Intertwining construction of flat bands

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T. Mizoguchi, H. Katsura, I. Maruyama, and
Y. Hatsugai, Phys. Rev. B **104**, 035155 (2021)

Institute for Physics of Intelligence

Trans-Scale Quantum Science Institute

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Outline

1. Introduction & Motivation
   - What are flat bands
   - My recent activity
2. Intertwining relation
   - Graph theory in a nutshell
   - ADE Dynkin diagrams
   - Graph intertwiner
3. Application to flat bands
   - Decorated honeycomb lattice
   - Decorated Haldane model
   - Decorated diamond lattice in 3D and 4D
4. Summary

What are flat bands

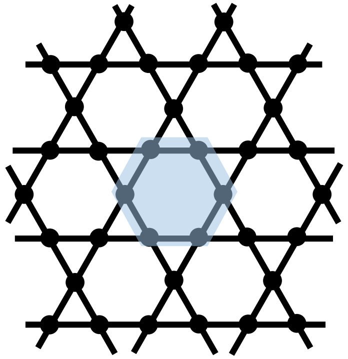
- Single-particle Schrödinger equation
  - It may happen that there exists an energy eigenvalue with *macroscopic degeneracy*.
  - Flat band: space of states spanned by these degenerate eigenstates
- Examples
  - Continuous space: Landau levels
  - Lattice: Kagome, pyrochlore, …
  - Old subject… Weaire-Thorpe, Phys. Rev. B **4** (1971)
- What are they good for?
  - Kinetic energy is quenched
  - Interesting playground for studying correlation physics
    Fractional quantum Hall effect, ferromagnetism, superconductivity, …

$$\hat{H}\psi = \epsilon\psi$$

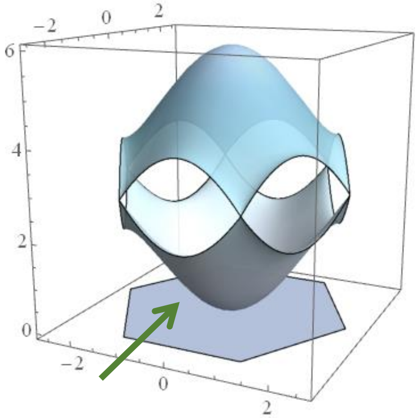
$$\lim_{V\to\infty} \frac{deg.}{V} = r > 0$$

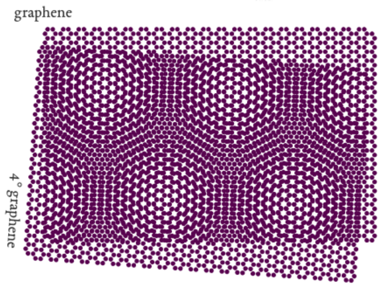
$deg.$: degeneracy
V : volume

Kagome lattice



Band structure



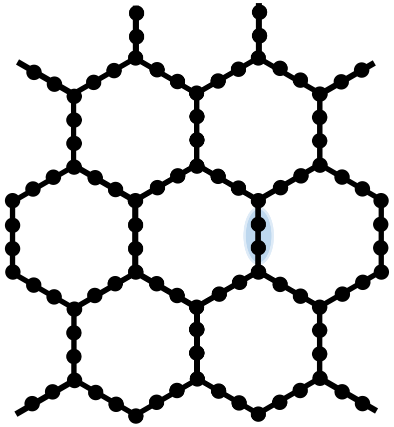


From Wikipedia

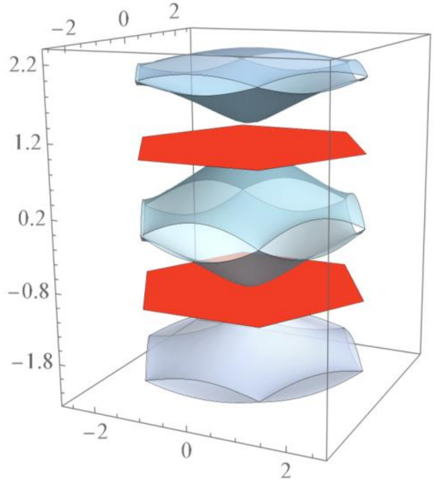
Today's subject

- How to construct tight-binding models with flat bands?
  - Various constructions
    - Line-graph construction: Mielke
    - Cell construction: Tasaki, (recent extension: Hatsugai, Mizoguchi)
    - Imbalance-type: Sutherland, …
    - Resonance-type: Katsura-Maruyama, …
  - What is the *mathematical* structure behind them?
- Intertwining relation
  - Two matrices A and $\tilde{A}$
  - $AC = C\tilde{A}$
  - A and $\tilde{A}$ have common eigenvalues
  - Covers many known examples
- Applications to tight-binding models

Decorated honeycomb



Band structure



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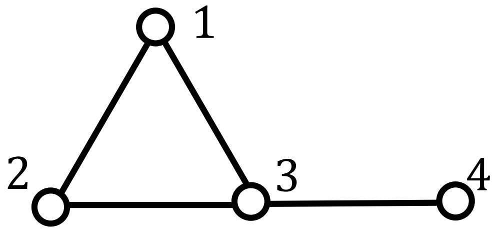
Graph Theory in a nutshell

Math.	Phys.
graph	lattice
vertex	site
edge	bond/link

- Graph $G(V, E)$
  - A pair of *V*, a set of vertices, and *E*, a set of edges
  - Sometimes called *undirected graph* $(i,j) = (j,i)$
- Example
  - 4-site graph



$$V = \{1,2,3,4\}$$
$$E = \{(1,2),(1,3),(2,3),(3,4)\}$$

- Adjacency matrix $A(G)$
  - $i, j \in V$ are said to be *adjacent* if there exists $(i,j) \in E$
  - Matrix elements

$$a_{i,j} = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

$$A(G) = \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \end{array} \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array}$$

  - Spectrum of *A(G)* is an important characteristic of *G*!

$$\mathrm{spec}(A(G)) = \{-1.48..., -1, 0.31..., 2.17...\}$$

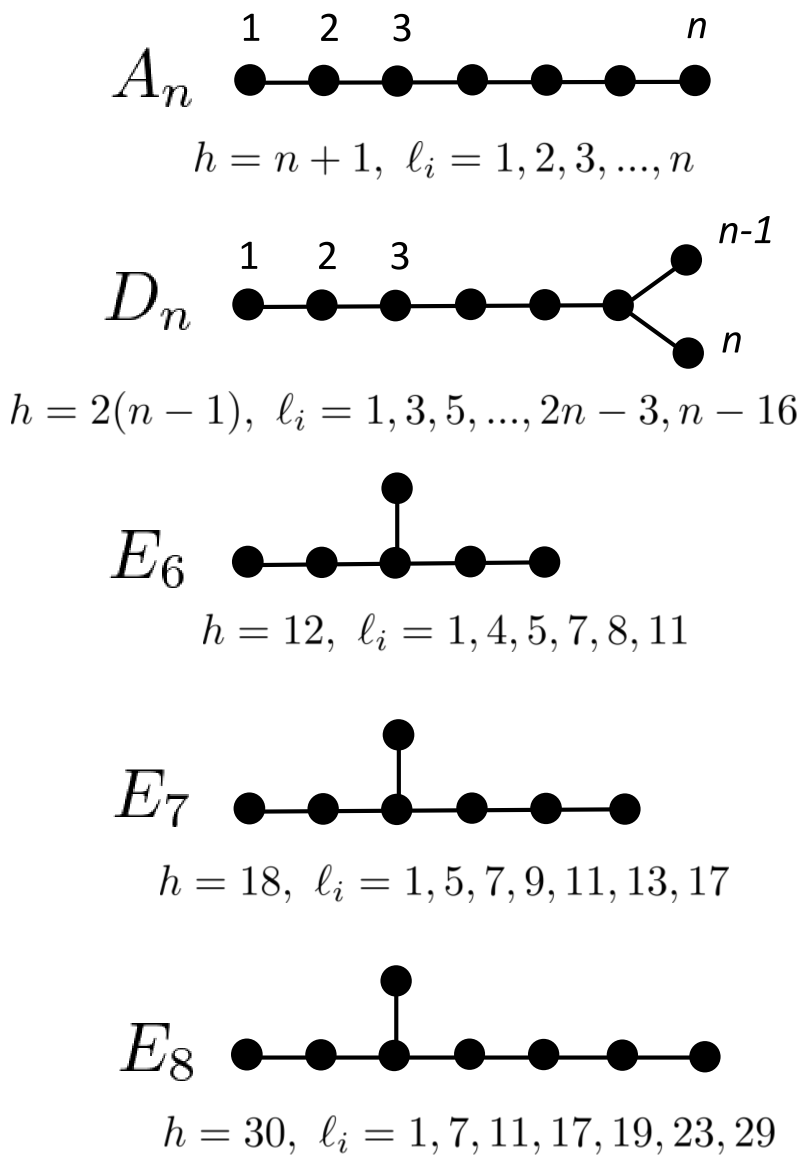
ADE Dynkin diagrams

- Ubiquitous in Math. and Phys.
  - Classification of semisimple Lie algebras
  - Classification of modular invariant partition functions of 2d CFT
  - Perron-Frobenius eigenvector of $A(G)$ → Solution of Yang-Baxter eq.
- Miraculous property
  - Spectrum of adjacency matrix

$$\lambda_i = 2\cos\left(\frac{\pi \ell_i}{h}\right) \qquad \begin{array}{ll} h: & \text{Coxeter number} \\ \ell_i: & \text{exponents} \end{array}$$

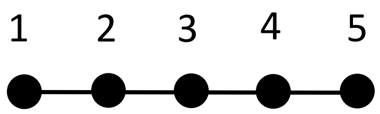
  - Eigenvectors can also be obtained analytically. They are written solely by trigonometric functions.

Why common eigenvalues for different graphs?



Example: $A_5 \leftrightarrow D_4$

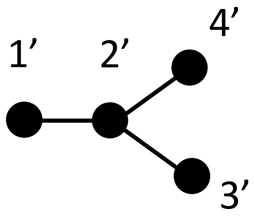
Graph | Adjacency matrix | eigenvalues



$$A(A_5) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\lambda = 0, \pm 1, \pm\sqrt{3}$$

They share eigenvalues



$$A(D_4) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

$$\lambda = 0, 0, \pm\sqrt{3}$$

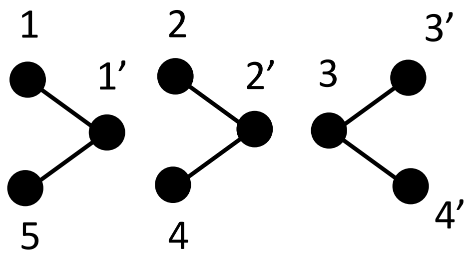
- Intertwining relation

$$A(A_5)\, C = C\, A(D_4)$$

$$C = \begin{array}{c c} & \begin{array}{cccc} 1' & 2' & 3' & 4' \end{array} \\ & \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \end{array}$$

  - C: graph intertwiner

P. A. Pearce & Y-K. Zhou, Int. J. Mod. Phys. B**7**, 3649 (1993)



Can construct C for any $(A_n, D_{\frac{n+3}{2}})$

Graph intertwiner

- Common eigenvalues
  - Let A and $\tilde{A}$ be adjacency matrices.
    If there exists $C \neq O$ such that $AC = C\tilde{A}$, *Intertwining relation*
    then $\mathrm{spec}(A) \cap \mathrm{spec}(\tilde{A}) \neq \emptyset$.
  - Proof) Suppose $\boldsymbol{v}$ is an eigenvector of $\tilde{A}$ with eigenvalue λ.
    Then $C\boldsymbol{v}$ is an eigenvector of A with eigenvalue λ,
    provided that $C\boldsymbol{v} \neq \mathbf{0}$.

$$A(C\boldsymbol{v}) = C\underbrace{\tilde{A}\boldsymbol{v}}_{= \lambda\boldsymbol{v}} = \lambda(C\boldsymbol{v})$$

    Since $C \neq O$, there is at least one eigenvector of $\tilde{A}$ which is not annihilated by C.

- Generalization: A and $\tilde{A}$ may not necessarily be adjacency matrices.

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Tight-binding model

- Lattice (Graph) $G(V,E)$ Can be infinite
- Single-particle Schrödinger equation $$\sum_{j\in V} t_{i,j}\varphi_j = \epsilon\varphi_i, \quad \forall i \in V$$
- Hopping matrix

$$T = (t_{i,j})_{i,j\in V}$$

  - Hermitian matrix
  - $t_{i,j} \neq 0 \quad \text{if } (i,j) \in E$
  - Generalization of adjacency matrix

- Spectrum of *T*
  - Assume translation invariance.
  - (Discrete version of) Bloch theorem:

$$\varphi_{\boldsymbol{k}}(\boldsymbol{r}_\alpha + \boldsymbol{R}) = e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\varphi_{\boldsymbol{k}}(\boldsymbol{r}_\alpha)$$

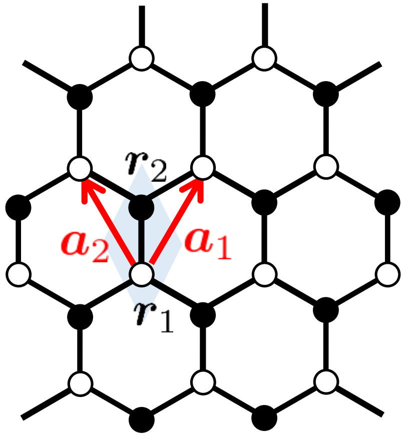
$\boldsymbol{k}$: crystal momentum

$\boldsymbol{r}_\alpha$: position within unit cell

$\alpha = 1, 2, ..., n$

$\boldsymbol{R} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$

Graphene

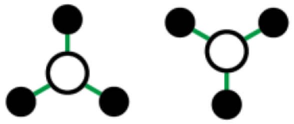


  - Diagonalization boils down to that of $n\times n$ matrix

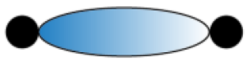
$$H(\boldsymbol{k}) = \begin{pmatrix} 0 & tf(\boldsymbol{k}) \\ tf^*(\boldsymbol{k}) & 0 \end{pmatrix} \quad f(\boldsymbol{k}) = 1 + e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_1} + e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_2}$$

Decorated honeycomb lattice (1)

- Motivation
  - *α*-graphyne
    - Each edge of graphene is replaced with -C≡C-.
      Baughman, Eckhardt, Kertesz, J. Chem. Phys. **87**, 6687 (1987)
  - 1*T*-TaS_2
    - Transition metal dichalcogenide with CDW order
    - Metallic network inside CDW domains
      Lee, Geng, Park, Oshikawa, Lee, Yeom, Cho,
      Phys. Rev. Lett. **124**, 137002 (2020)
- (Our) Terminology & convention
  - Linker

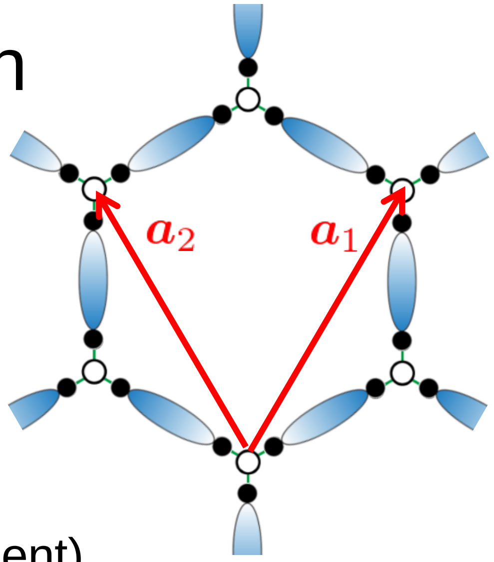


  - Linkage



  - Primitive translation vectors

$$\boldsymbol{a}_1 = (1/2, \sqrt{3}/2), \boldsymbol{a}_2 = (-1/2, \sqrt{3}/2)$$



Assume uniform hopping (for the moment)

Decorated honeycomb lattice (2)

- Hamiltonian in momentum space
  - (3q+2) × (3q+2) marix

$$H(\boldsymbol{k}) = \begin{pmatrix} 0 & t\boldsymbol{x}_q^T & t\boldsymbol{x}_q^T & t\boldsymbol{x}_q^T & 0 \\ t\boldsymbol{x}_q & H_{\mathrm{mol}} & O_q & O_q & te^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_1}\boldsymbol{y}_q \\ t\boldsymbol{x}_q & O_q & H_{\mathrm{mol}} & O_q & te^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_2}\boldsymbol{y}_q \\ t\boldsymbol{x}_q & O_q & O_q & H_{\mathrm{mol}} & \boldsymbol{y}_q \\ 0 & te^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_1}\boldsymbol{y}_q^{\mathrm{T}} & te^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_2}\boldsymbol{y}_q^{\mathrm{T}} & t\boldsymbol{y}^{\mathrm{T}} & 0 \end{pmatrix}$$

$$\boldsymbol{x}_q = (1, \overbrace{0, \ldots, 0}^{q-1})^{\mathrm{T}}$$

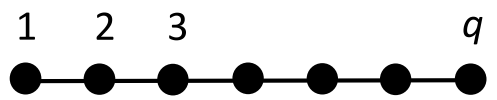
$$\boldsymbol{y}_q = (\overbrace{0, \ldots, 0}^{q-1}, 1)^{\mathrm{T}}$$

$$O_q : \ q \times q \text{ zero matrix}$$

- Molecular Hamiltonian for linkage
  - $q \times q$ matrix (independent of $\boldsymbol{k}$)

$$H_{\mathrm{mol}} = \begin{pmatrix} 0 & t & & & \\ t & 0 & t & & \\ & t & 0 & \ddots & \\ & & \ddots & \ddots & t \\ & & & t & 0 \end{pmatrix} = tA(A_q)$$

A_q



- Eigenvalues and eigenvectors are known explicitly

$$\epsilon_n = 2t\cos\left(\frac{\pi n}{q+1}\right), \quad n = 1, 2, \ldots, q$$

Flat-band energies = Eigen-enegies of H_{mol}

- Intertwining relation

$$H(\boldsymbol{k})C(\boldsymbol{k}) = C(\boldsymbol{k})H_{\mathrm{mol}}$$

  - Intertwiner
    $(3q+2)\times q$ matrix

$$C(\boldsymbol{k}) = \begin{pmatrix} \overbrace{0 \ \cdots \ 0}^{q} \\ [\boldsymbol{\lambda}(\boldsymbol{k})]_1 I_q \\ [\boldsymbol{\lambda}(\boldsymbol{k})]_2 I_q \\ [\boldsymbol{\lambda}(\boldsymbol{k})]_3 I_q \\ 0 \ \cdots \ 0 \end{pmatrix}$$

$I_q : \ q \times q$ identity matrix

$$\boldsymbol{\lambda}(\boldsymbol{k}) = \begin{pmatrix} 1 - e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_2} \\ -1 + e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_1} \\ -e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_1} + e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_2} \end{pmatrix}$$

Orthogonal to

$$(1,1,1)^{\mathrm{T}}, \ (e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_1}, e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{a}_2}, 1)^{\mathrm{T}}$$

- Implications
  - Multiple flat bands!

$$\epsilon_n = 2t\cos\left(\frac{\pi n}{q+1}\right), \quad n = 1, 2, \ldots, q$$

  - Eigenvectors $(\boldsymbol{k} \neq \boldsymbol{0})$

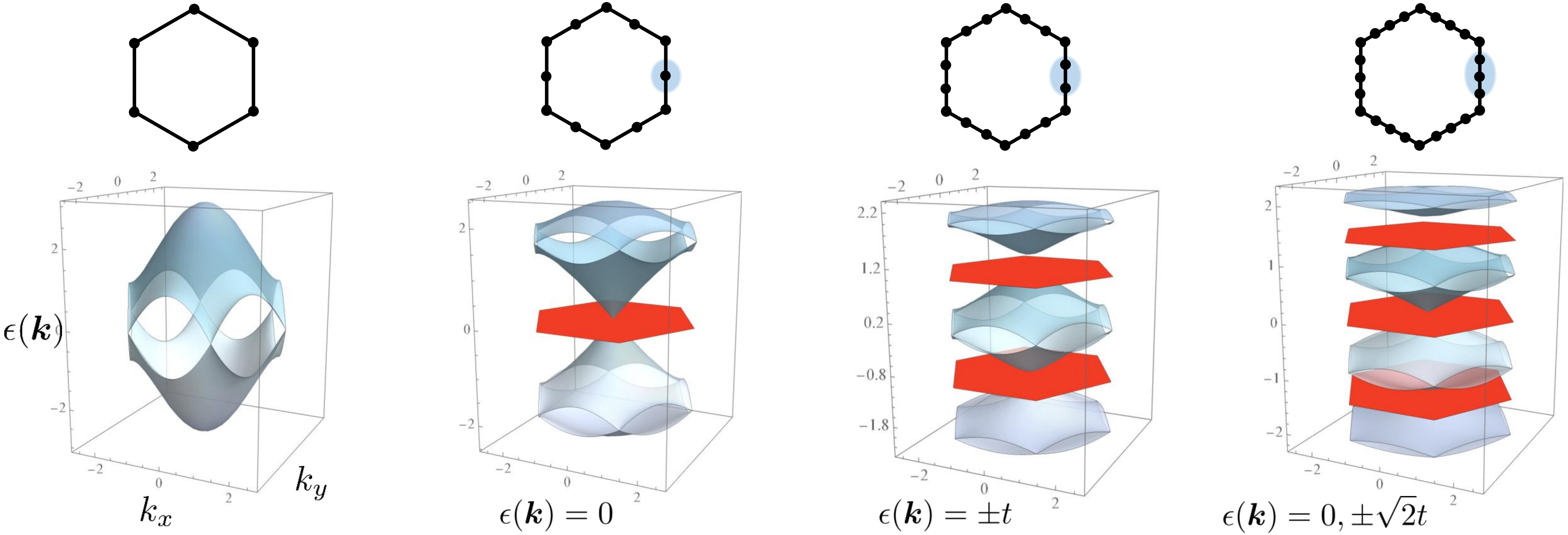
$$\psi_n(\boldsymbol{k}) = \frac{1}{\mathcal{N}_n(\boldsymbol{k})} C(\boldsymbol{k})\phi_n$$

$\mathcal{N}(\boldsymbol{k}) : \ $ Normalization const.

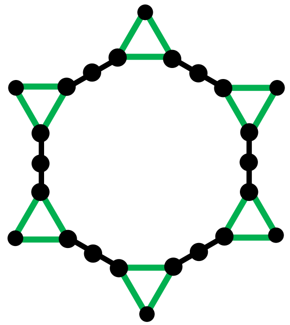
$\phi_n : \ n-$th eigenvector of H_{mol}

Examples

- q=0
- q=1
- q=2
- q=3



- Band touching occurs at $\boldsymbol{k}$=0 (at which $C(\boldsymbol{k})$=0)
- Combining the idea of line graph, one can also study decorated kagome lattice (related to COF, e.g., triptycene)



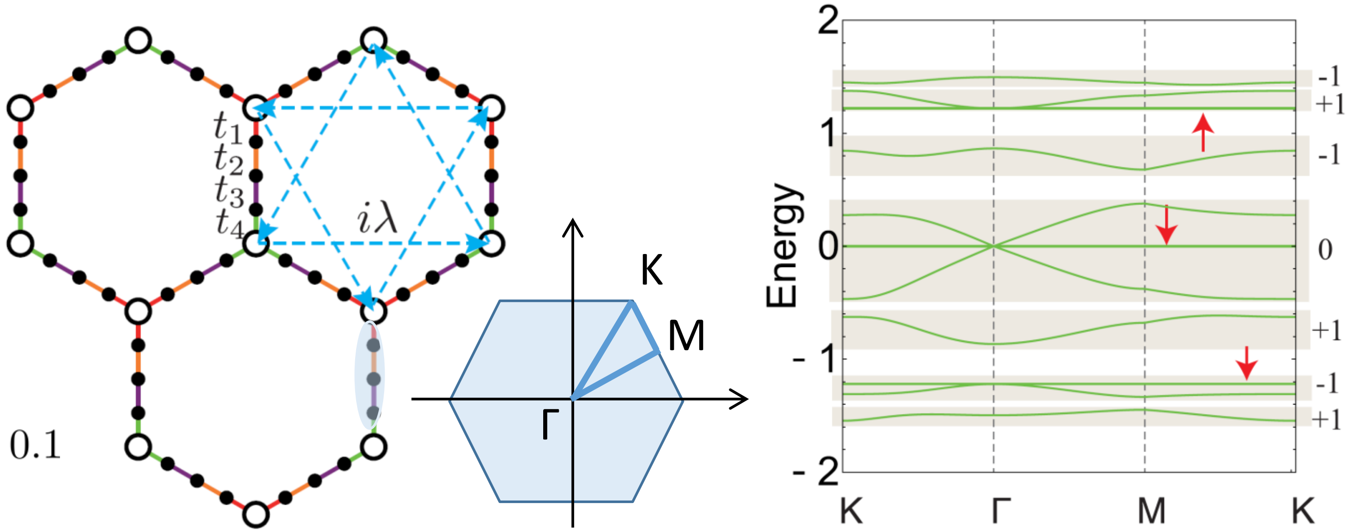
Mizoguchi et al., Phys. Rev. Mater. **3**, 114201 (2019).

Other applications

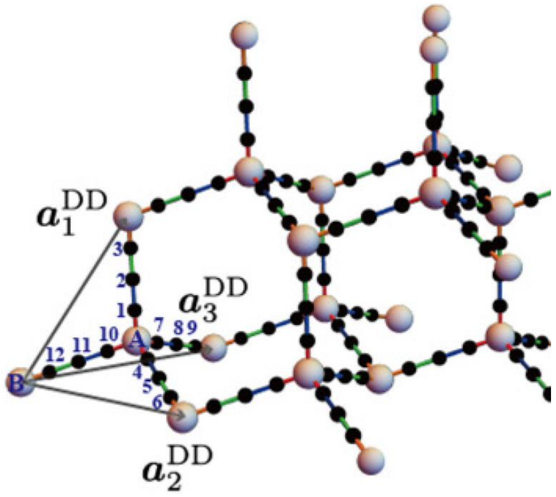
- Decorated Haldane model
  - Toy model for integer quantum Hall effect

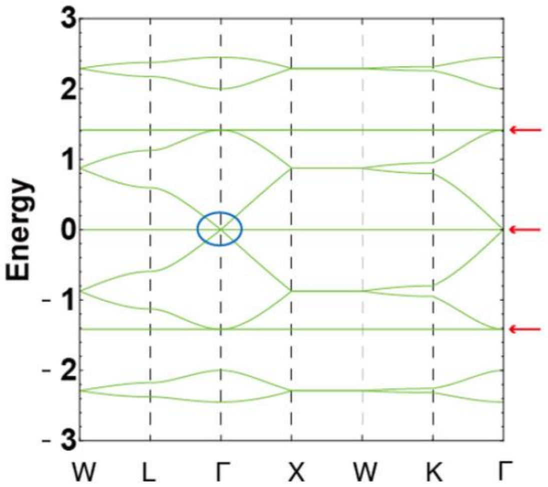
    Haldane, Phys. Rev. Lett. **61**, 2015 (1988).
  - Parameters

    $t_1 = 0.5,\ t_2 = 0.7,\ t_3 = 1.0,\ t_4 = 0.5,\ \lambda = 0.1$

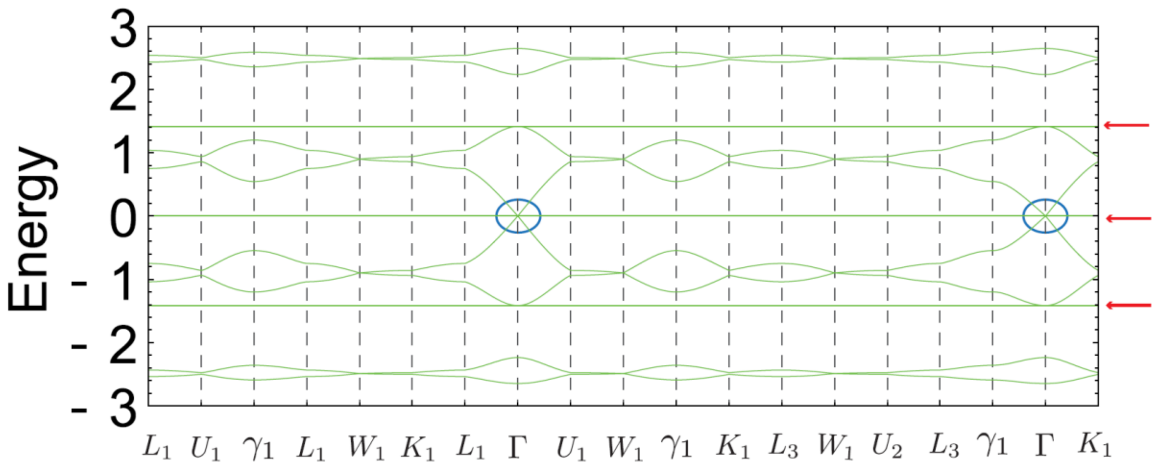


- Decorated diamond lattice (q=3)



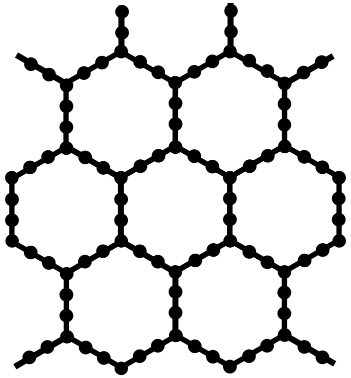


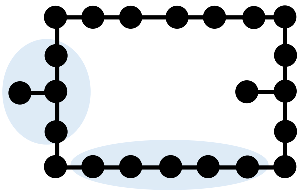
- 4D decorated diamond (q=3)



Summary

- Intertwining relation $AC = C\tilde{A}$
- Applicable to finite and infinite graphs
- Underlying mechanism behind flat bands
  - Decorated honeycomb lattices
  - Decorated diamond lattices in 3D, 4D, …





Future directions

- Inhomogeneous generalizations?
  - Possible in some cases, e.g., q=1 decorated honeycomb
- What abut the effect of interactions?
  - Localized "exciton" states?
- Intertwining relation in many-body systems?