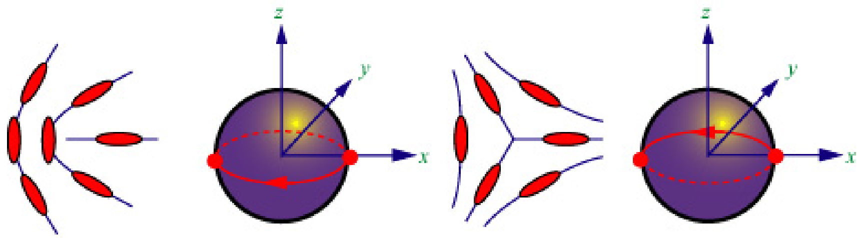
Topological Phonons, Edge States, and Guest Modes

Topological Defects

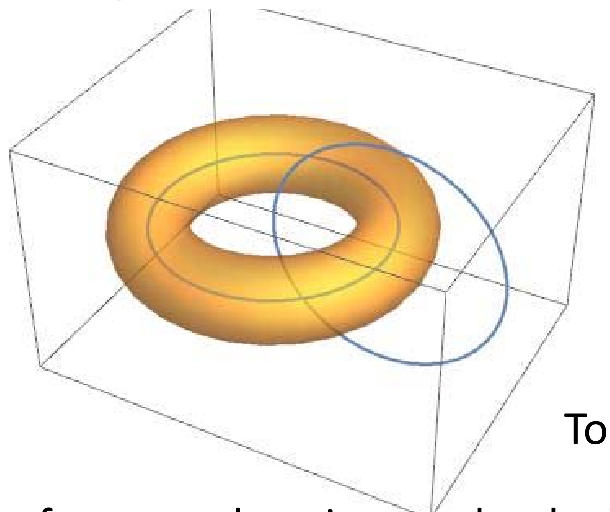
Closed path in real space

Path in order parameter space: topological invariant



"k=1/2" "k=-1/2"

Periodic Brillouin Zone



Function on torus

Torus

Closed path of function

It no defects on surface, topology is completely determined by two winding numbers, i.e., by a lattice vector

Topology and Adiabatic Continuity

Insulators are topologically equivalent if they can be continuously deformed into one another without closing the energy gap

genus = 0

Are there "topological phases" that are not adiabatically connected to the trivial insulator (ie the vacuum) ?

genus = 1

Topological Electronic States and Topological Insulators

A major theme in theory or electronic states:

Berry's phases

Polyacetylene

Quantum Hall effect

Topological Insulators – surface conducting states (Graphene - + 3d): Charlie Kane, Gene Mele, Liang Fu, Shoucheng Zhang

Kane and Mele, PRL 95, 226801; PRL 95 146802 (2005)
Hasan and Kane, Rev. Mod. Phys. 82, 3046 (2012)
S.-C. Zhang and B. Yan, Rept. Prog. Phys. 75, 096501 (2012)

Gapped states can have different topological classifications leading to different surface states.

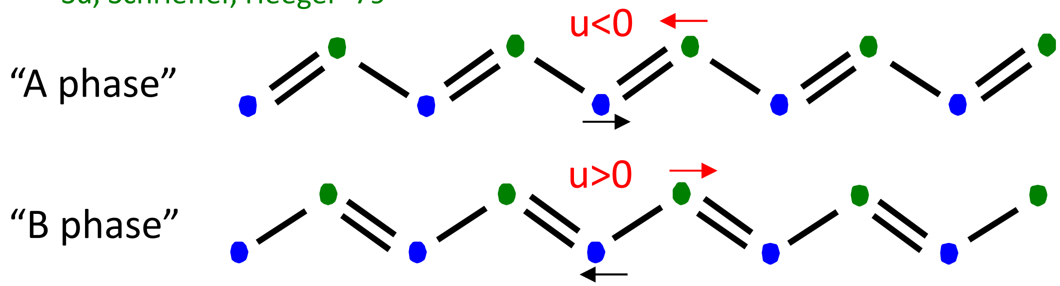
Charlie Kane

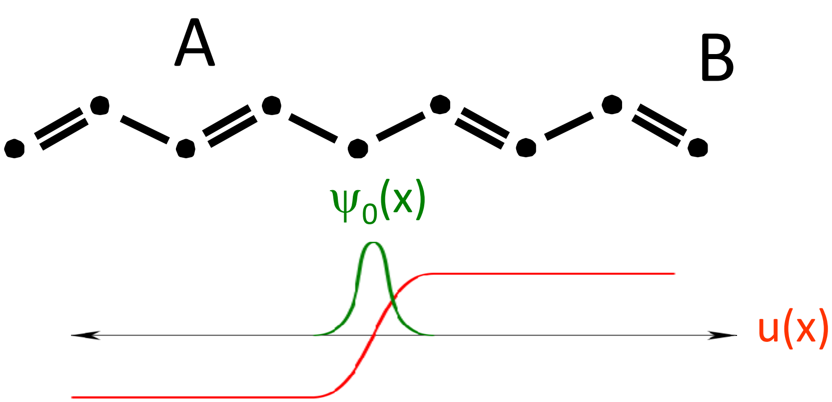
Gene Mele

Topology in hbar physics

Polyacetalene: 1D chain with dimerization $u = \pm u_0$

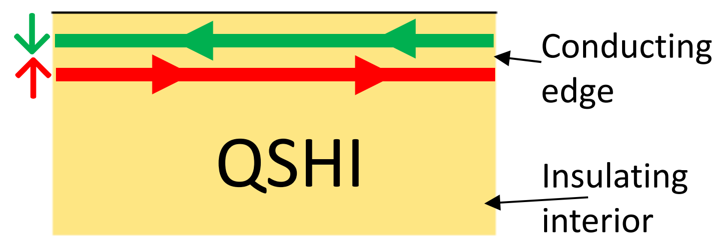
Su, Schrieffer, Heeger '79

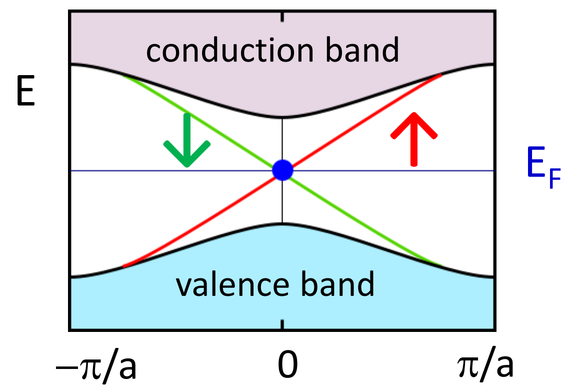




Two Dimensions: Quantum spin Hall insulator

Kane and Mele '05



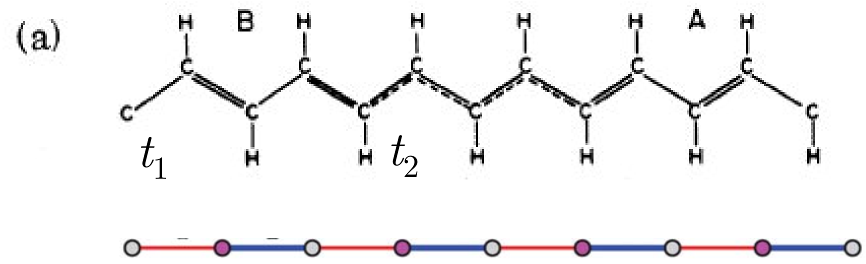


Outline

- Topological index and edge states in the SSH model
- A Mechanical SSH model
- Kagome-based lattices with distinct topological properties
- Topological count and edge states in kagome-based lattices
- Guest elastic modes
- Weyl modes and lines
- 3D Lattices
- Jamming

Su-Schrieffer-Heeger Model

Two types of sites: 1 and 2:
1 connects to 2 but not 1 to 1 or 2 to 2



$$H = \sum_l \left[t_1 \psi^\dagger_{l,1} \psi_{l,2} + t_2 \psi^\dagger_{l,2} \psi_{l+,1} + h.c. \right]$$

$$= \sum_{l,l'} [\psi^\dagger_{l,1} Q_{ll'} \psi_{l',2} + \psi^\dagger_{l,2} Q^\dagger_{ll'} \psi_{l',1}]$$

$$= \sum_k \Psi^\dagger(k) H(k) \Psi(k); \; \Psi = (\psi_1, \psi_2)$$

$$Q_{ll'} = t_1 \delta_{ll'} + t_2 \delta_{l-1,l'};$$

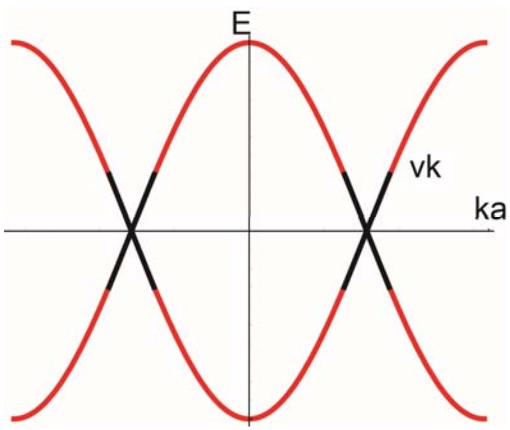
$$Q^T_{ll'} = t_1 \delta_{ll'} + t_2 \delta_{l+1,l'} = C_{ll'}$$

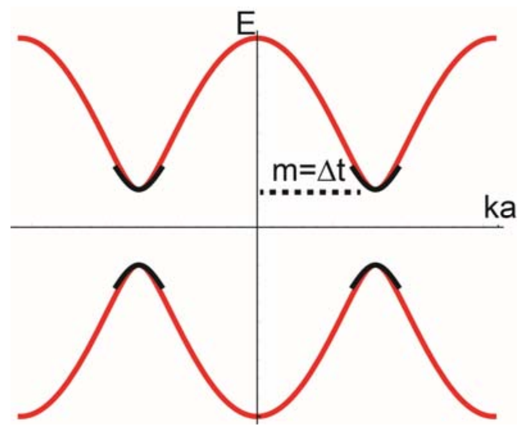
$$C(k) = Q^*(k) = t_1 + t_2 e^{ika}$$

$$H(k) = \begin{pmatrix} 0 & t_1 + t_2 e^{-ik} \\ t_1 + t_2 e^{ik} & 0 \end{pmatrix} \equiv \begin{pmatrix} 0 & Q(k) \\ Q^*(k) & 0 \end{pmatrix}$$

Gapped Spectrum

$$E = \pm |Q(k)| = \pm\sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos ka}$$
$$\xrightarrow{t_1=t_2=t} \pm 2t\,|\cos(ka/2)|$$
$$\xrightarrow{ka=\pm\pi} \pm |t_1 - t_2|$$





Spectrum has zeros at $ka = \pm\pi$ when $t_1 = t_2$ and a gap of $E_g = 2|t_1 - t_2|$ when $t_1 \neq t_2$.

Zero modes localized at endpoints

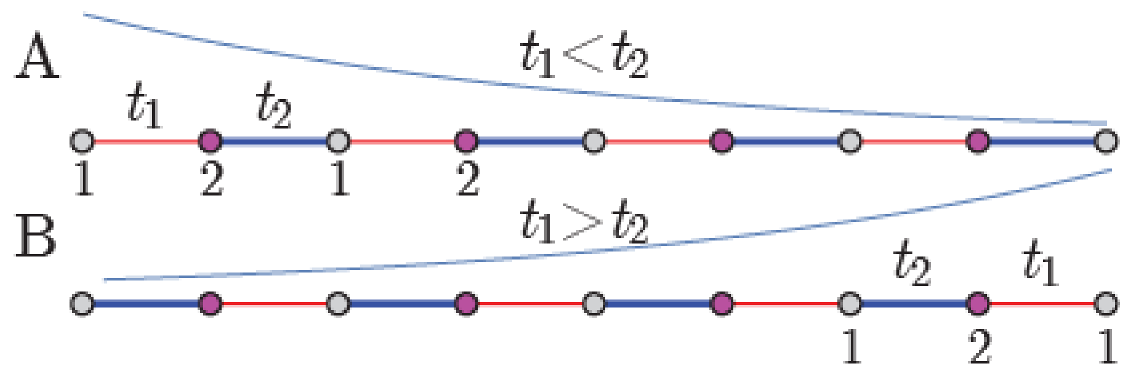
$$H(k)=\begin{pmatrix} 0 & Q(k) \\ C(k) & 0 \end{pmatrix}$$

$$C(k)=\begin{pmatrix} t_1 & t_2 & 0 & 0 \\ 0 & t_1 & t_2 & 0 \\ 0 & 0 & t_1 & t_2 \\ 0 & 0 & 0 & \ddots \end{pmatrix}$$

$$\begin{aligned} &E\psi_{l2} = t_1\psi_{l1} + t_2\psi_{l+1,1}; E = 0 \\ &\Rightarrow \psi_{l+1,1} = -(t_1 / t_2)\psi_{l,1}; \\ &\quad \psi_{l-1,1} = -(t_2 / t_1)\psi_{l,1}; \qquad \psi_{l,2} = 0 \end{aligned}$$

$$\begin{aligned} &E\psi_{l1} = t_1\psi_{l2} + t_2\psi_{l-1,2}; E = 0 \\ &\Rightarrow \psi_{l-1,2} = -(t_1 / t_2)\psi_{l,2}; \\ &\quad \psi_{l+1,2} = -(t_2 / t_1)\psi_{l,2}; \qquad \psi_{l,1} = 0 \end{aligned}$$

Decaying sol'n
on sites 1 from right
if $|t_1| < |t_2|$;
from left if $|t_1| > |t_2|$



Topological Charge of Gapped States

$$\boxed{C(k) = t_1 + e^{ik} t_2 \equiv t_1 + z t_2 = C(z) \quad (=0, \quad \text{at } z = -t_1 / t_2)}$$

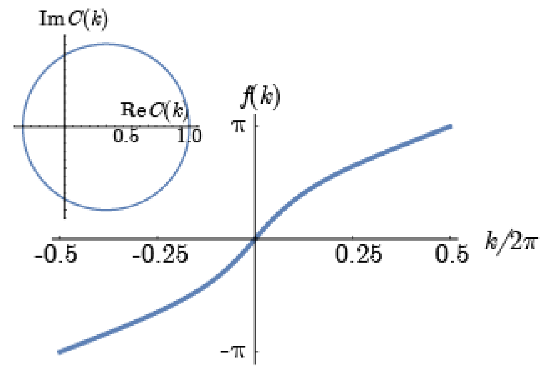
Cauchy's Argument Principle

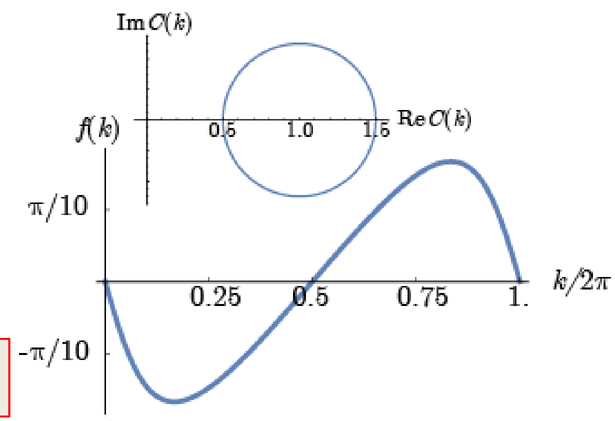
$$\nu = \frac{1}{2\pi i} \oint dz \frac{g'(z)}{g(z)} = \frac{1}{2\pi i} \int_0^{2\pi} dk \frac{d}{dk} \ln g(e^{ik})$$
$$= \#\,\text{zeros - } \#\text{ poles} = \text{integer}$$
$$g(z) = 0; \quad |z| = |e^{ik}| < 0; \text{ no poles}$$
$$\Rightarrow \text{Im } k > 0\text{: decaying soln}$$

$$\boxed{\nu = P = \frac{1}{2\pi} \int_0^{2\pi} dk \frac{d}{dk} \ln C(k) = 1, 0}$$

Phase of *C*

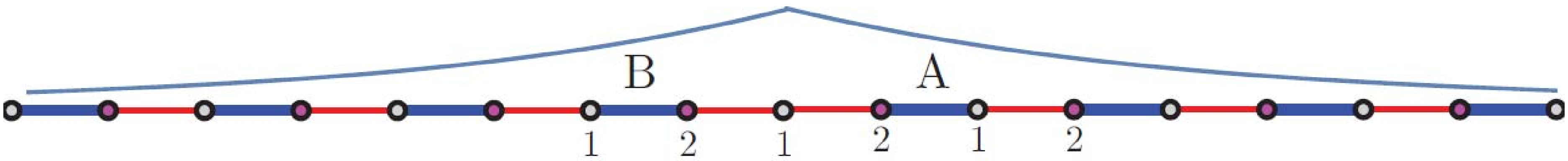
$t_1 < t_2$





$t_2 < t_1$

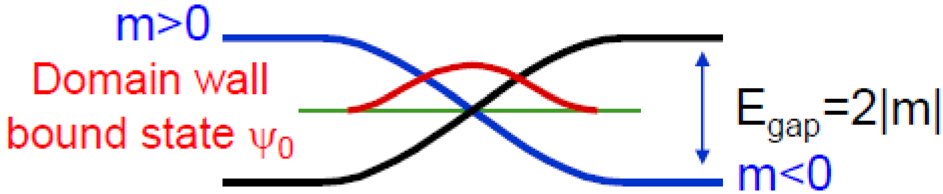
Domain-wall states



Tie right and left decaying states together to create a zero-energy mode localized at the domain wall

$$\sigma_z H \sigma_z = -H$$

For every state with energy E, there is a state with energy –E ("particle-hole symmetry"): There is a topologically protected zero mode at the boundary between the two distinct topological phases.



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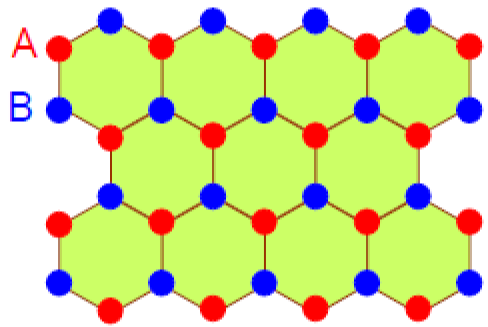
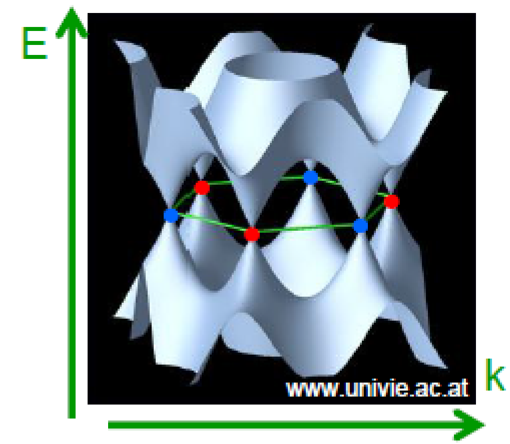
Graphene



Two band model $H = -t\sum_{<ij>} c_{Ai}^{\dagger} c_{Bj}$

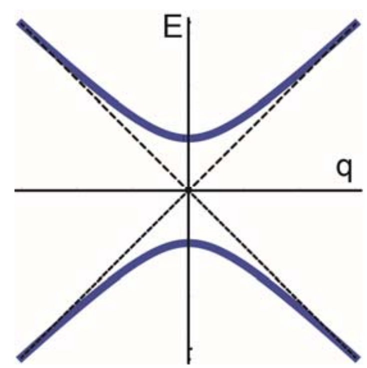
$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \vec{\sigma}$$

$$E(\mathbf{k}) = \pm |\mathbf{d}(\mathbf{k})|$$



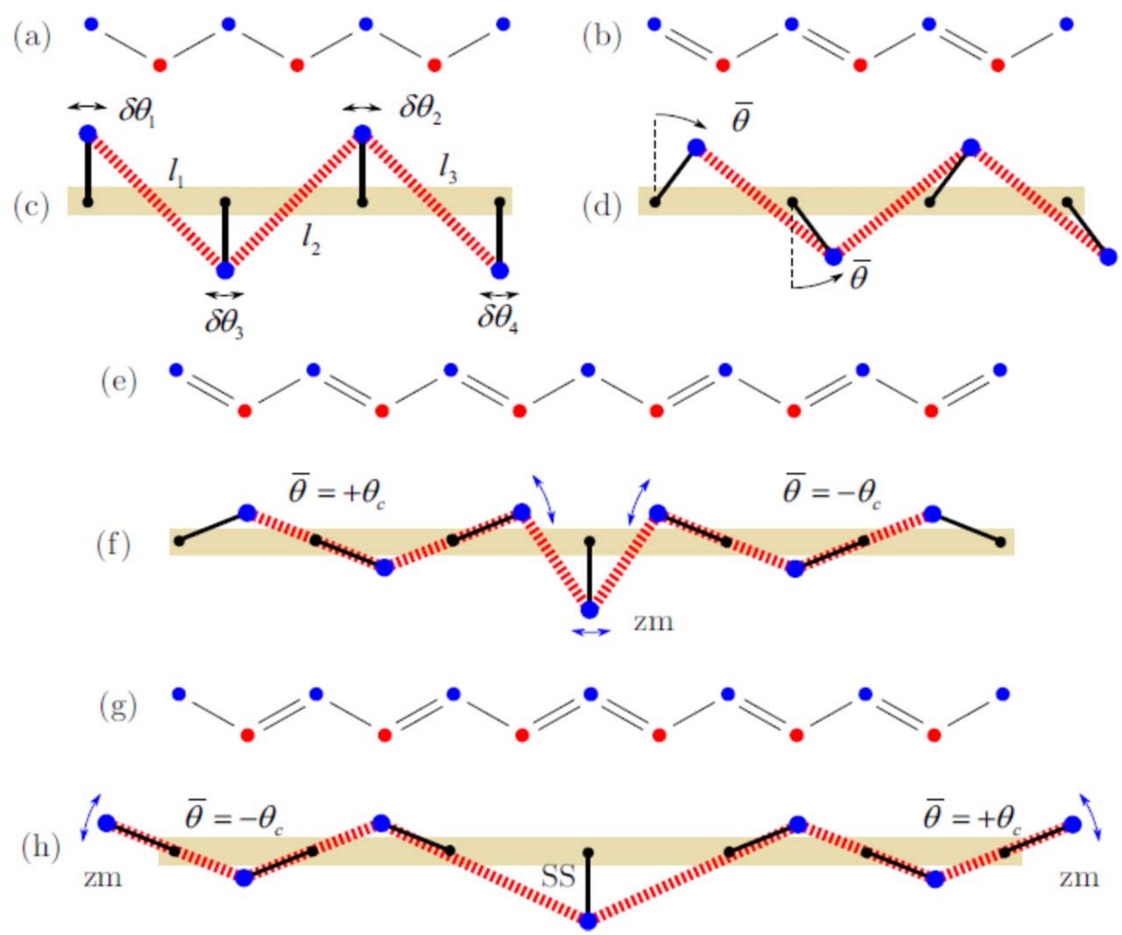
$H(\pm\mathbf{K} + \mathbf{q}) = \mathrm{v}\vec{\sigma} \cdot \mathbf{q}$ Massless Dirac Hamiltonian

Various perturbations break the symmetry and lead to gaps at the Dirac points. Note similarity to gapping of phonon states in the twisted kagome lattice. [Graphene: rotational symmetry about vertical axis; kagome – pattern for every q_x.]



1D Topological Mechanical Model

Blue SSH site -> site: Red SSH site -> bond



Mechanical SSH Model

$$\delta\ell_\beta = C_{\beta,s}\delta\theta_s$$

$$C_{\beta,s} = c_1(\bar{\theta})\delta_{s,\beta} - c_2(\bar{\theta})\delta_{\beta,s+1}$$

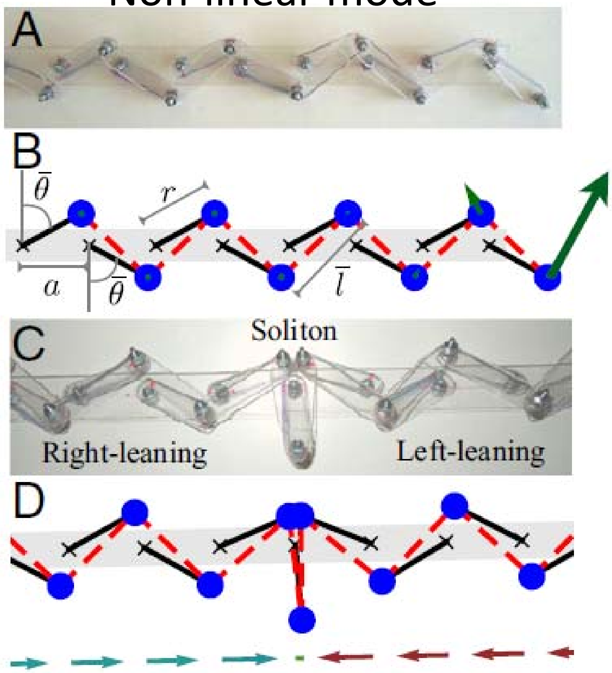
$$C_{\beta,s}(q) = c_1(\bar{\theta}) - c_2(\bar{\theta})e^{iqa}$$

$$c_{1(2)} = \frac{(a \pm 2r\sin\bar{\theta})r\cos\bar{\theta}}{\sqrt{a^2 + 4r^2\cos^2\bar{\theta}}}$$

$$E = \tfrac{1}{2}k\sum_\beta\left(\delta l_\beta\right)^2$$
$$= \tfrac{1}{2}k\sum_{s,\beta,s'}\delta\theta_s C^T_{s,\beta}C_{\beta,s'}\delta\theta_{s'}$$
$$= \tfrac{1}{2}k\sum_s\left(c_1\delta\theta_s - c_2\delta\theta_{s+1}\right)^2$$
$$= \tfrac{1}{2}\delta\vec{\theta}^T D\delta\vec{\theta}$$

Same spectrum as SSH:
Zero mode on left (right) if $c_1 < c_2 (c_1 > c_2)$.

Non-linear mode



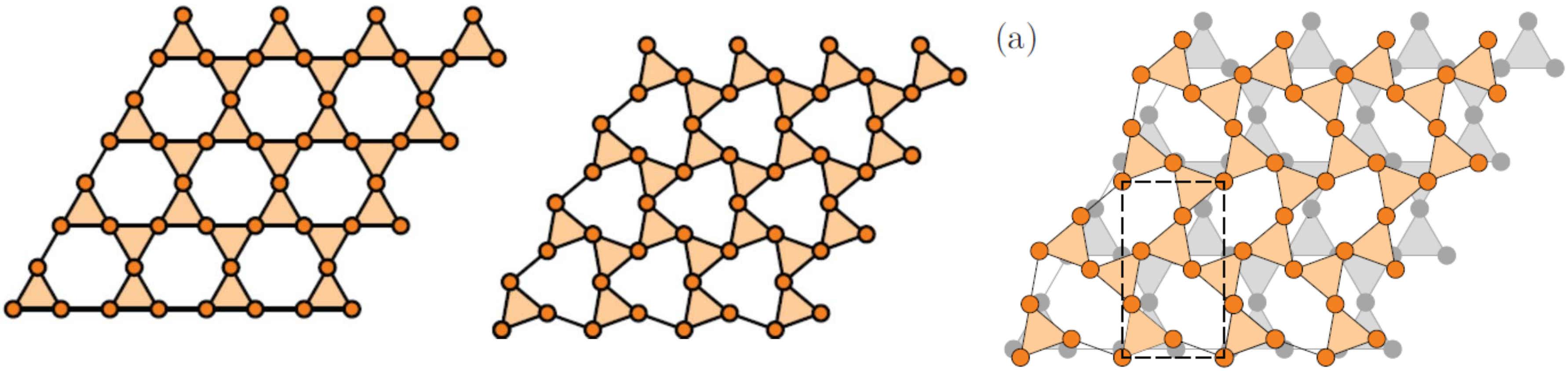
B. G. G. Chen, N. Upadhyaya, V. Vitelli
PNAS **111**, 13004-13009 (2014).

Topological Mechanics

Bryan Chen, Nitin Upadhyaya, Vincenzo Vitelli (Leiden) PNAS, **111**,13004,(2014)

2 D Maxwell Lattices: z=2d=4

Maxwell Lattice – one that under periodic boundary conditions have $z=2d$ exactly, i.e., $z=4$ in two-dimensions and $z=6$ in three dimension (Isostatic later)



Kagome Lattices

Topological States in Isostatic Lattices

$$\boxed{H = \frac{1}{2}kQQ^T \rightarrow \frac{1}{2}kQ(k)Q^{\dagger}(k)}$$

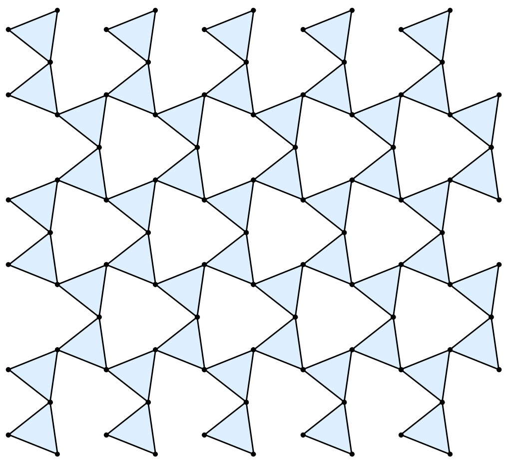
Not clear how to extract topological information from this: Introduce a model coupling sites to bonds. Remember that in the periodic case, $N_B = dN$, and Q is a square matrix.

$$\boxed{\mathsf{H} = k\begin{pmatrix} 0 & Q \\ Q^T & 0 \end{pmatrix}; \quad \mathsf{H}^2 = k^2\begin{pmatrix} QQ^T & 0 \\ 0 & Q^TQ \end{pmatrix}}$$

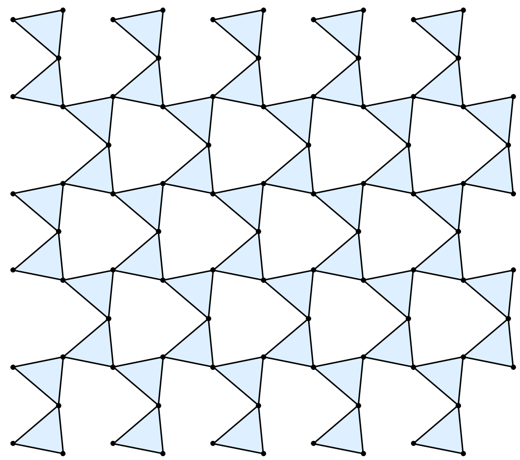
H^2 has the same spectrum as H, except for zero modes

Topological information is contained in Q. To get nontrivial topological states, constraint of equal-length (but not $z=4$) bonds must be relaxed.

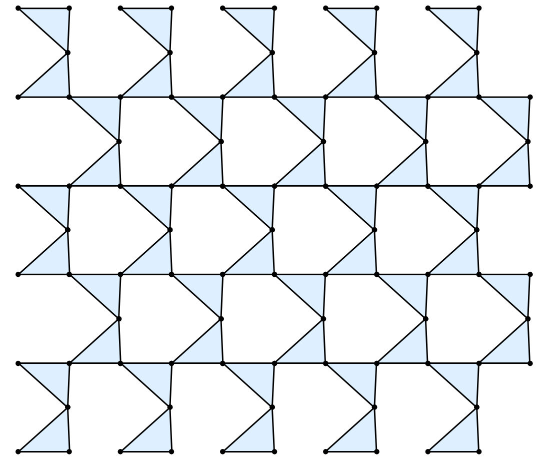
Transitions between Topological States



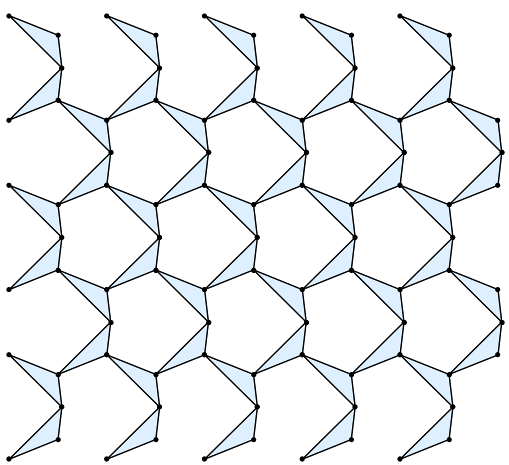
$\mathbf{P}_T = 0$



$\mathbf{P}_T = 0$

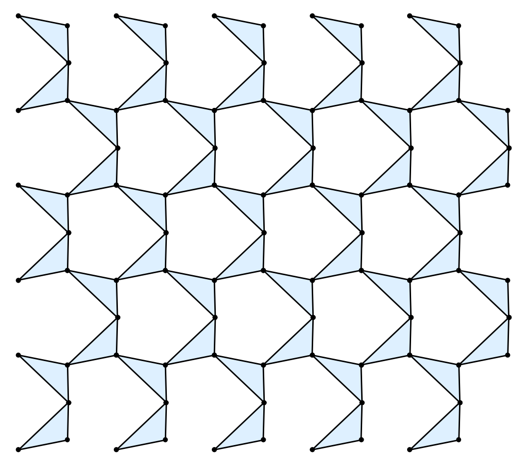


Transition state with states of self-stress



$\mathbf{P}_T = -\mathbf{a}_1$

Different topological states ,characterized by a polarization vector **P**$_T$ classes are separated by gapless states produced by states of self stress



$\mathbf{P}_T = -\mathbf{a}$

Polarizations

Choose symmetric unit cell;
Calculate Q

Place charge +2 at each site bond: zero net charge in unit cells; polarization is zero in symmetric cell

Topological Polarization

$$\nu_T = \frac{1}{V_{\text{cell}}}\int_{\partial S} d\mathbf{S}\cdot\mathbf{P}_T$$

$$\mathbf{P}_T = \frac{1}{V_{BZ}}\int_{BZ} d^2k\nabla_{\mathbf{k}}\,\mathrm{Im}\,\mathrm{Tr}\ln Q = \mathbf{R}_T = \sum_i n_i\mathbf{a}_i$$

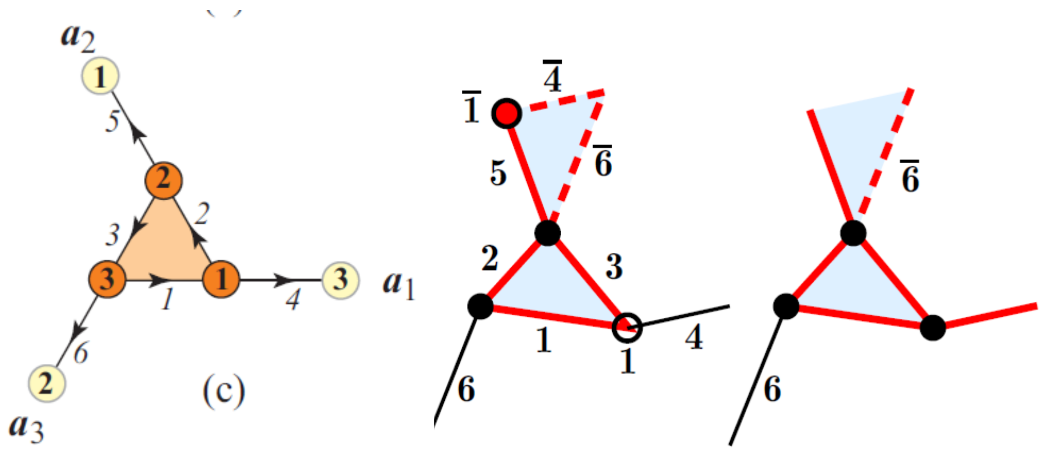
$$\nu_T = N_{\text{cell}}\mathbf{G}\,\mathbf{R}_T/2\pi; \quad \mathbf{G} = \sum_i k_i\mathbf{b}_i; \quad \mathbf{b}_i\,\mathbf{a}_j = 2\pi\delta_{ij}$$

$$\nu_L = N_{\text{cell}}\mathbf{G}\,\mathbf{P}_L/2\pi$$

$$\mathbf{P}_L = \mathbf{R}_L = \text{Polarization of surface cell}$$

$$= d\sum_{\text{sites } s}\Delta\mathbf{r}_s - \sum_{\text{bonds } b}\Delta\mathbf{r}_b$$

$$\nu = \nu_L + \nu_T = n_0 - s$$



$$1 \to \bar{1}: \text{ charge } 2 \to \mathbf{a}_2$$

$$4 \to \bar{4}: \text{ charge -1} \to \mathbf{a}_2$$

$$6 \to \bar{6}: \text{ charge -1} \to -\mathbf{a}_3$$

$$\mathbf{P}_L = 2\mathbf{a}_2 - (\mathbf{a}_2 - \mathbf{a}_3) = -\mathbf{a}_1$$

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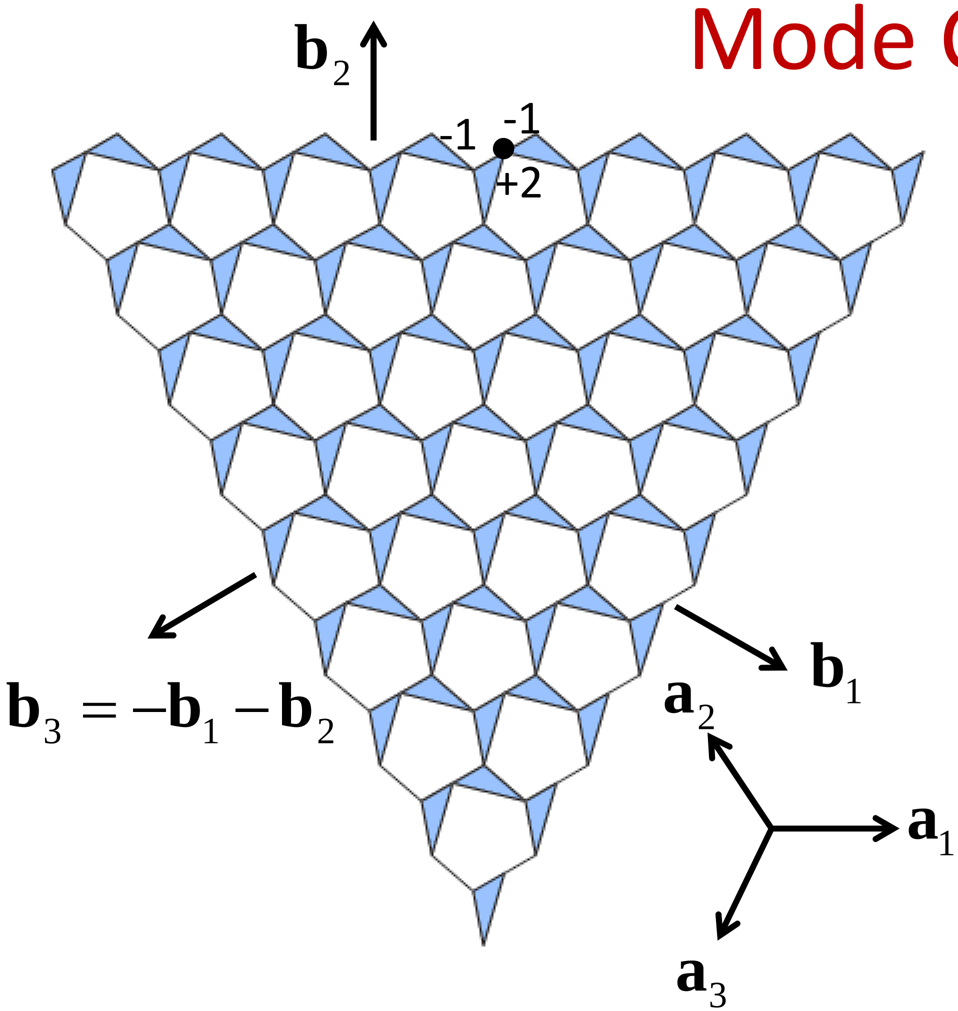
Mode Count



First recall $dN = N_B$. Assign charge +2 to each site and -1 to each bond (like Pebble game – Thorpe). The periodic lattice is charge neutral, but charge distribution within cells can have a dipole moment.

Spectrum is gapless with modes with frequency $\omega \sim q^2$

Define: $\nu = N_0 - S = dN - N_B$

$\nu = \nu_L + \nu_T$

$\nu_L =$ local count = surface charge

$\nu_T =$ Topological count

= "Polarization" charge

Symmetric and Surface Gauges

$$w_n = e^{i\mathbf{q}\cdot\mathbf{a}_n}; \quad S_n = w_n - 1$$

$$\det C_{\text{sym}} = g_1 S_2 S_3 + g_2 S_3 S_2 + g_3 S_1 S_2 + g_0 S_1 S_2 S_3$$

$$= a + \sum_{n=1}^{3} b_n w_n + \sum_{n=1}^{3} c_n w_n^{-1}$$

$$z_x = e^{iq_x x}; \quad z_y = e^{i\sqrt{3}q_y y/2}$$

$$w_1 = z_x; \quad w_2 = z_x^{-1/2} z_y; \quad w_2 = z_x^{-1/2} z_y^{-1}$$

$\Rightarrow$ One pole in z_y

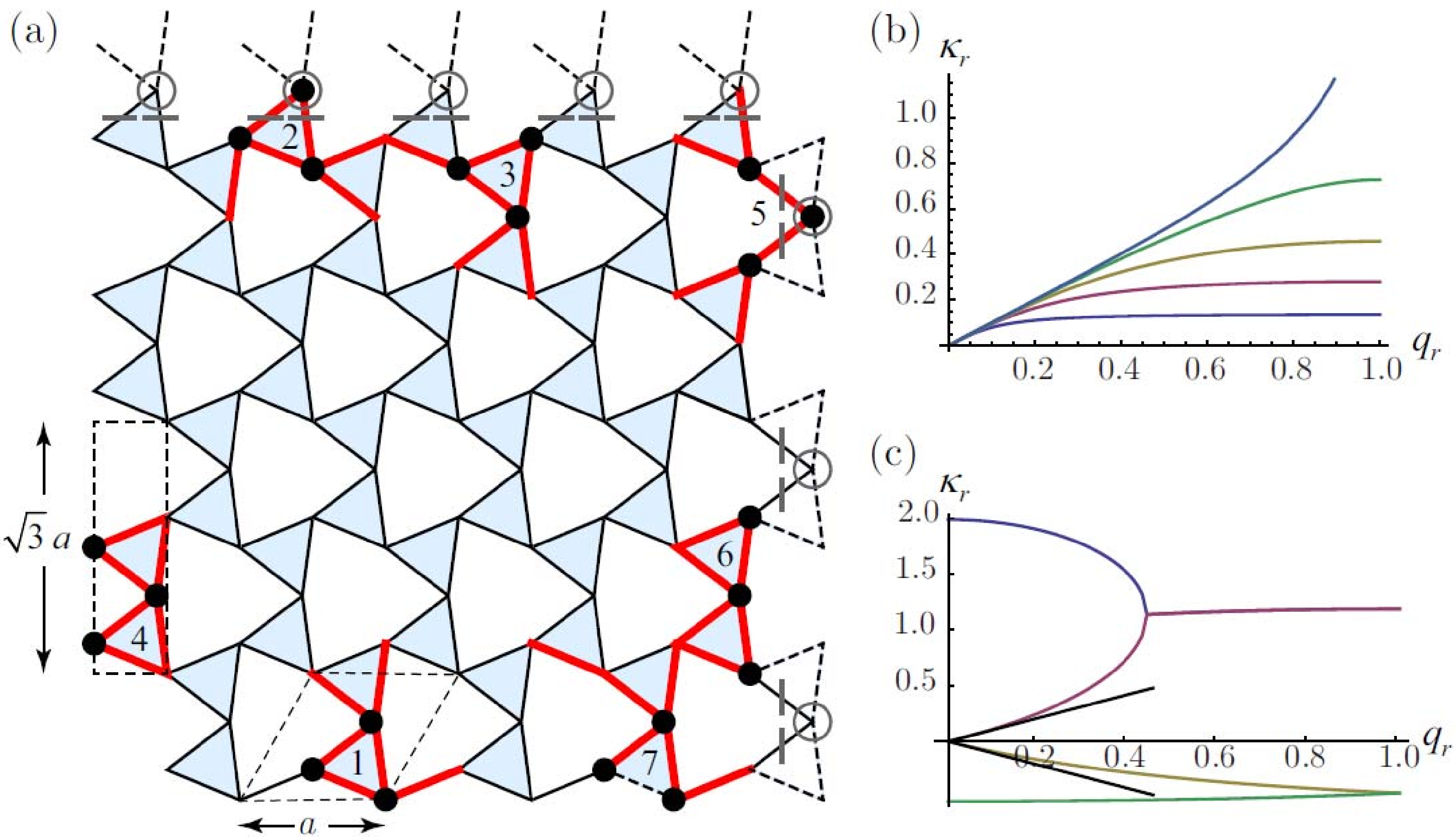
$$\det C_{\text{surf}} = e^{-i\mathbf{q}\cdot\mathbf{R}_L} \det C_{\text{sym}}$$

$\Rightarrow$ No poles, only zeros:

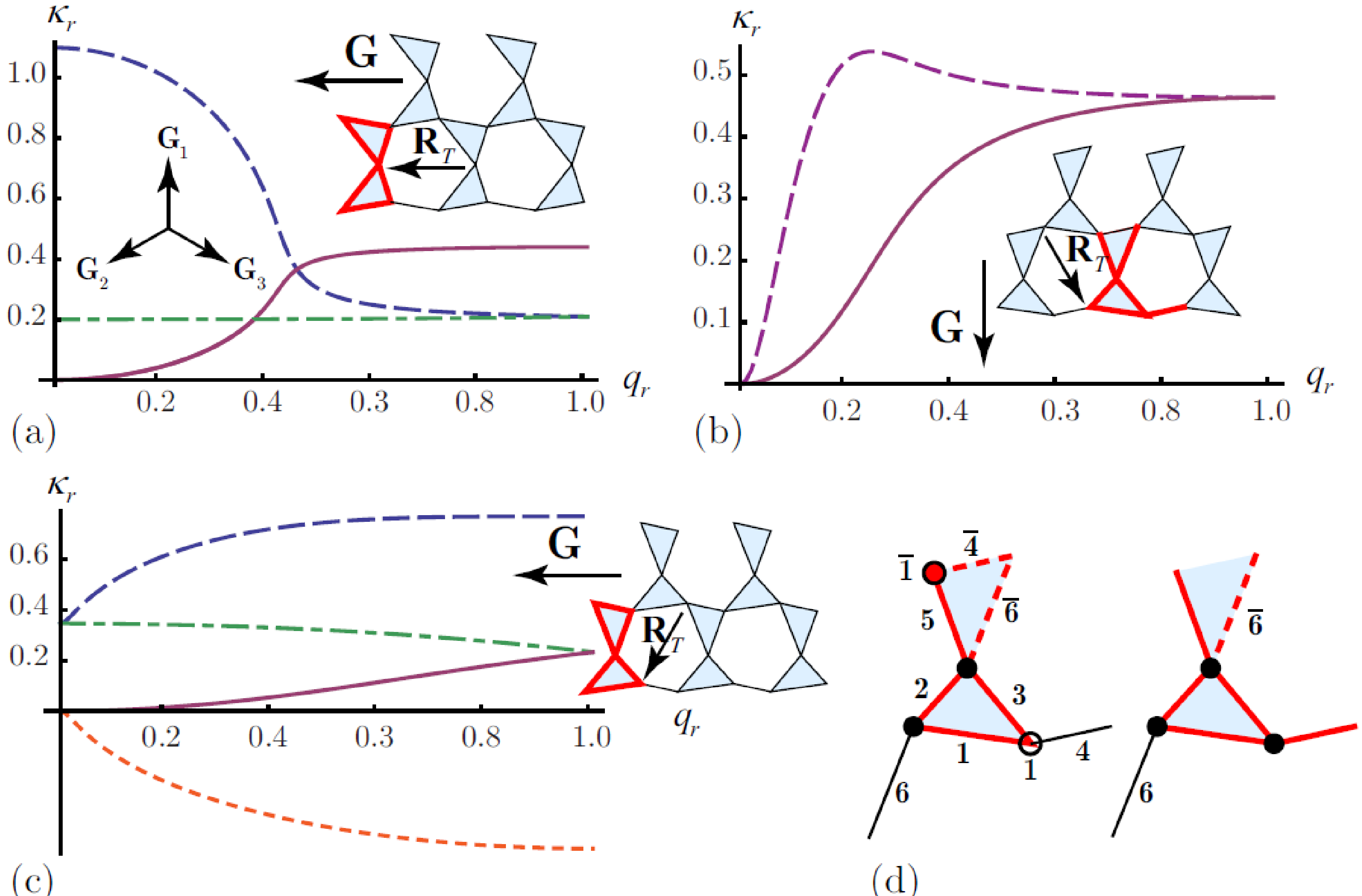
Topological charge of surface compatible unit cells simply counts the total number of zero modes at the surface!

Twisted Kagome Surface States

$$\boxed{\mathbf{P}_T = \mathbf{R}_T = 0}$$



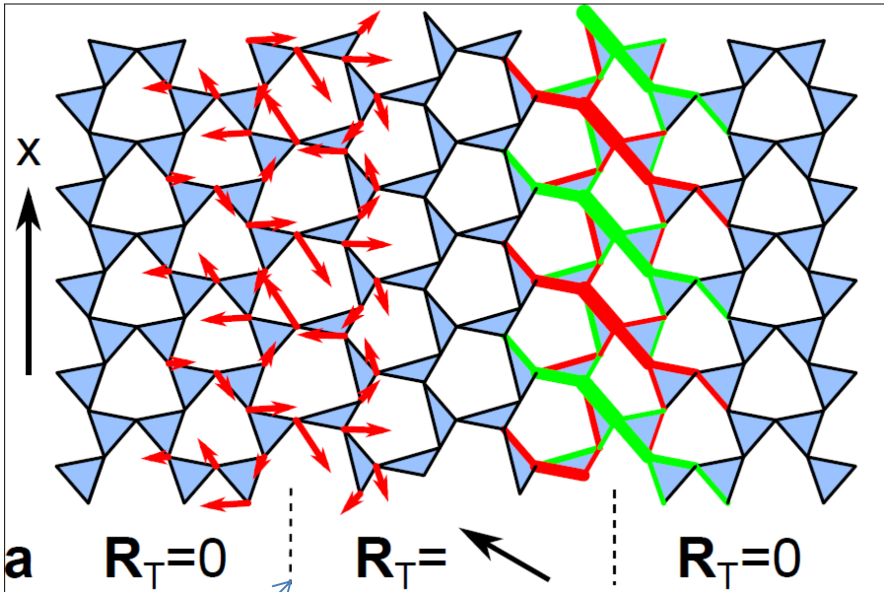
Topological Surface States

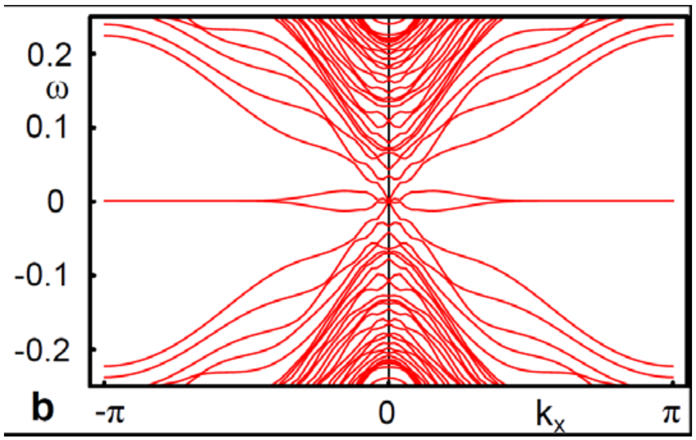


Non-zero R_T moves zero modes from one surface to the opposite one.

Domain Wall

$$\mathbf{G} = -\mathbf{b}_1 \qquad \mathbf{G} = -\mathbf{b}_1$$





$$\nu_T = \frac{\mathbf{G}\cdot(\mathbf{R}_T^l - \mathbf{R}_T^r)}{2\pi} = 1$$

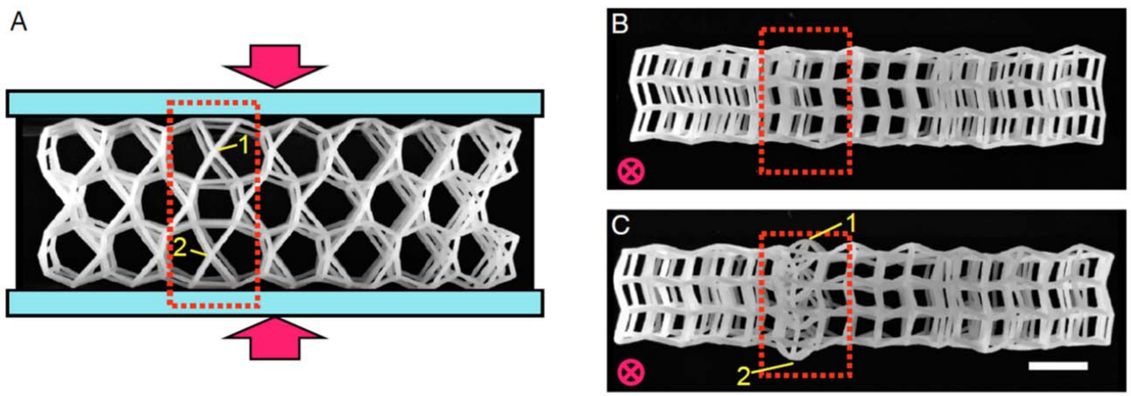
zero modes

$$\nu_T = \frac{\mathbf{G}\cdot(\mathbf{R}_T^l - \mathbf{R}_T^r)}{2\pi} = -1$$

States of Self Stres

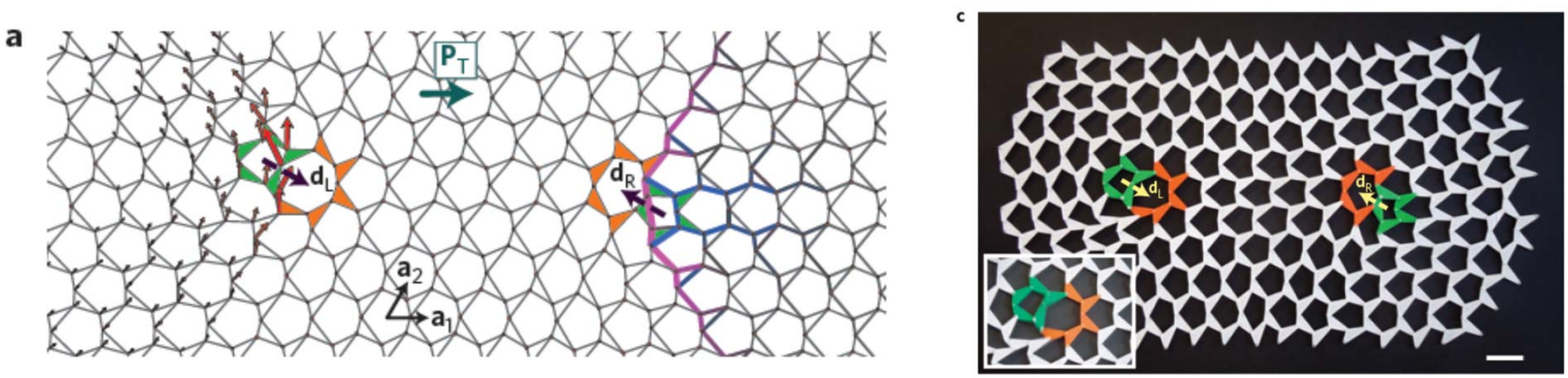
Modes of full H with zero modes from Q (States of self stress) and form Q^T (zero modes)

Stresses and zero modes at defects



Stress is concentrated at self-stress domain wall causing mechanical failure

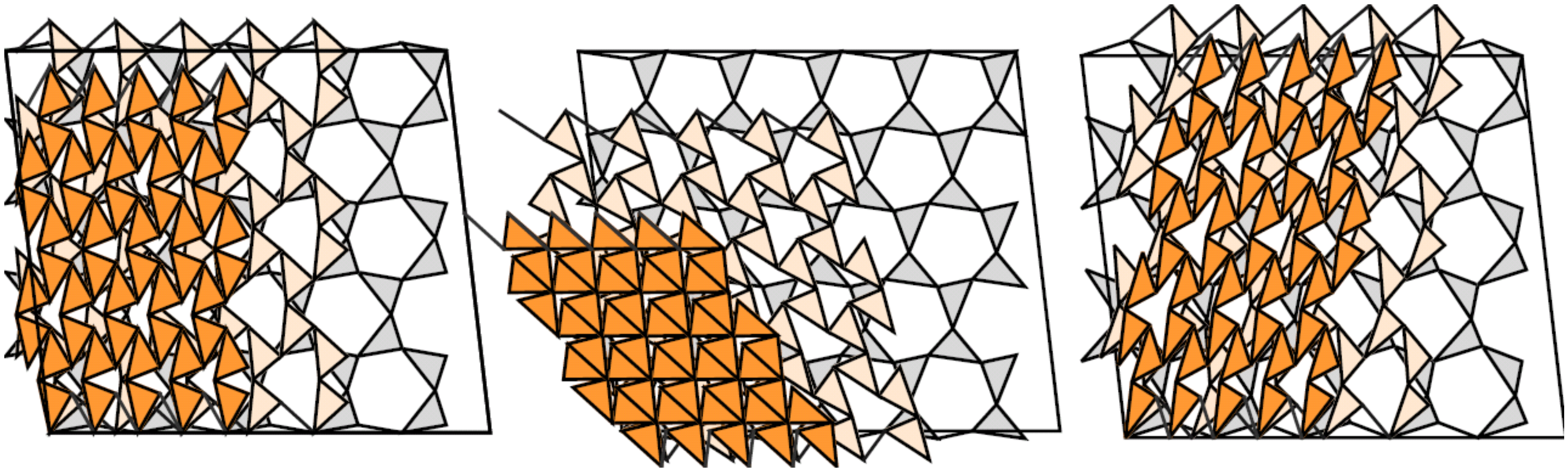
J. Paulose, B. G. G. Chen, V. Vitelli, *Nature Physics* **11**, 153-156 (2015).



Dislocations localize soft modes and self stress:

J. Paulose, A. S. Meeussen, V. Vitelli, PNAS **112**, 7639-7644 (2015)

Guest Modes



$$\mathbf{K} = \begin{pmatrix} K_{xxxx} & K_{xxyy} & K_{xxxy} \\ K_{xxyy} & K_{yyyy} & K_{yyxy} \\ K_{xxxy} & K_{yyxy} & K_{xyxy} \end{pmatrix}; \quad \mathbf{u}^G = \begin{pmatrix} u^G_{xx} & u^G_{xy} \\ u^G_{xy} & u^G_{yy} \end{pmatrix} \rightarrow \begin{pmatrix} u^G_{xx} \\ u^G_{yy} \\ u^G_{xy} \end{pmatrix}$$

Zeros to linear order in $\mathbf{q}$ if

$$q_y = \frac{q_x}{u^G_{xx}}\left(u^G_{xy} \pm \sqrt{-\det \mathbf{u}^G}\right)$$

Elastic Energy

$$\boxed{f = \tfrac{1}{2} K[(u_{xx} - a_1 u_{yy})^2 + 2a_4 u_{xy}^2]}$$

$$\boxed{\text{Soft Mode: } u_{xx} = a_1 u_{yy}}$$

$$\boxed{\det Q^T = A[k_x^2 + a_1 k_y^2 + ic(k_x^3 - 3k_x k_y^2)] + O(k^4)}$$

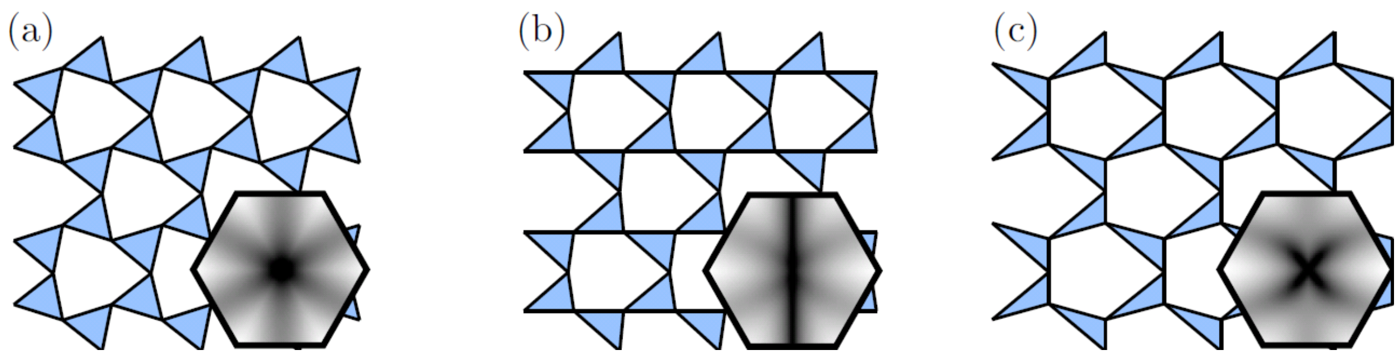
$a_1 > 0:$ Negative Poisson ratio and $\mathbf{R}_T = 0$;

$\det Q^T = O(k^2)$ near origin

$a_1 < 0:$ Positive Poisson ratio and $\mathbf{R}_T \neq 0$;

$\det Q^T = O(k^3)$ along $k_x = \pm\sqrt{a_1} k_y; \omega \sim k^2$

Show Mathematica animation!



$a_1 > 0$ $a_1 < 0$

Penn

Bulk Modes of Topological Lattices

$$\vec{k} = k_{\perp}\vec{n} + k_{||}\hat{z}\times\hat{n};\ \ \hat{n} = \text{Surface normal}$$

$$k_{\perp}^{\pm} = \frac{\sin\theta \pm i\sqrt{a_1}\cos\theta}{\cos\theta \mp i\sqrt{a_1}\sin\theta}k_{||} + \frac{i(3+a_1)d}{2(\cos\theta \mp i\sqrt{a_1}\sin\theta)^3}k_{||}^2$$

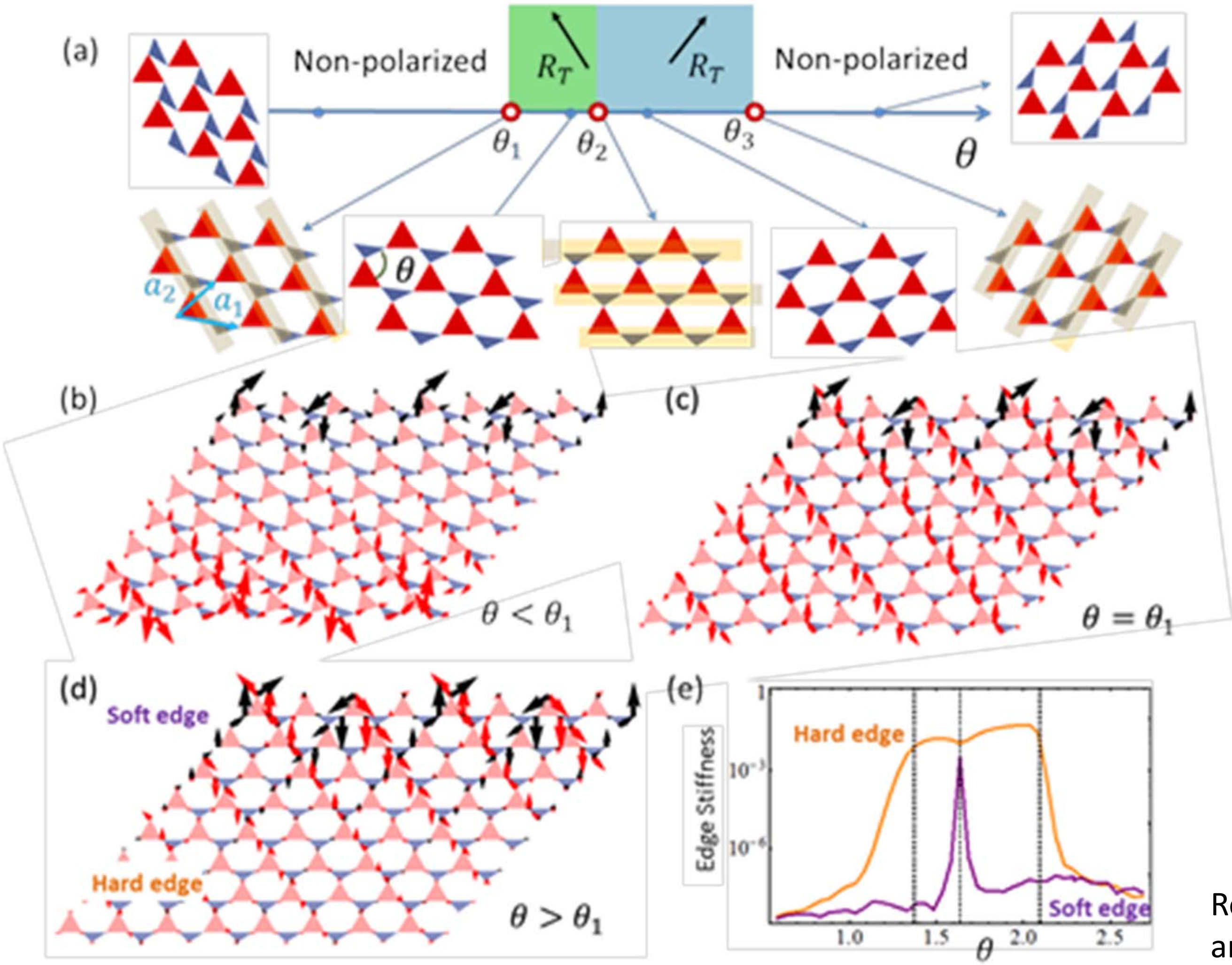
$a_1 > 0 : \mathrm{Im}k_{\perp}^{\pm} \sim \pm k_{||}$

Opposite signs on opposite surfaces

$a_1 < 0 : \mathrm{Im}k_{\perp}^{\pm} \sim k_{||}^2$

Number surface modes (1 or 2) depends on θ

Strain-shifted zero modes



Rocklin, Zhou, Sun, Mao, arXiv:1510.06389

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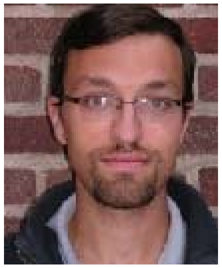
Topological Square Lattices

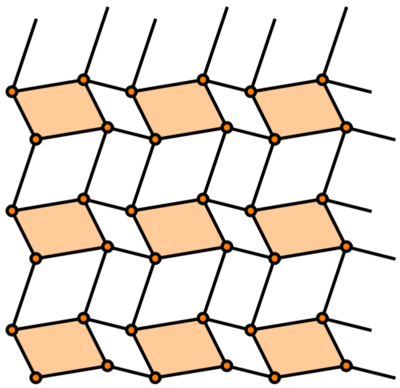


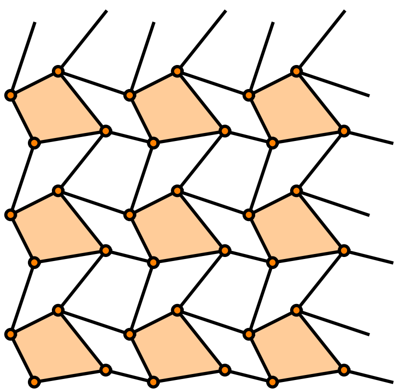
Zeb
Rocklin
Michigan

Bryan Chen
UMass

Vincenzo Vitelli
Leiden
+Martin Falk

D. Z. Rocklin, B. G.-g. Chen, M. Falk, V. Vitelli, TCL, *arXiv:1510.04970* (2015)

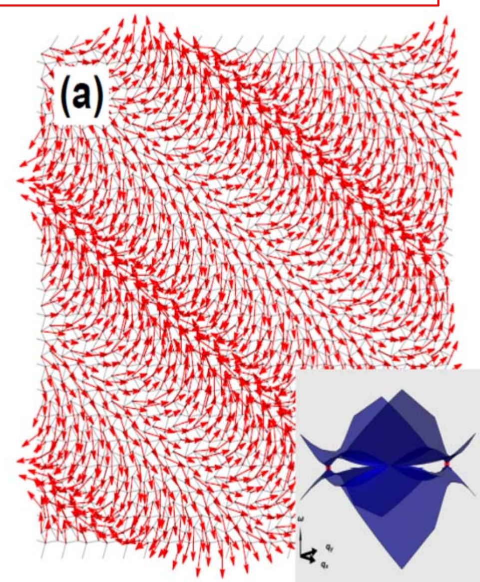




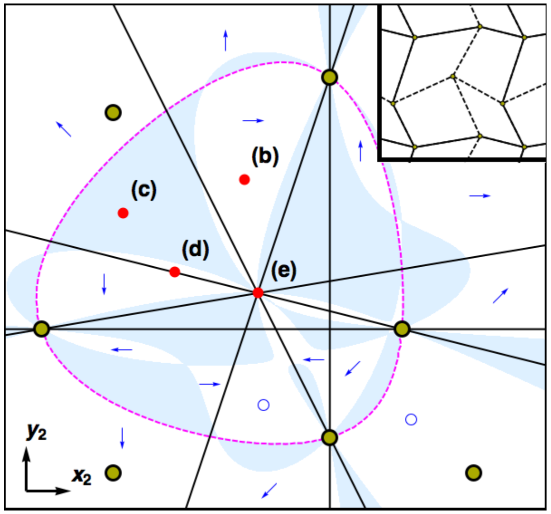
Two q=0 states of self stress but no elasticity.

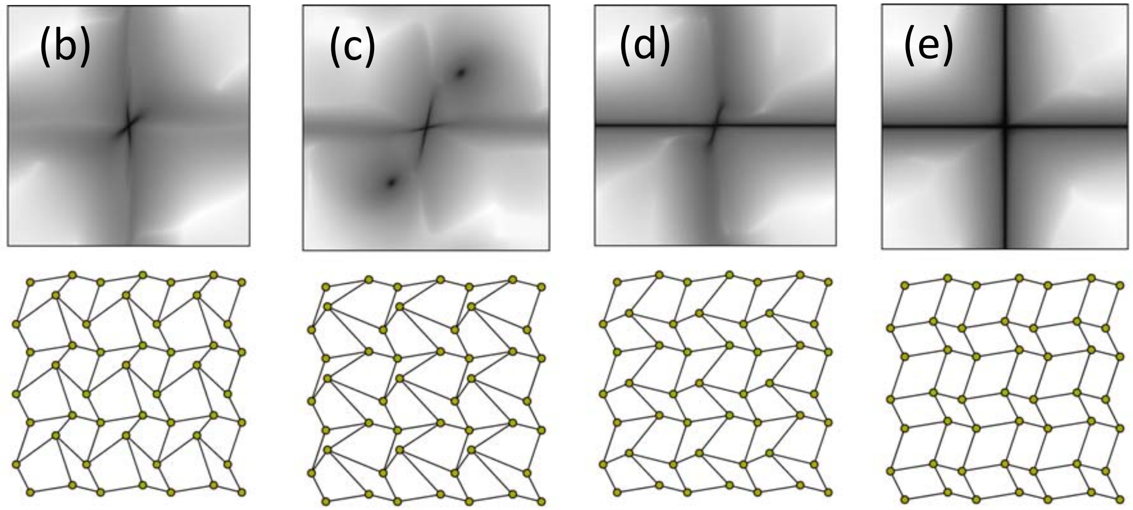
Weyl modes have interesting and non-trivial effect nonlinear dynamics (Bryan Chen) - Rule rather than exception for large unit-cell lattices

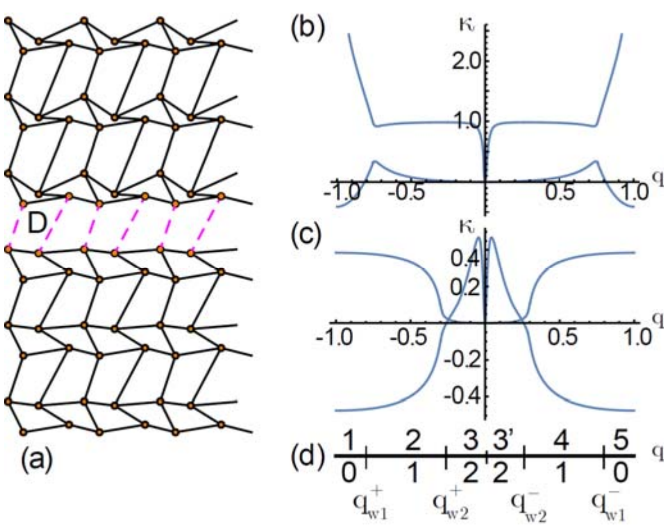
Topological lattice with zero (Weyl) modes at q \neq 0 (like graphene Dirac point) with non-zero winding number: Topological Polarization depends on surface q_s, and zero modes change surfaces with q_s. Sample traversing state of self stress when q_s corresponds to Weyl q.



Weyl Phase diagram and domain-wall zero modes







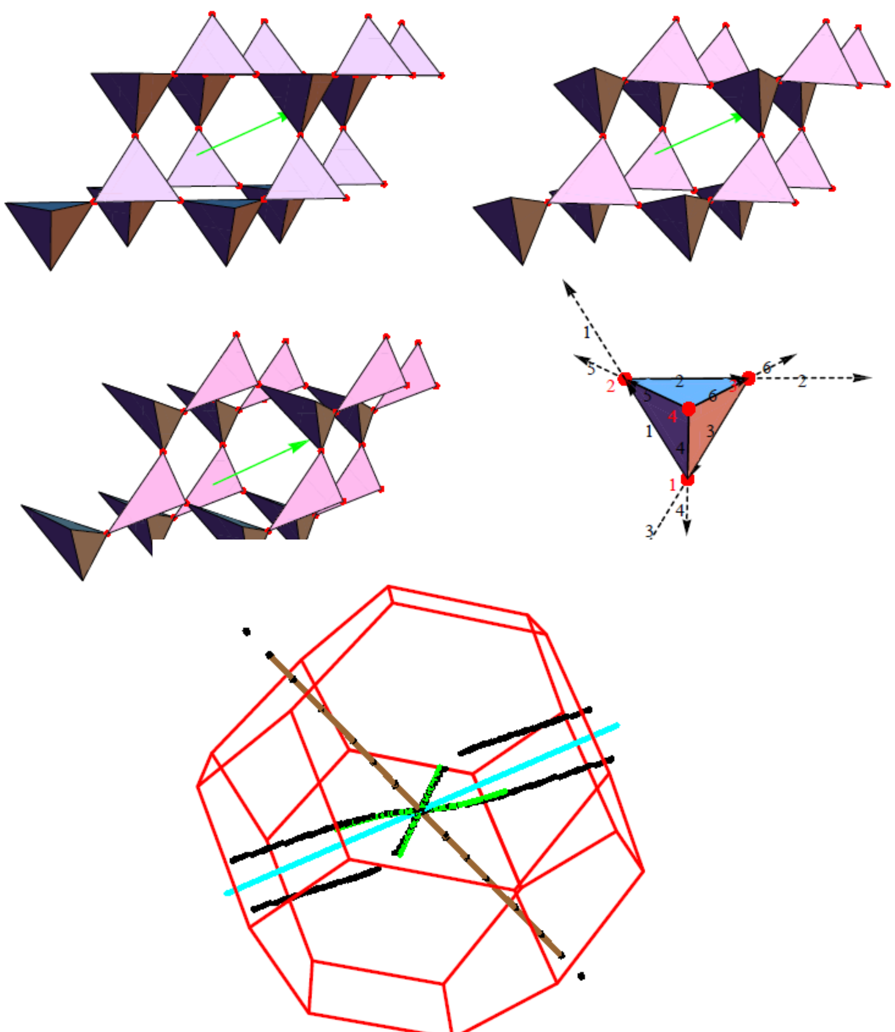
(b) In region without Weyl modes – like kagome
(c) Region with a pair of Weyl modes – enter at origin and disappear at zone edge
(d) Transition region – line of zero modes and SSS
(e) Double critical lines of zero modes and SSS in two diretions

$$n_0^{(U,L)}(q) = \text{ No. zero modes at } q \text{ on free upper (lower) surface}$$

$$n_B = \text{ No. of "binding bonds" added}$$

$$n_0^D(q) = n_0^U(q) + n_0^L(q) - n_B$$
$$= \text{No. of zero modes in DW}$$

Topological Pyrochlore Lattices



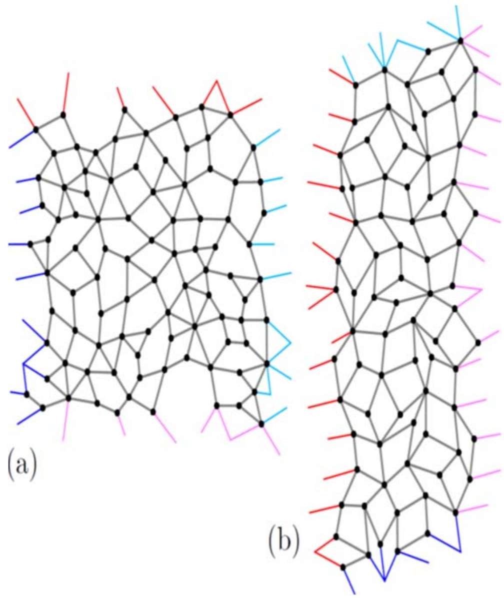
Olaf Stenull, CL Kane, TCL: Work in Progress

- Topologically distinct 3D phases, constructed following procedures developed for kagome lattices
- Weyl lines instead of Weyl points with associated transition of zero modes from one side of sample to other as Weyl lines are crossed.
- 3 zero modes at q=0: and 3 soft and 3 hard elastic directions (like origami).

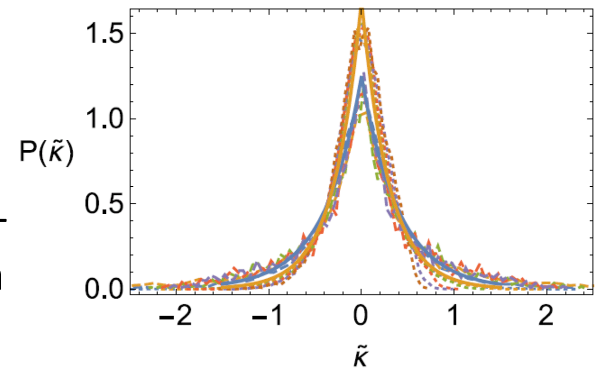
Weyl points at jamming

(a) Jammed Maxwell Lattice

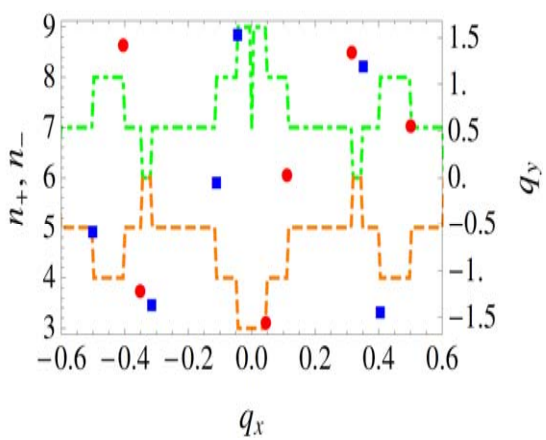
(b) Randomized quasicrystal approximate



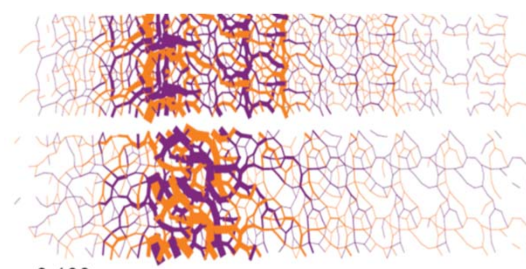
Probability distribution of inverse penetration depth: + on right, - on left

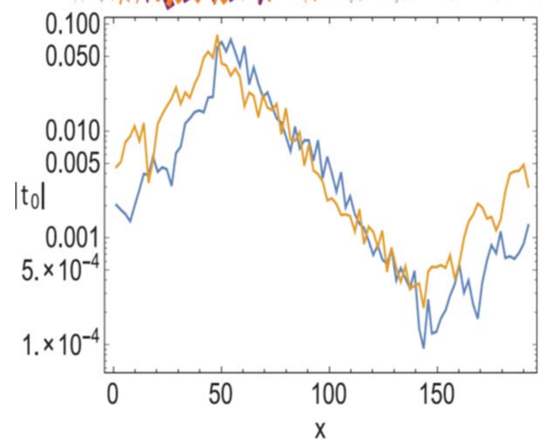


No. of zero modes on two surfaces and positions of Weyl modes.



Two independent states of self stress at domain wall dividing two jammed Maxwell lattices

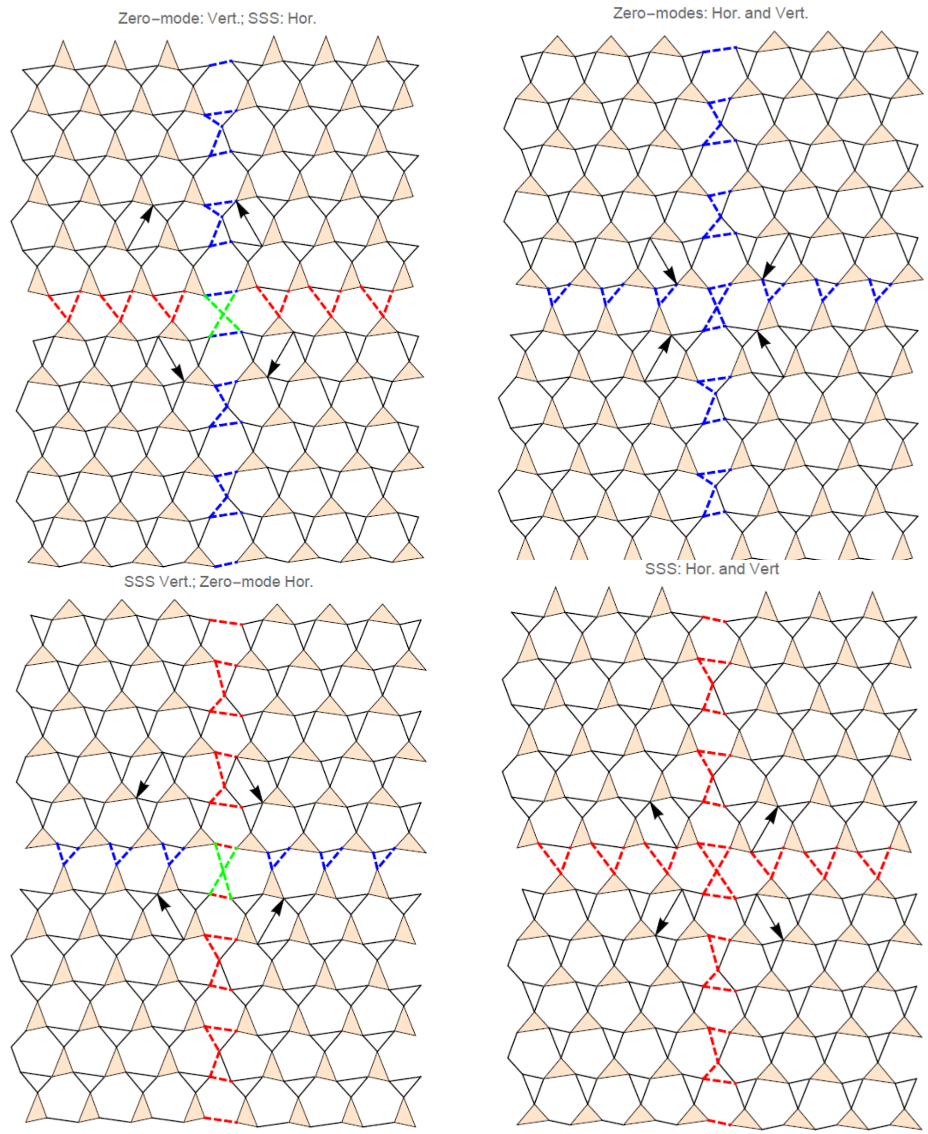




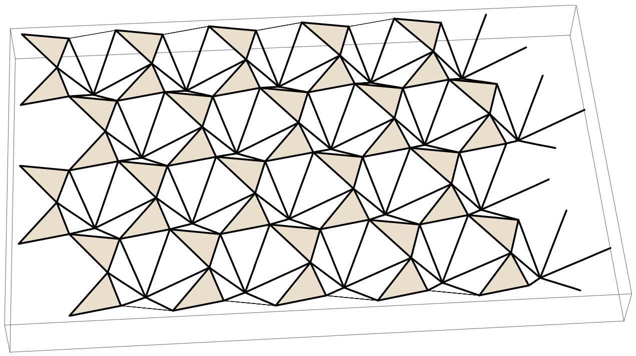
Large antagonistic unit cells

Red: wall of states of self stress

Blue: Zero energy domain wall



Origami – In Progress



Thanks to Chris Santangelo and Bryan Chen

d=3; n=4; n_b=12; dn-n_b =0: A Maxwell lattice

- Twisted kagome and “topological” versions gapped – apparently no topological distinction between two
- 3 states of self stress and 3 zero modes at q=0: 3 soft “elastic modes” that involve 2d elasticity and change in “thickness” of membrane (zz-strain). Relax latter: One soft mode of inplane distortion, like flat kagome.
- Effective elastic energy has Helfrich bending energy (up-down symmetry is broken) and strain curvature coupling (suggestive of Ron Resch)

In Progress

- Nonlinear response: Weyl Modes and their interactions with Guest Modes; Elastic and periodic Weyl modes mix producing interesting instabilities. (B. Chen, Z. Rocklin, V. Vitelli, TCL. Extend to 3D Weyl lines (O. Stenull, TCL)
- Real systems: Perfect physical Maxwell lattices do not exist. They either have bending forces between bonds at vertices or effective further neighbor interactions, but these interactions can be small in engineered materials. How does turning on small NNN or bending forces modify elastic response and zero modes (X. Mao, O. Stenull, Shu Yang, TCL) :
  - Long-wavelength: (d-1) Rayleigh modes on each surface; Shorter wavelengths; crossover to behavior similar to Maxwell lattice behavior but with low-frequency surface modes
  - Domain-wall modes develop a finite frequency and become localized propagating phonons: Domain wall acts like a wave guide. Can we control phonon propagation by controlled placement of domain walls
  - Self-stress domain walls concentrate stress [Paulose, Meeussen,Vitelli PNAS **112**, 7639-7644 (2015)] . Can we control these stresses and places at which material breakdown occurs?

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