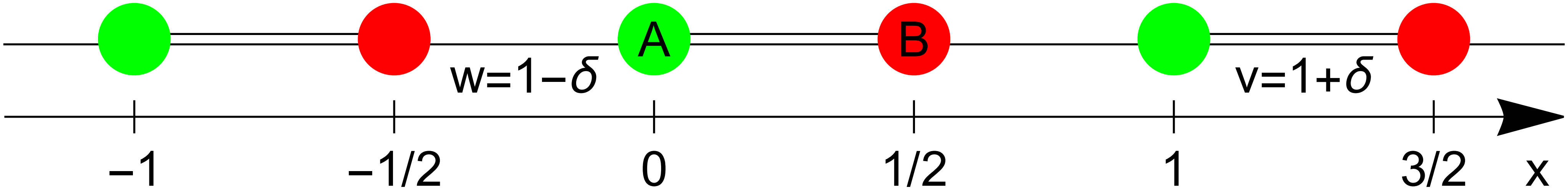
Su, Schrieffer & Heeger 1979
Also Jackiw & Rebbi 1976

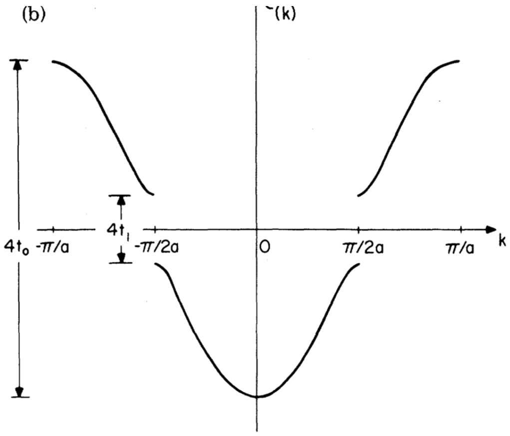
SSH model

1D tight-binding model for π-electrons ($2p_z$ orbitals)

Alternating weak and strong hopping amplitudes v and w

Two bands if $\delta \neq 0$. At half-filling: band insulator.





$$E_{\pm}(k) = \pm\sqrt{4\cos^2\frac{k}{2} + 4\delta^2\sin^2\frac{k}{2}}$$

$$\text{gap} = 2E_{+}(\pi) = 4|\delta|$$

Two dimerizations $\delta > 0$ or $\delta < 0$.

Su, Schrieffer & Heeger 1979

2) SSH as textbook topol. insulator

$$\mathcal{H}(k) = \begin{pmatrix} 0 & v + we^{ik} \\ v + we^{-ik} & 0 \end{pmatrix}$$

$$\mathcal{H}(k) = (v + w\cos k)\sigma_x - w\sin k\sigma_y$$

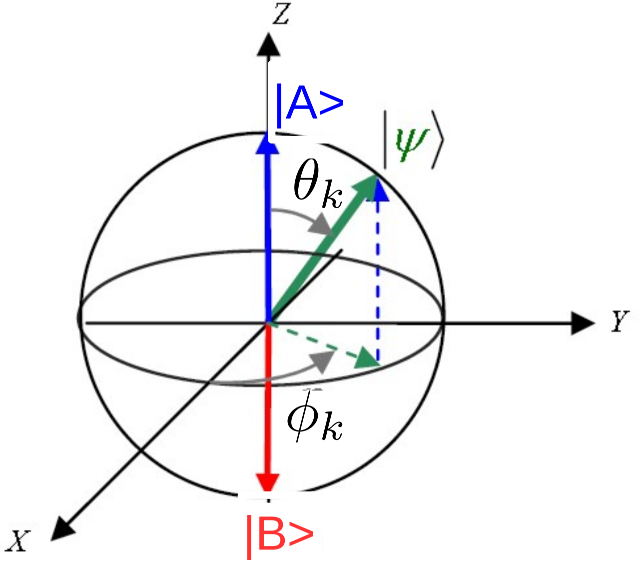
$\mathcal{H}(k+2\pi) = \mathcal{H}(k)$ periodic Bloch Ham.

Brillouin zone (BZ) $-\pi \leq k < \pi$

SSH: no $\sigma_z \rightarrow$ equator of Bloch sphere (chiral symmetry)

map from BZ $= S^1$ to equator $= S^1$

$\Pi_1(S^1) = \mathbb{Z}$, winding number $\mathcal{W}$



Since ~2010. For review see C. Kane 2013; Book by Asboth et al. 2016; Chiu, Teo, Schnyder, Ryu, RMP 2016

SSH in the ten-fold periodic table

chiral (sublattice) sym. $\sigma_z \mathcal{H}(k) \sigma_z = -\mathcal{H}(k)$

time-reversal sym. $\mathcal{H}(-k)^* = \mathcal{H}(k)$

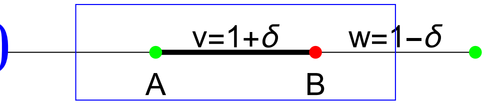
particle-hole sym. $\sigma_z \mathcal{H}(-k)^* \sigma_z = -\mathcal{H}(k)$

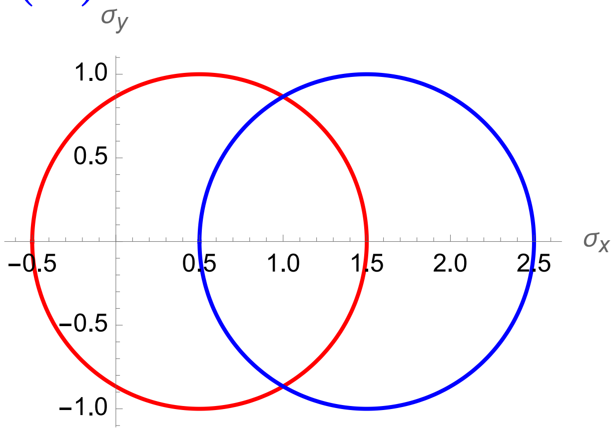
System	Cartan nomenclature	TRS	PHS	SLS	$d=1$	$d=2$	$d=3$
standard (Wigner-Dyson)	A (unitary)	0	0	0	-	**Z**	-
	AI (orthogonal)	+1	0	0	-	-	-
	AII (symplectic)	−1	0	0	-	$\mathbf{Z}_2$	$\mathbf{Z}_2$
chiral (sublattice)	AIII (chiral unit.)	0	0	1	**Z**	-	**Z**
	BDI (chiral orthog.)	+1	+1	1	**Z**	-	-
	CII (chiral sympl.)	−1	−1	1	**Z**	-	$\mathbf{Z}_2$
BdG	D	0	+1	0	$\mathbf{Z}_2$	**Z**	-
	C	0	−1	0	-	**Z**	-
	DIII	−1	+1	1	$\mathbf{Z}_2$	$\mathbf{Z}_2$	**Z**
	CI	+1	−1	1	-	-	**Z**

Schnyder, Ryu, Furusaki, Ludwig 2008; Kitaev 2009

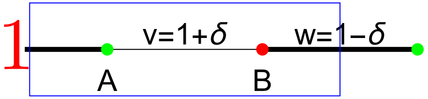
Topological phase transition in SSH

$$v > w : \mathcal{H}_{w=0}(k) = v\sigma_x \to \mathcal{W} = 0$$





$$v < w : \mathcal{H}_{v=0}(k) = w(\cos k\sigma_x - \sin k\sigma_y) \to \mathcal{W} = -1$$

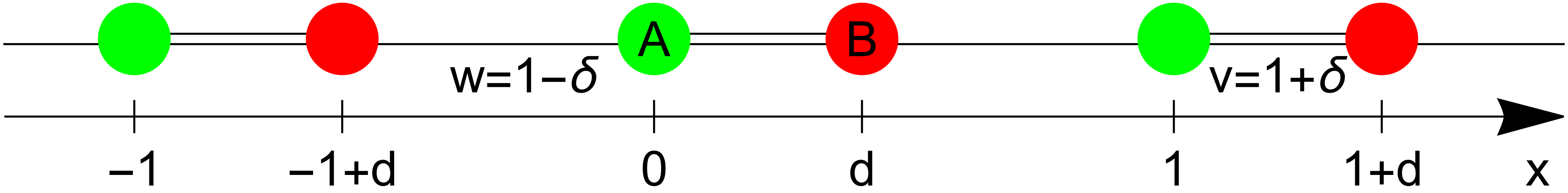


Topological phase transition between:

- topo insulator $\mathcal{W} \neq 0$ ($v < w$, weak intra-cell hopping)
- trivial insulator $\mathcal{W} = 0$ ($v > w$, strong intra-cell hopping)

Topo invariant $\mathcal{W}$ protected by chiral symmetry

Bloch Hamiltonian: basis I/II issue



$$x_A = m \in \mathbb{Z} \qquad x_B = m + d = x_A + d$$

$\mathcal{H}(k)$ "=" $e^{-ik\hat{R}} H e^{ik\hat{R}}$ (basis I, periodic, cell-dep., d-indep.)

one unit cell: $\mathcal{H}(k) = (v + w\cos k)\sigma_x - w \sin k \sigma_y = H_{d=0}(k)$

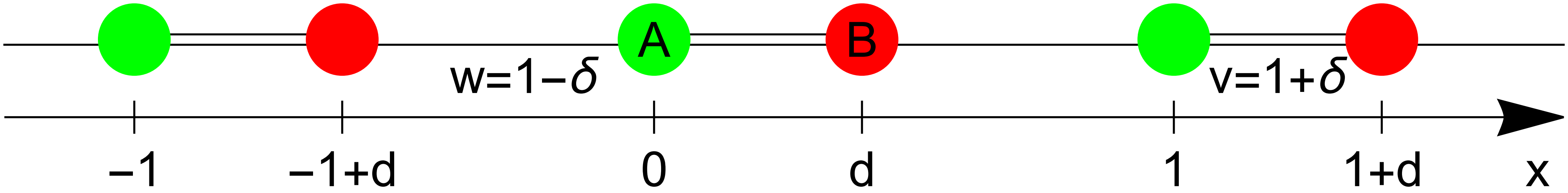
another unit cell: $\tilde{\mathcal{H}}(k) = (w + v\cos k)\sigma_x + v \sin k \sigma_y = H_{d=1}(k)$

Cell-dependent winding number : $\mathcal{W} = 0/-1,\ \tilde{\mathcal{W}} = 1/0$

Spatial embedding of orbitals is neglected

Bena & Montambaux 2009; For review see Cayssol & Fuchs 2021

Bloch Hamiltonian in “basis II”



$$x_A = m \in \mathbb{Z} \qquad x_B = m + d = x_A + d$$

$H(k)$ “$=$” $e^{-ik\hat{x}} H e^{ik\hat{x}}$ (basis II, not periodic, canonical, d-dep.)

$$H_d(k) = 2\cos\frac{k}{2}\sigma_x(k,d) - 2\delta\sin\frac{k}{2}\sigma_y(k,d)$$

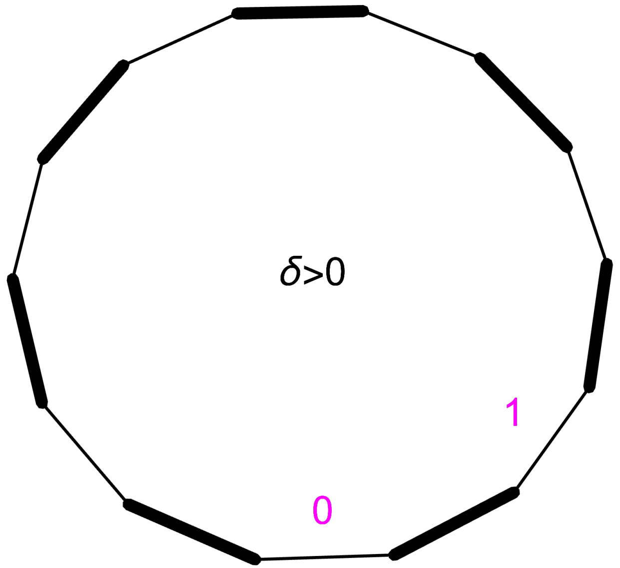
$$\sigma_j(k,d) = e^{ik(d-1/2)\sigma_z/2}\sigma_j e^{-ik(d-1/2)\sigma_z/2} = \sigma_j \text{ if } d = 1/2$$

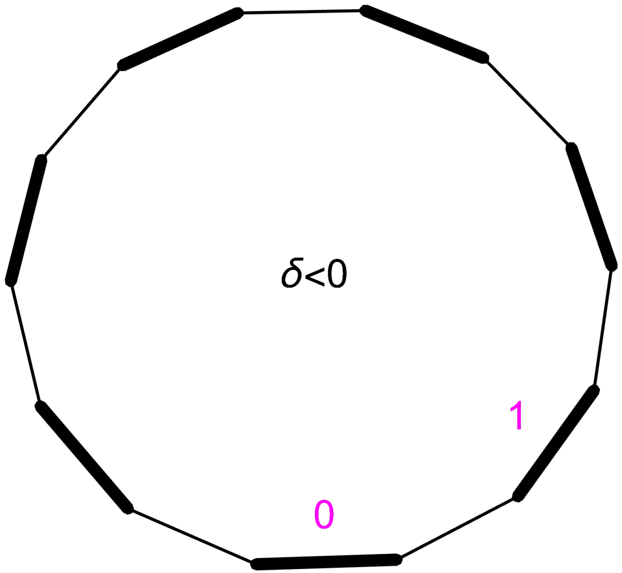
No bulk winding number : $W = \emptyset$

Spatial embedding of orbitals is taken into account.

Bena & Montambaux 2009; For review see Cayssol & Fuchs 2021

SSH on a ring (PBC)





No measurable bulk quantity can depend on sign δ.
Single phase when $\delta \neq 0$.

3) Inversion-symmetric insulators: quantized electric polarization

Electric polarization = P = dipole moment per unit volume
Defined in neutral insulators (dielectrics)

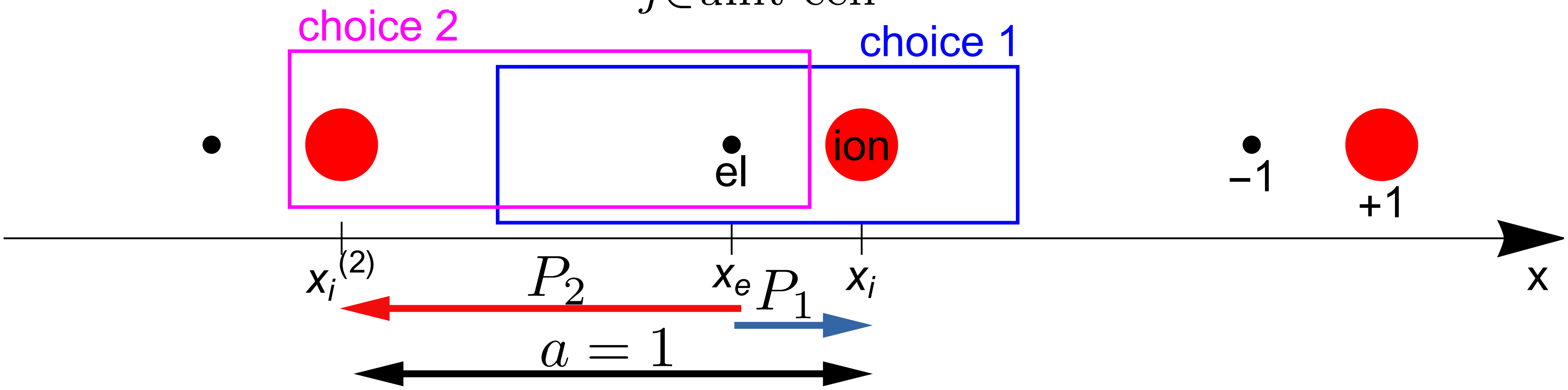
Inversion symmetry: $P \to -P = P \Rightarrow P = 0$

Bulk electric polarization P of a crystal is an angle:
P defined modulo P_q ("quantum" of polarization)
Fact of classical electrostatics (remains true in QM)

$\mathbb{Z}_2$ topological invariant: either $P = 0$ or $P = P_q/2 \bmod P_q$
(SSH has bond inversion symmetry)

« Quantum » of polarization

$$P = \frac{1}{a} \sum_{j \in \text{unit cell}} q_j x_j$$



$$P_1 = -x_e + x_i$$

$$P_2 = -x_e + x_i^{(2)} = -x_e + x_i - 1 = P_1 - 1$$

$$\Rightarrow P_q = 1$$

P is defined modulo $P_q = 1$ $(e \equiv 1,\ a \equiv 1)$

Vanderbilt & King-Smith 1993. For review, see Vanderbilt's 2018 book

Where are the electrons in an insulator?

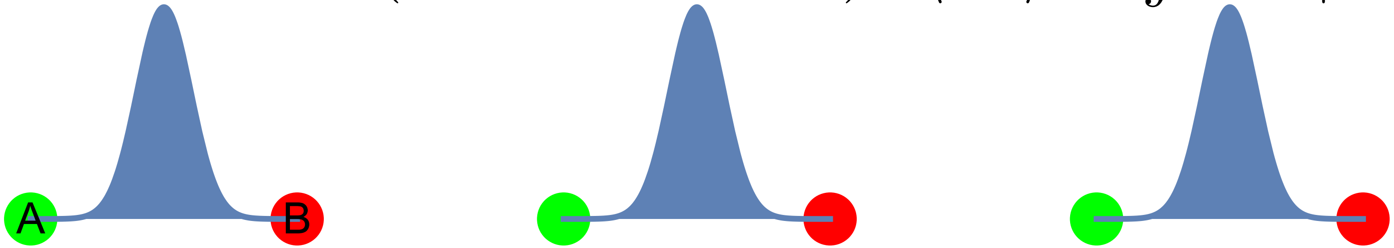
$$|u_{n,k}(x_A)|^2 = |u_{n,k}(x_B)|^2 = 1/N_s??$$

Wannier function for a given filled band $w_n(x)$

$w_{n,R}(x) = \int dx \psi_{n,k}(x) e^{-ikR} = w_{n,0}(x-R)$

Exponentially localized (Wannier spread)

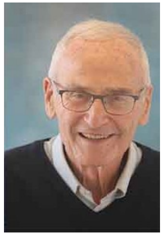
Wannier center (or band center): $\langle x_n \rangle = \int dx x |w_n(x)|^2$



$$\langle x_n \rangle = a\frac{Z_n}{2\pi} \text{ depends on the phase of } u_{n,k}(x)$$

Wannier (1937)

Kohn (1964)



Zak (1989)

Review by Resta 2011, *The insulating state of matter : a geometrical theory*

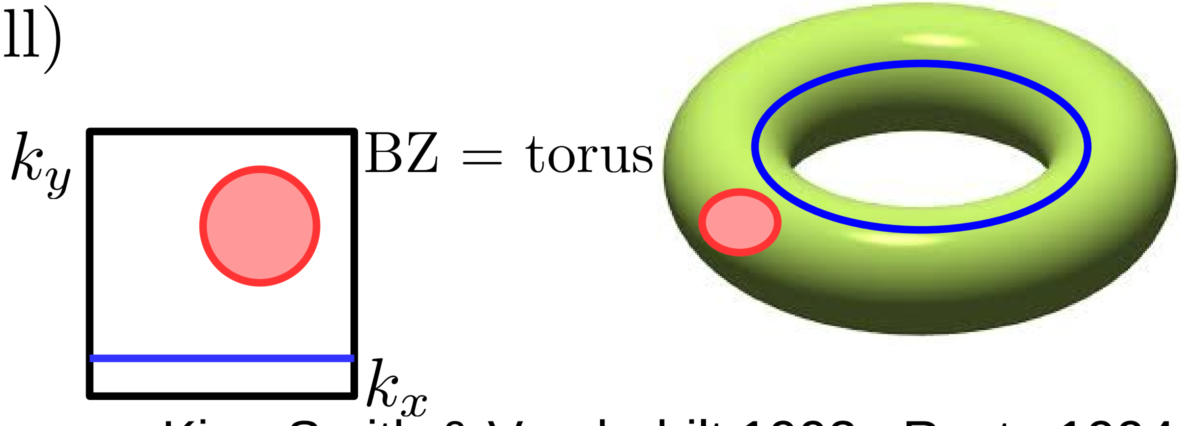
Polarization from Zak phase

$$P = P_{\text{el}} + P_{\text{ion}} = -\langle x_- \rangle + x_i = -\frac{Z_-}{2\pi} + x_i \bmod P_q = 1$$

$$Z_n = \int_{-\pi}^{\pi} dk \langle u_n(k) | i\partial_k u_n(k) \rangle + \arg \langle u_n(-\pi) | e^{i2\pi x} | u_n(\pi) \rangle \bmod 2\pi$$

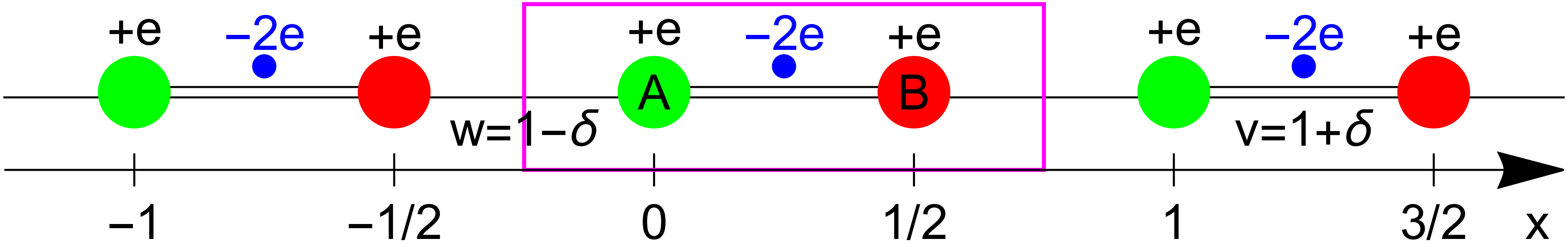
Zak phase = peculiar Berry phase (non-contractible path in BZ)
= Wannier center

Inversion symmetry ⇒ Wannier center on inversion center
(in 1D: 2 centers per unit cell)



King-Smith & Vanderbilt 1993 ; Resta 1994

Original SSH model (SSH$_{1/2}$)



Ionic charges on every carbon site.

Neutrality ⇒ ionic charge = $+e$ (if spinful electrons)

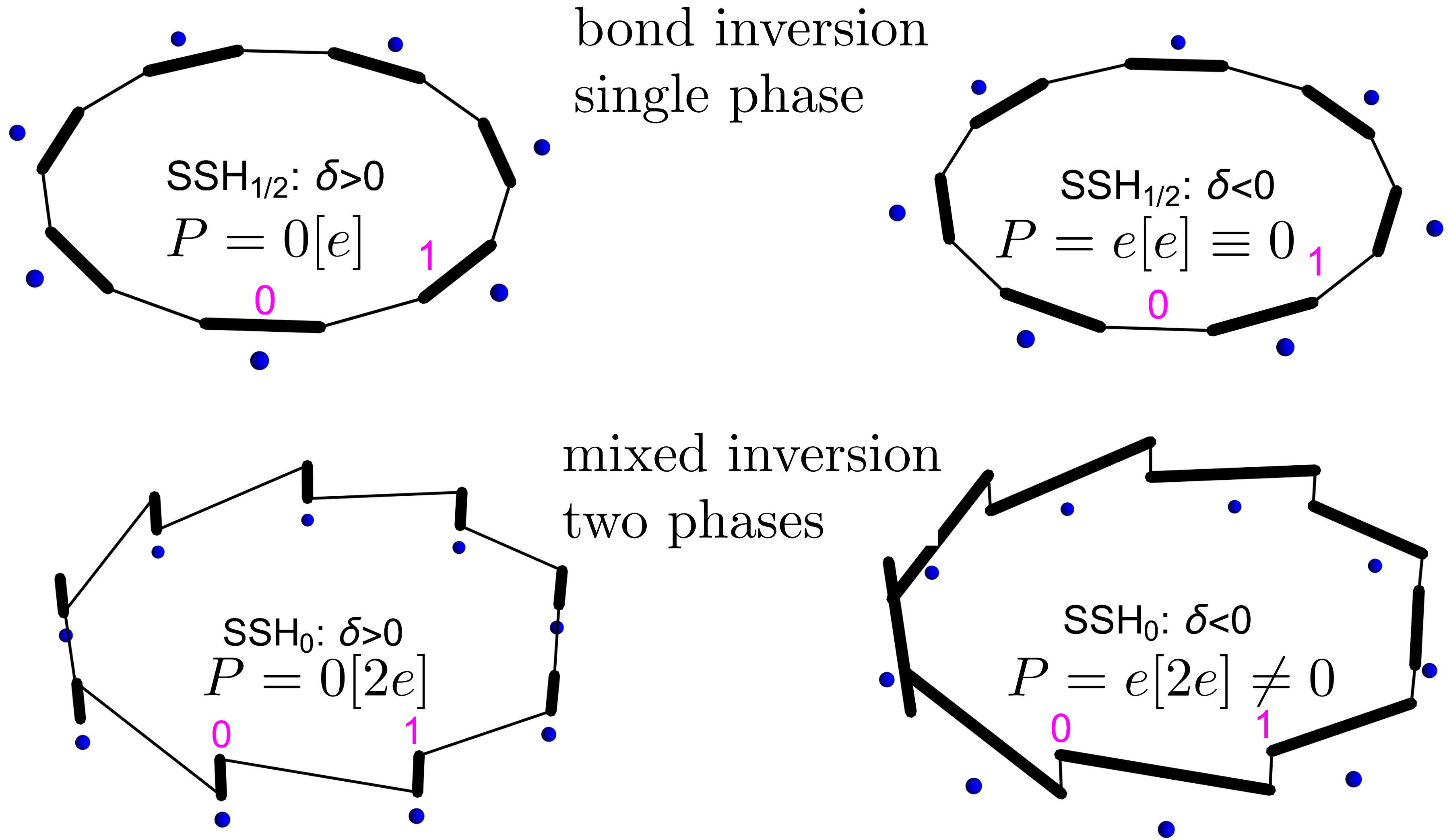
Quantum of polarization: $P_q = e$ (and not $2e$!)

Bulk polarization: $P = P_{\text{el}} + P_{\text{ions}} \bmod P_q$

$$P_{\text{ions}} = \frac{1}{a} \sum_{j \in \text{unit cell}} q_j x_j = e/2$$

$$P_{\text{el}} = -2e\langle x_- \rangle = -2e \text{ sign } \delta/4$$

$$P = 0 \text{ or } e \bmod e \equiv 0 \text{ for both dimerizations}$$



bond inversion
single phase
SSH$_{1/2}$: $\delta>0$
$P = 0[e]$
0
1
SSH$_{1/2}$: $\delta<0$
$P = e[e] \equiv 0$
0
1
mixed inversion
two phases
SSH$_0$: $\delta>0$
$P = 0[2e]$
0
1
SSH$_0$: $\delta<0$
$P = e[2e] \neq 0$
0
1

Take-home messages

- Z_2 SSB Peierls instability : two-fold degenerate groundstate
- Importance of spatial embedding of orbitals : basis I/II, no bulk winding number (despite chiral symmetry)
- Periodic insulator : where are the electrons ? Wannier center (Zak phase, no ordinary Berry phase)
- Neutral insulator : importance of ionic model
- Periodic insulator : quantum of polarization depends on el & ions
- Inversion symmetry in crystal (TCI) : quantized P (Z_2 topo invariant)
- SSH has P=0 mod e for both dimerizations : no topo phase transition

With F. Piéchon, “Orbital embedding and topology of one-dimensional insulators’’,
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Review with J. Cayssol, “Topological and geometrical aspects of band theory’’,
J. Phys. Mater. **4**, 034007 (2021), arXiv:2012.11941