A graph-theoretic characterization of free-fermion-solvable spin models

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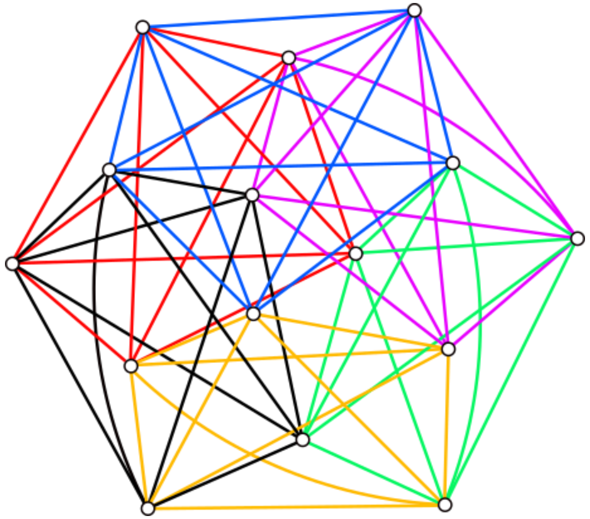
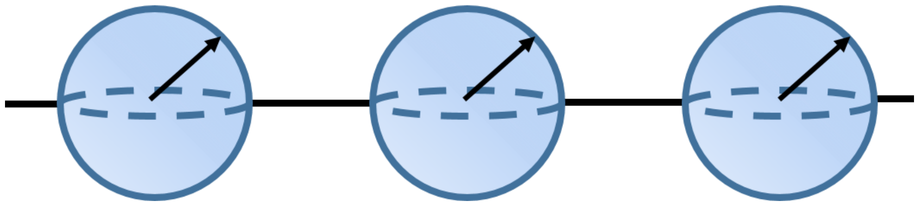
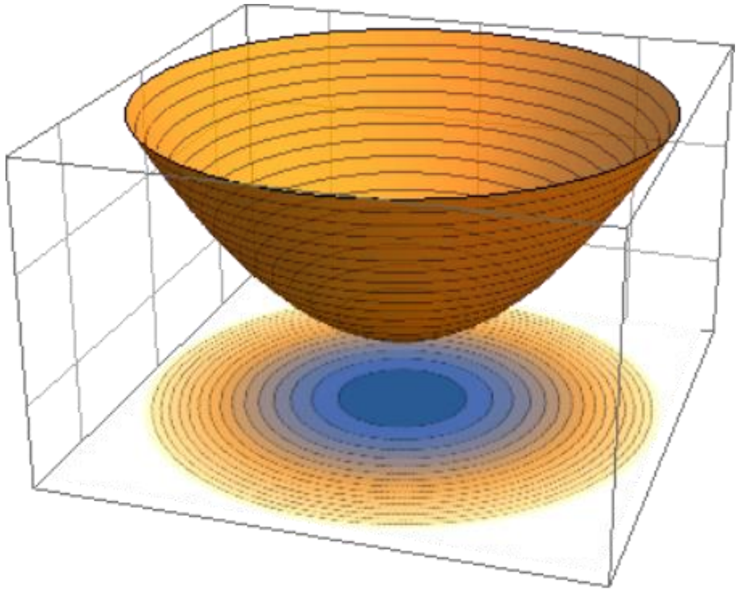


Motivation – Exact solutions for spin models

- Mapping to free-fermions is a workhorse method
    - Mathematically elegant.
    - Starting point for perturbation theory
- Rich connection to complexity
    - Matchgate circuits [1-4]
    - FKT algorithm [5-7]
    - Sensitivity conjecture [8,9]
- Graph theory plays a central role.



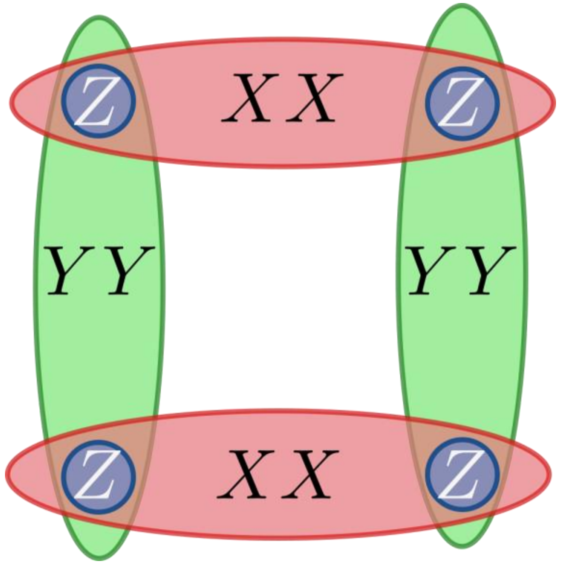


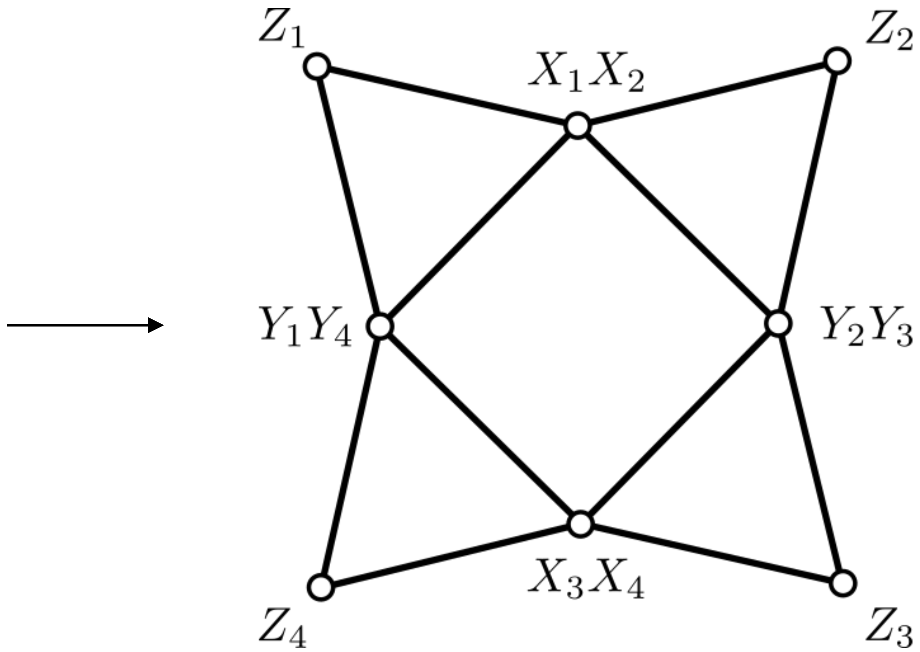
[1] B.M Terhal and D.P. DiVincenzo, PRA **65**, 032325 (2002).
[2] S. Bravyi. PRA **73**, 042313 (2006).
[3] R. Jozsa and A. Miyake, *Proc. R. Soc. A* **464**, 3089-3106 (2008).
[4] D. J. Brod and A.M. Childs, *Quantum Info. Comput.* **14**, 901 (2014).
[5] P. W. Kasteleyn. *Physica*, **27**(12):1209 – 1225, 1961.
[6] H. N. V. Temperley and M. E. Fisher. *The Philosophical Magazine: A Journal of Theoretical Experimental and Applied Physics*, **6**(68):1061–1063, 1961.
[7] L. Valiant. *SIAM J. Computing* **31**:4, 1229-1254, 2002. L. Valiant. *SIAM J. Computing* **37**:5 1565-1594, 2007.
[8] H. Huang. arXiv:1907.00847 [math.CO] (2019).
[9] Y. Gu and X.-L. Qi. arXiv:1908.06322 [cond-mat.stat-mech] (2019).

Graphs of Hamiltonians

A **graph** $G = (V, E)$ consists of sets $\begin{cases} V & \text{vertices} \\ E \equiv \{(i,j) \mid i,j \in V\} & \text{edges} \end{cases}$

$$H = \sum_{j=1}^{n/2} (X_{2j-1}X_{2j} + Y_{2j}Y_{2j+1}) + \sum_{j=1}^{n} Z_j$$



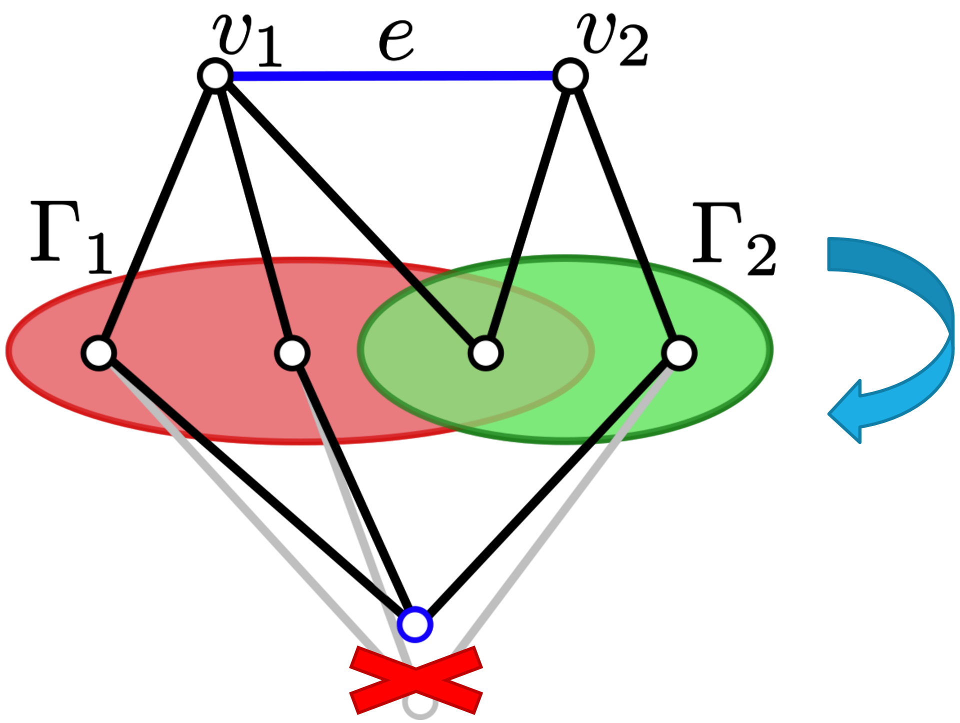


The **anti-compatibility graph** of a Hamiltonian has vertices corresponding to Pauli terms, which are neighboring if corresponding Paulis anticommute.

Anti-Compatibility Graphs – A “Game of Life”

Given a graph $G = (V, E)$, for every edge $(v_1, v_2) \in E$:

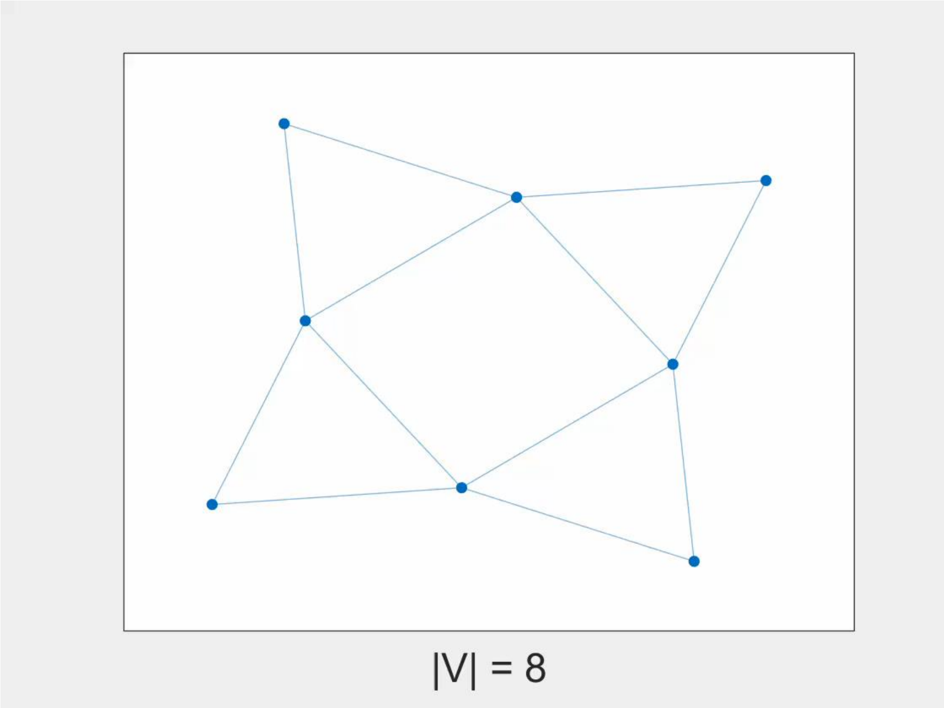
1. Add a vertex whose neighbors are vertices neighboring exactly one of either v_1 or v_2.
2. Do not add a vertex if there is already a vertex with the same neighbors.
3. Repeat until no more vertices can be added.



Anti-Compatibility Graphs – A "Game of Life"

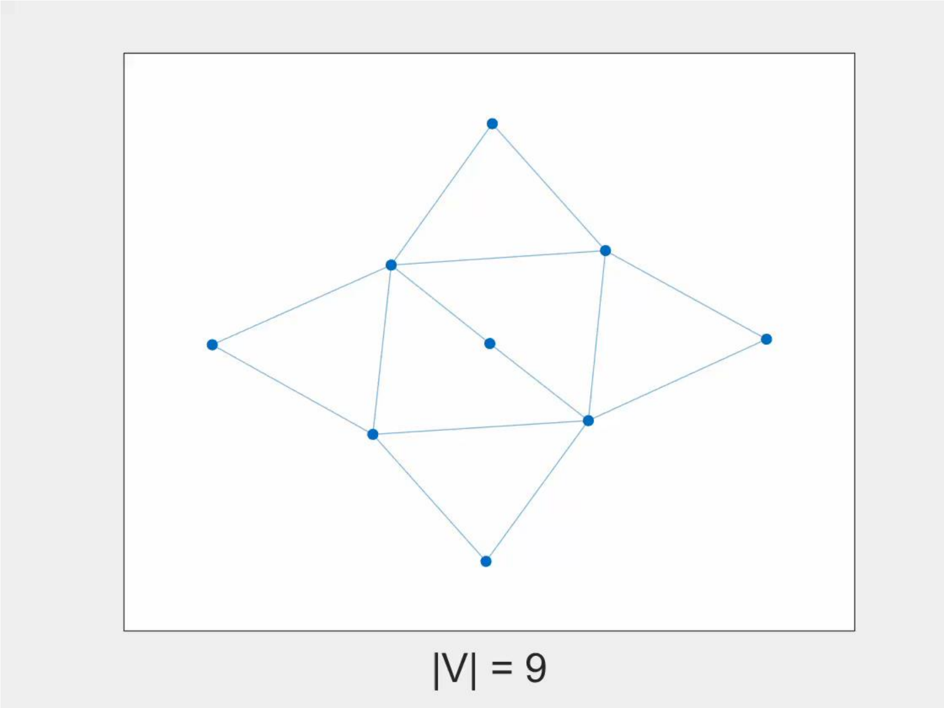
Solvable

$$H_{\text{int}} = \sum_{j=1}^{n/2} (X_{2j-1}X_{2j} + Y_{2j}Y_{2j+1}) + \sum_{j=1}^{n} Z_j$$



Not Solvable

$$H_{\text{nint}} = \sum_{j=1}^{n/2} (X_{2j-1}X_{2j} + Y_{2j}Y_{2j+1}) + \sum_{j=1}^{n} Z_j + Z_1 Z_2$$



Somehow these graphs know the difference!

Free Fermions

Consider the “solvable” case:

$$H_{\text{int}} = \sum_{j=1}^{n/2} (X_{2j-1}X_{2j} + Y_{2j}Y_{2j+1}) + \sum_{j=1}^{n} Z_j$$

Apply the **Jordan-Wigner Transformation [10]**
$$\begin{cases} c_{2j-1} = Z^{\otimes(j-1)} \otimes X_j \otimes I^{\otimes(n-j)} \\ c_{2j} = Z^{\otimes(j-1)} \otimes Y_j \otimes I^{\otimes(n-j)} \end{cases}$$

Canonical anticommutation relations $\{c_\mu, c_\nu\} \equiv c_\mu c_\nu + c_\nu c_\mu = 2\delta_{\mu\nu} I$

Hamiltonian terms are quadratic in the Majorana operators

$$\begin{array}{rl} Z\,Z\,Z\,Z\,Y\;I\,I\,I\,I & c_{10} \\ \text{x}\;\; \underline{Z\,Z\,Z\,Z\,Z\,X\,I\,I\,I} & c_{11} \\ i\,I\;\;I\;\;I\;\;I\,X\,X\,I\,I\,I & = c_{10}c_{11} \end{array}$$

[10] P. Jordan and E. Wigner, Zeitschrift für Physik **47**, 631 (1928).

Free Fermions

Consider the "solvable" case:

$$H_{\text{int}} = \sum_{j=1}^{n/2} (X_{2j-1}X_{2j} + Y_{2j}Y_{2j+1}) + \sum_{j=1}^{n} Z_j$$

Apply the **Jordan-Wigner Transformation**

$$H_{\text{int}} = -i\sum_{j=1}^{n/2} (c_{4j-2}c_{4j-1} - c_{4j-1}c_{4j+2}) - i\sum_{j=1}^{n} c_{2j-1}c_{2j}$$

$$H_{\text{int}} \equiv -i\mathbf{c}\cdot\mathbf{h}\cdot\mathbf{c}^{\mathrm{T}} \qquad \mathbf{h} = -\mathbf{h}^{\mathrm{T}} \in \mathbb{R}^{2n\times 2n}$$

Majorana operators transform covariantly

$$e^{iH_{\text{int}}}c_\mu e^{-iH_{\text{int}}} = \sum_\nu \left(e^{-4\mathbf{h}}\right)_{\mu\nu} c_\nu \qquad e^{-4\mathbf{h}} \in \mathrm{SO}(2n)$$

Can find spectrum and eigenvectors by diagonalizing $\mathbf{h}$.

$$e^{4\mathbf{w}}\cdot\mathbf{h}\cdot e^{-4\mathbf{w}} = \bigoplus_{j=1}^{n}\begin{pmatrix} 0 & -\lambda_j \\ \lambda_j & 0 \end{pmatrix}$$

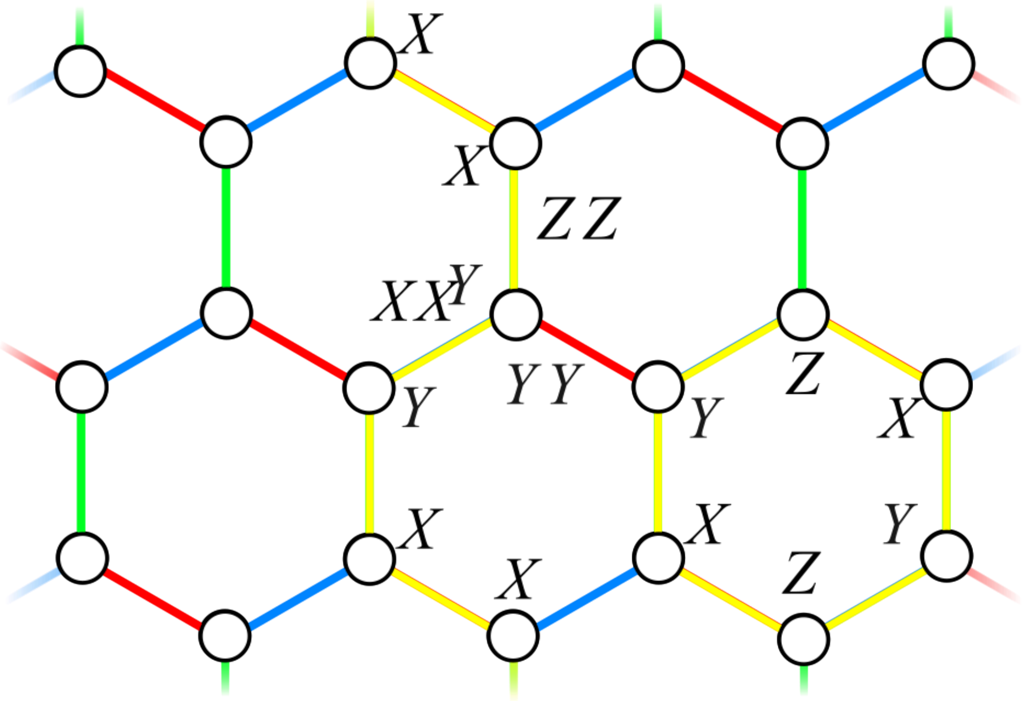
$$e^{-\mathbf{c}\cdot\mathbf{w}\cdot\mathbf{c}^{\mathrm{T}}} H e^{\mathbf{c}\cdot\mathbf{w}\cdot\mathbf{c}^{\mathrm{T}}} = 2\sum_j \lambda_j Z_j$$

$$E_{\mathbf{x}} = 2\sum_j (-1)^{x_j}\lambda_j$$

Another free-fermion solution: Kitaev Honeycomb Model

$$H = -J_x \sum_{x-\text{links}} X_j X_k - J_y \sum_{y-\text{links}} Y_j Y_k - J_z \sum_{z-\text{links}} Z_j Z_k$$

- Compass model on Honeycomb lattice.
- Bonds on cycles multiply to constants.
- For an L_x x L_y lattice, the effective Hilbert space contains $O(L_x L_y)$ qubits in a mutual eigenspace of the cycles!
- A free-fermion mapping is needed to complete the solution.



[11] A. Kitaev. Ann. Phys. **321**, 2 (2006).

Another free-fermion solution: Kitaev Honeycomb Model

$$H = -J_x \sum_{x-\text{links}} X_j X_k - J_y \sum_{y-\text{links}} Y_j Y_k - J_z \sum_{z-\text{links}} Z_j Z_k$$

Map each qubit to **four** fermions

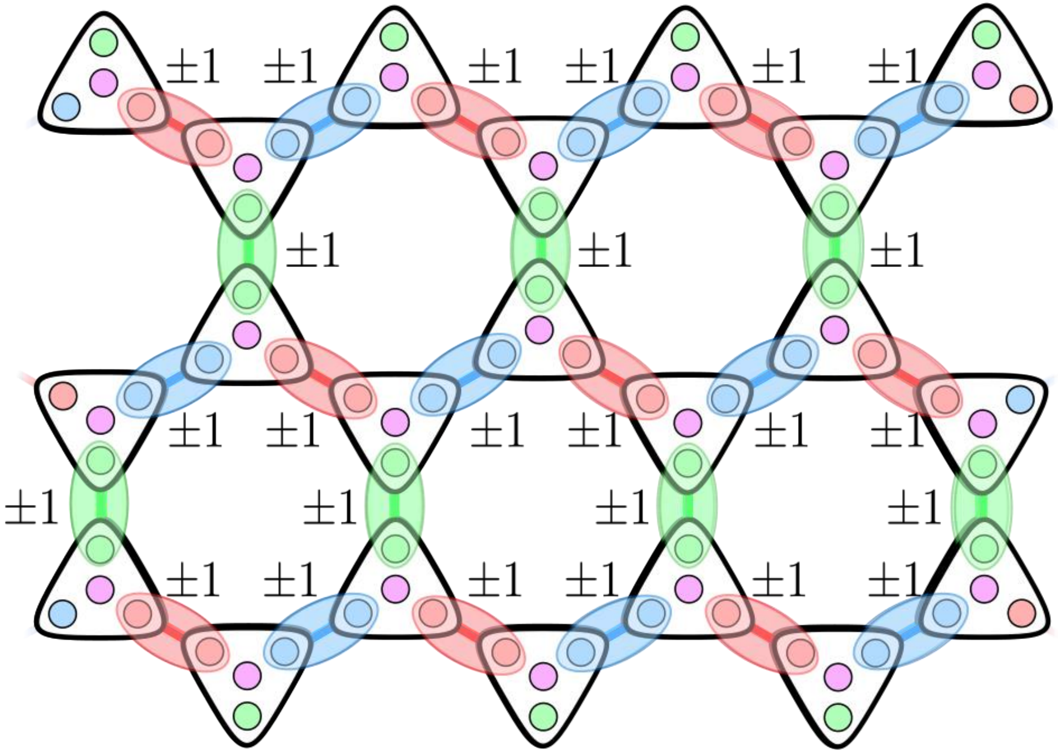
$$\sigma_k^\alpha = i b_k^\alpha c_k$$

with a new symmetry at each vertex

$$D_j \equiv b_j^x b_j^y b_j^z c_j$$

Bond fermions pair to constants of motion

$$u_{j,j+\hat{\boldsymbol{\alpha}}} \equiv i b_j^\alpha b_{j+\hat{\boldsymbol{\alpha}}}^\alpha$$



Solve the "matter" fermion Hamiltonian over each bond sector.

[11] A. Kitaev. Ann. Phys. **321**, 2 (2006).

Photo Credit: Anirban Chowdhury

When is a mapping to free fermions possible?

Given a general Pauli Hamiltonian

$$H = \sum_j h_j P_j$$

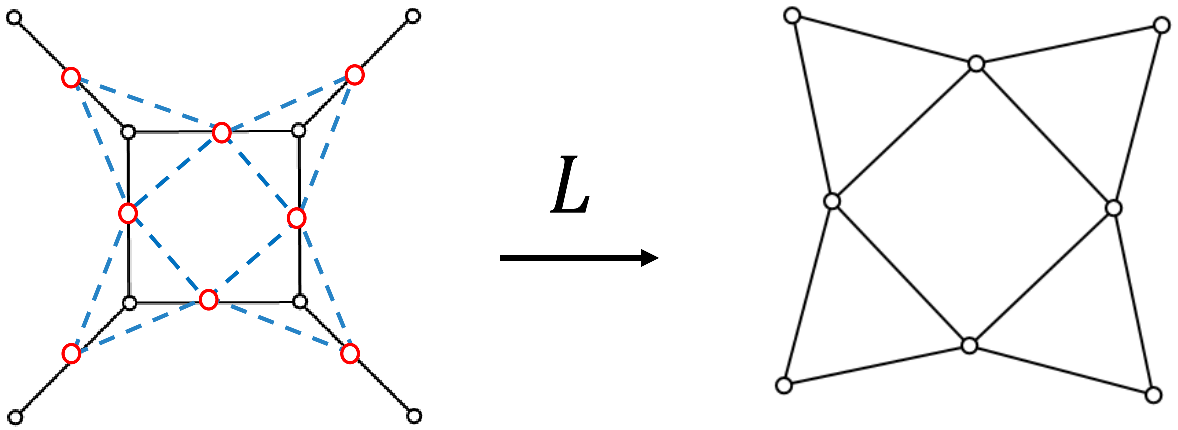
when can we define distinct quadratic fermion operators such that commutation relations are respected?

$$P_j \mapsto i c_{j_1} c_{j_2}$$ such that $$P_j P_k = (-1)^{|(j_1,j_2)\cap(k_1,k_2)|} P_k P_j$$

In graph theoretic terms: When can we label vertices of the anti-compatibility graph by subsets of size at most 2, such that neighboring vertices' subsets intersect in exactly one element?

Line Graphs!

The **line graph** of a root graph, $R = (V, E)$, is a graph $L(R) = (E, F)$, whose vertices correspond to the edges of R such that two vertices are neighboring in $L(R)$ if the corresponding edges in R share a vertex.



Fundamental Theorem: There exists a free-fermion description of a Pauli Hamiltonian iff its anti-compatibility graph is a line graph.

Krausz (1943): A graph is a line graph iff there exists an edge partition into cliques (complete graphs) such that every vertex belongs to at most two cliques.

[12] J. Krausz, Mat. Fiz. Lapok **50** (1943), 75-85

Proof Sketch

Theorem: Given the Pauli Hamiltonian

$$H = \sum_j h_j P_j$$

an injective mapping

$P_j \mapsto i c_{j_1} c_{j_2}$ such that $P_j P_k = (-1)^{|(j_1, j_2) \cap (k_1, k_2)|} P_k P_j$

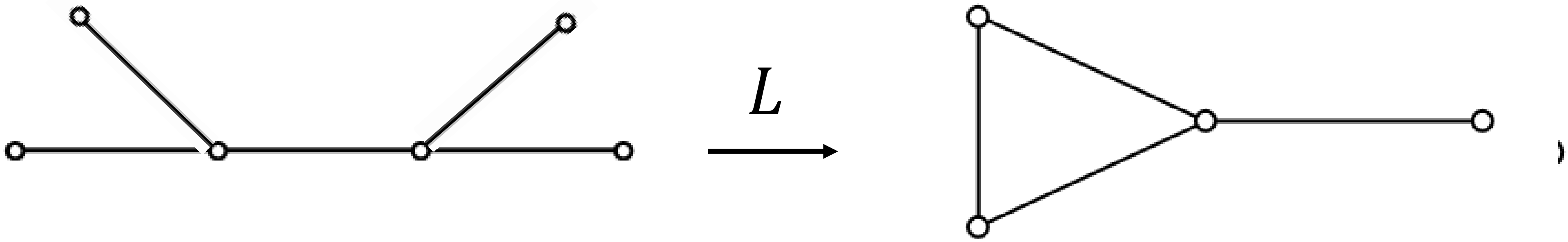
exists iff the anti-compatibility graph of H is the line graph $\mathrm{L}(R)$ for some root graph R.

⇒ (definitions coincide)

⇐ If the anti-compatibility graph of H is a line graph, associate a fermion to each clique in the Krausz decomposition, and give each Pauli the fermions corresponding to its cliques.

Example – The Claw

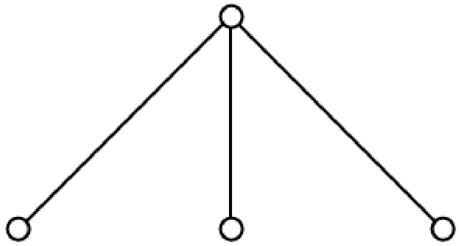
Consider the path graph P_3, whose line graph is P_2

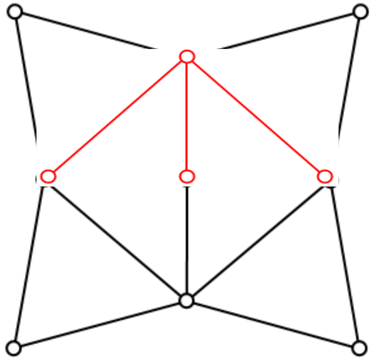


Clearly, no matter how an edge is (or edges are) added to the interior vertices, a triangle is created. Adding an edge to the ends only elongates.

(H_{nint})

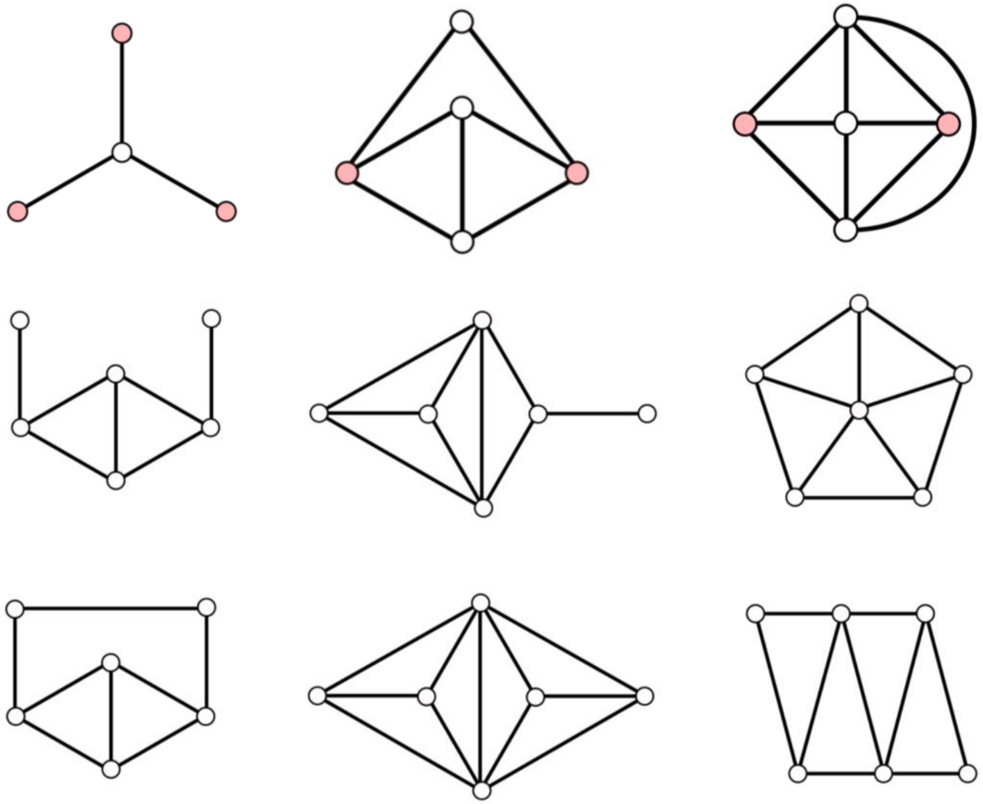
It is impossible for a line graph to contain a claw.





Forbidden Subgraph Characterization – Beineke (1970)

A graph is a line graph iff no subset of its vertices induces one of the nine ***forbidden subgraphs*** below.

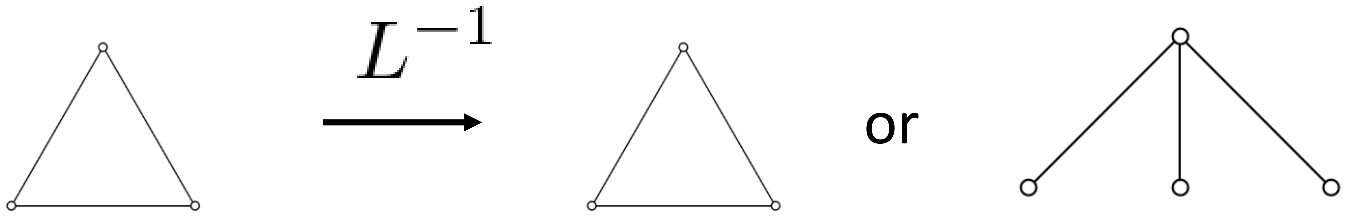


These nine anticommutation structures obstruct a free-fermion solution.

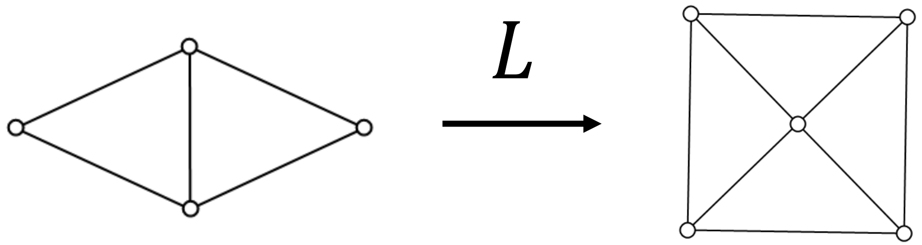
[13] L. W. Beineke, J. Comb. Theory, **9** (2): 129-135 (1970).

Isomorphism Theorems

Whitney (1932): Except for the triangle graph, K_3, the root graph of any line graph is unique.



Jung (1966): If two connected graphs are edge-isomorphic with more than four vertices, then they are also vertex-isomorphic, and this vertex isomorphism is unique.



Degiorgi and Simon (1995) utilized these theorems to develop a dynamical algorithm to recognize line graphs in $O(n)$ time. **Rossopoulos and Lehot (1973-1974)** earlier gave non-dynamical algorithms to perform this recognition.

[14] D.G. Degiorgi and K. Simon, Lecture Notes in Computer Science, **1017**, Berlin: Springer 37-48 (1995).
[15] N. D. Roussopoulos. Info. Proc. Lett., **2**(4):108 – 112, 1973. P. G. H. Lehot. ACM, **21**(4):569-575, 1974.

Photo Credit: Anirban Chowdhury

Graphical Symmetries

Given the Pauli Hamiltonian

$$H = \sum_j h_j P_j$$

look for products that commute with every term in the Hamiltonian.

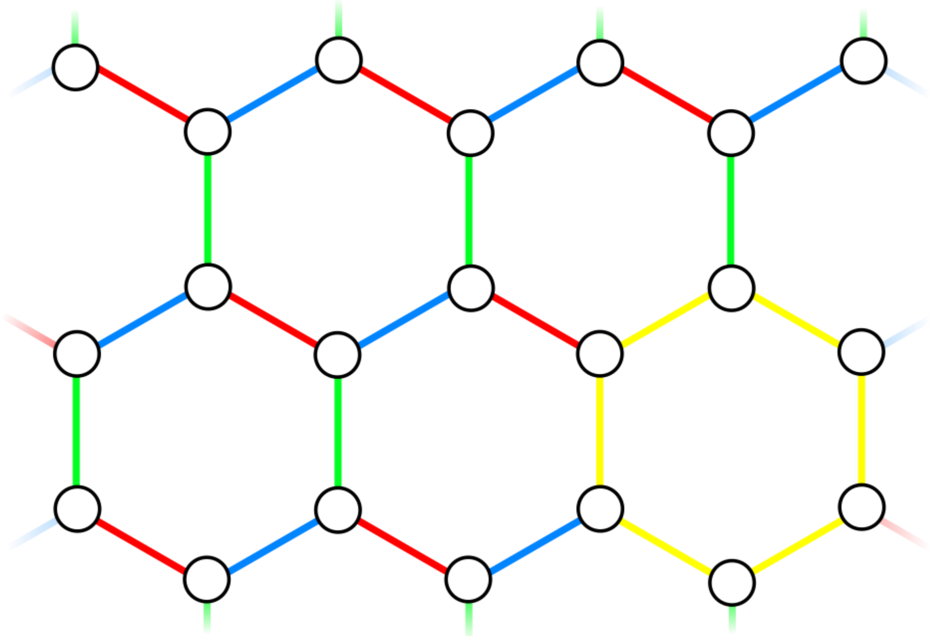
$$[\prod_{j \in S} P_j, P_k] = 0 \ \forall \ k$$

The subsets S arise as graphical structures:

(i) Twin vertices

(ii) Cycles in the root graph

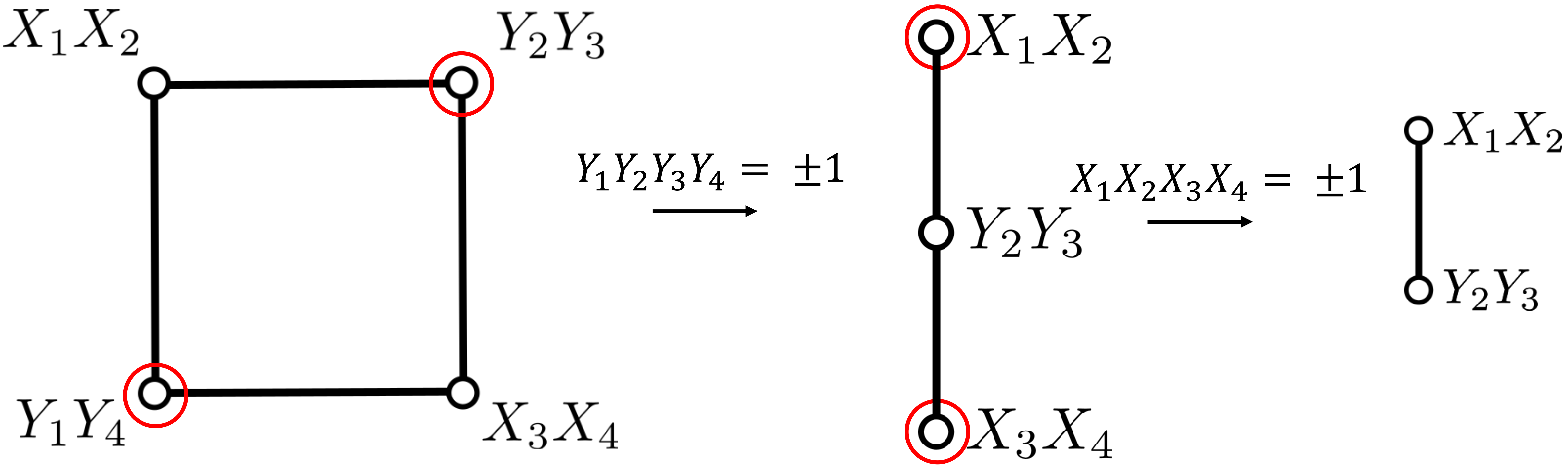
(iii) Fermionic parity operator



We solve the free-fermion model over each mutual eigenspace.

Twin vertices

If two vertices in the anti-compatibility graph have the same neighbors, then their product commutes with every term in the Hamiltonian. We can remove twins by fixing corresponding stabilizer values, e.g.



This can only be done for products of **pairs** of terms.

Root-graph symmetries: cycles and parity

The adjacency matrix of a line graph $L(R) = (E, F)$ with root $R = (V, E)$ can be factorized as

$$\mathbf{A} = \mathbf{B}\mathbf{B}^{\mathrm{T}} \pmod 2$$

$\mathbf{B}$ is the root graph incidence matrix

$$B_{ij} = \begin{cases} 1 & \text{if vertex } j \in V \text{ belongs to edge } i \text{ in } E \\ 0 & \text{otherwise} \end{cases}$$

Graphical symmetries are vectors $\mathbf{v} \in \{0, 1\}^{\times |E|}$ in the kernel of $\mathbf{A}$

$$\mathbf{A} \cdot \mathbf{v} = \mathbf{0} \pmod 2$$

We have two cases

(i) $\mathbf{B}^{\mathrm{T}} \cdot \mathbf{v} = \mathbf{0} \quad \Rightarrow$ $\mathbf{v}$ is a subgraph of even degree (a cycle)

(ii) $\mathbf{B} \cdot (\mathbf{B}^{\mathrm{T}} \cdot \mathbf{v}) = \mathbf{0} \quad \Rightarrow \mathbf{B}^{\mathrm{T}} \cdot \mathbf{v} = \mathbf{1}$, the all ones vector (fermionic parity operator)

What about the sign?

The sign of a term is changed by exchanging $j_1 \leftrightarrow j_2$ in the mapping

$$P_j \mapsto i c_{j_1} c_{j_2}$$

This corresponds to an orientation of the root graph, but is not fixed by the commutation relations between the Paulis.

We choose this orientation when we fix the cycle-symmetry eigenvalues:

1. Choose a spanning tree of the root graph
2. Orient the edges on this tree arbitrarily
   a) This cannot change the spectrum of $\mathbf{h}$.
   b) This changes the eigenvectors of $\mathbf{h}$ by a diagonal ± 1 single-particle matrix.
3. For each edge not in the spanning tree, choose orientation according to the sign of the unique corresponding independent cycle.

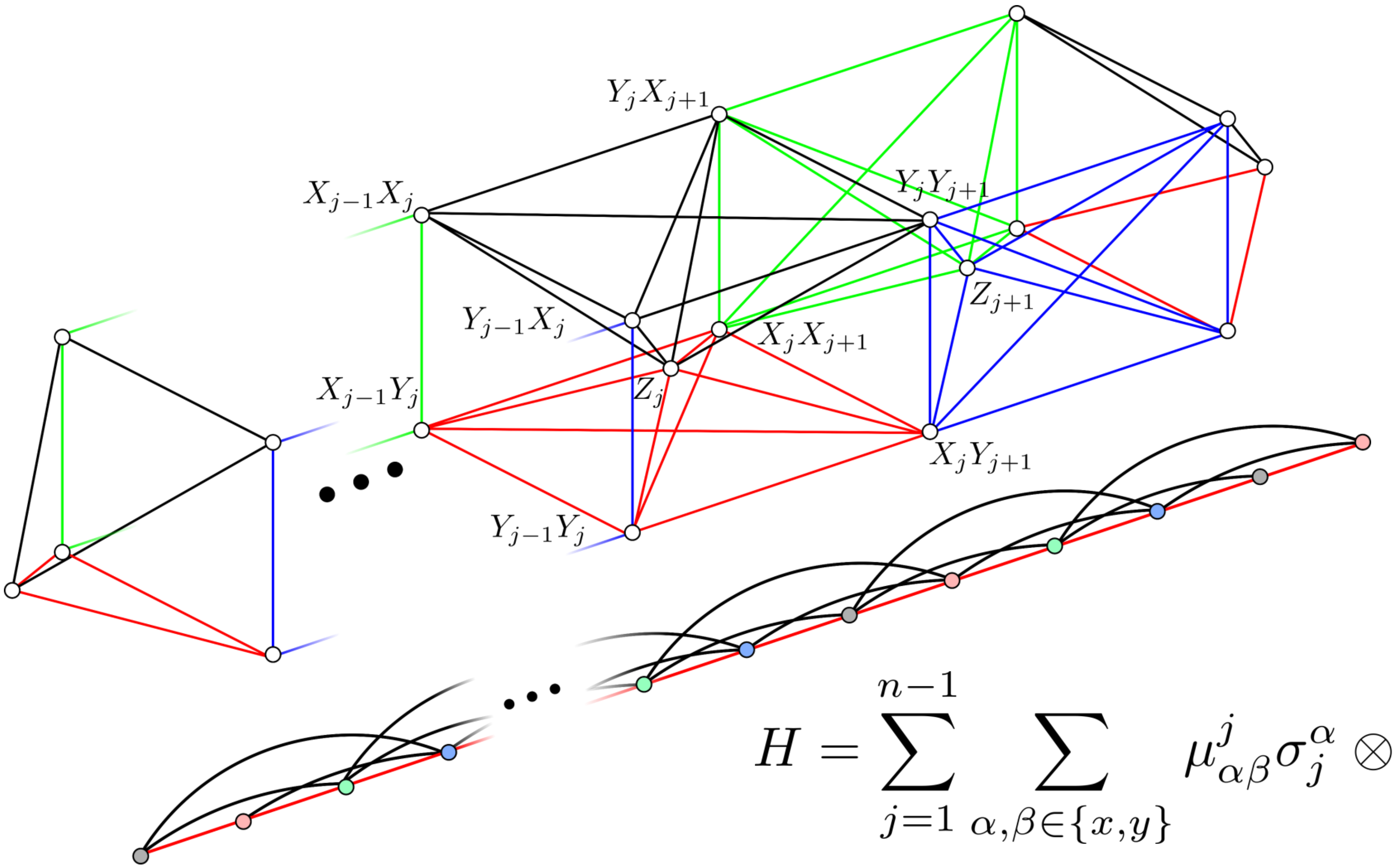
Putting Things Together

Given a general Pauli Hamiltonian

$$H = \sum_j h_j P_j$$

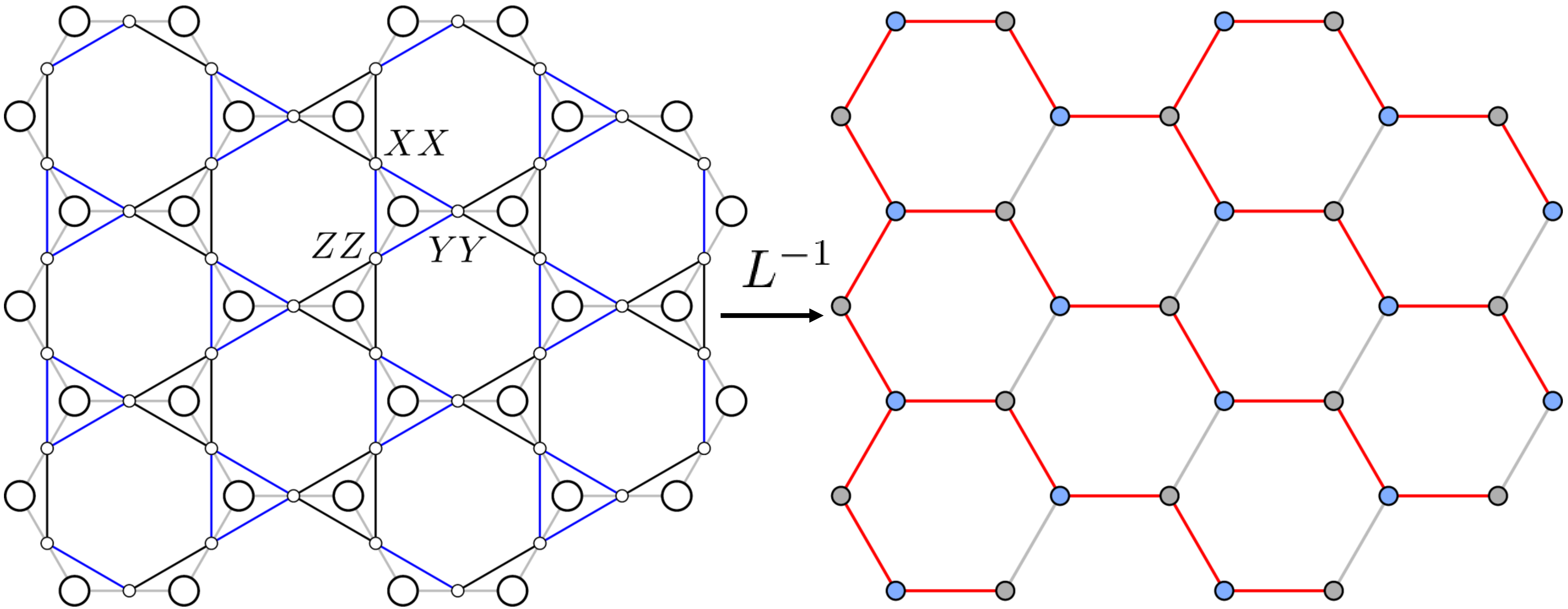
1. Check if the anti-compatibility graph is a line graph, possibly removing twins if necessary.
2. If a line graph, find the graphical symmetries
3. For each symmetry eigenvalue configuration, choose an orientation as described.
4. Solve the free-fermion Hamiltonian with the resulting single-particle transition matrix, restricting onto a fixed-parity eigenspace if necessary.

General Nearest-Neighbor 1-d Model



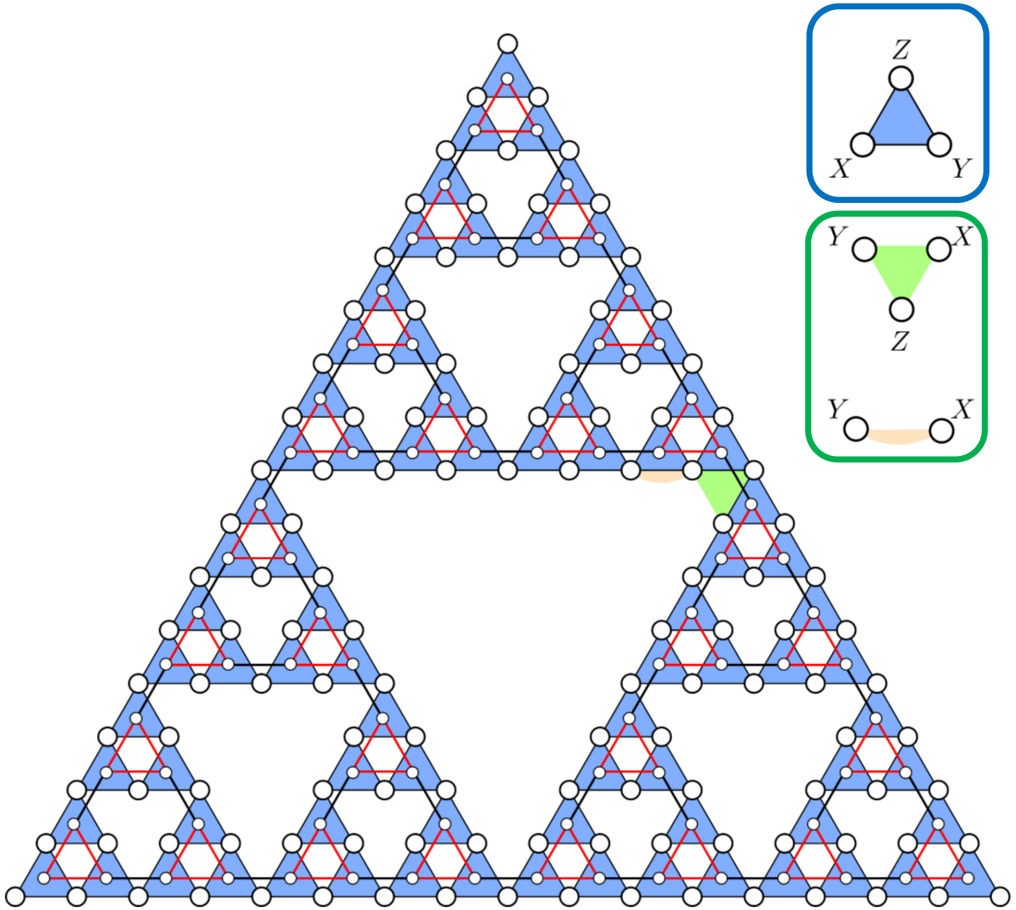
$$H = \sum_{j=1}^{n-1} \sum_{\alpha,\beta \in \{x,y\}} \mu_{\alpha\beta}^{j} \sigma_j^{\alpha} \otimes \sigma_{j+1}^{\beta} + \sum_{j=1}^{n} \nu_j Z_j$$

Kitaev Honeycomb Model



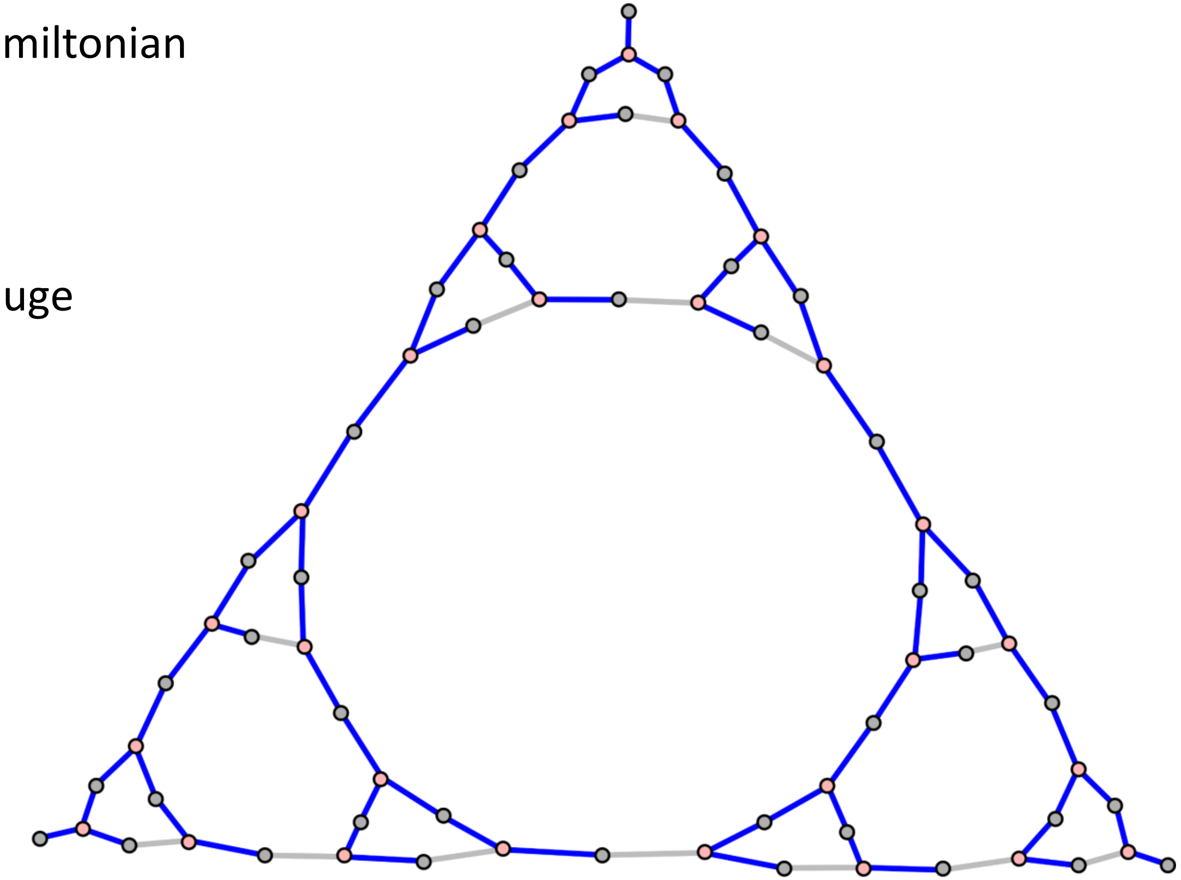
- The anti-compatibility graph is the line graph of the honeycomb graph.
- Conserved bond operators keep track of the edge-orientation outside the spanning tree, but strictly speaking are more redundant than necessary.

Sierpinski-Hanoi Model



Hamiltonian

Gauge



- Anti-compatibility graph describes allowed towers of Hanoi transitions
- Model encodes logical qubits at a constant asymptotic rate of $\frac{11}{18}$.

Future work - Free parafermions and circle graphs

- Joint work with Samuel Elman at University of Sydney.
- Parafermions satisfy twisted commutation relations

$$\gamma_i \gamma_j = \omega^{\mathrm{sgn}(i-j)} \gamma_j \gamma_i \qquad \gamma_j^d = \gamma_j \gamma_j^\dagger = I$$

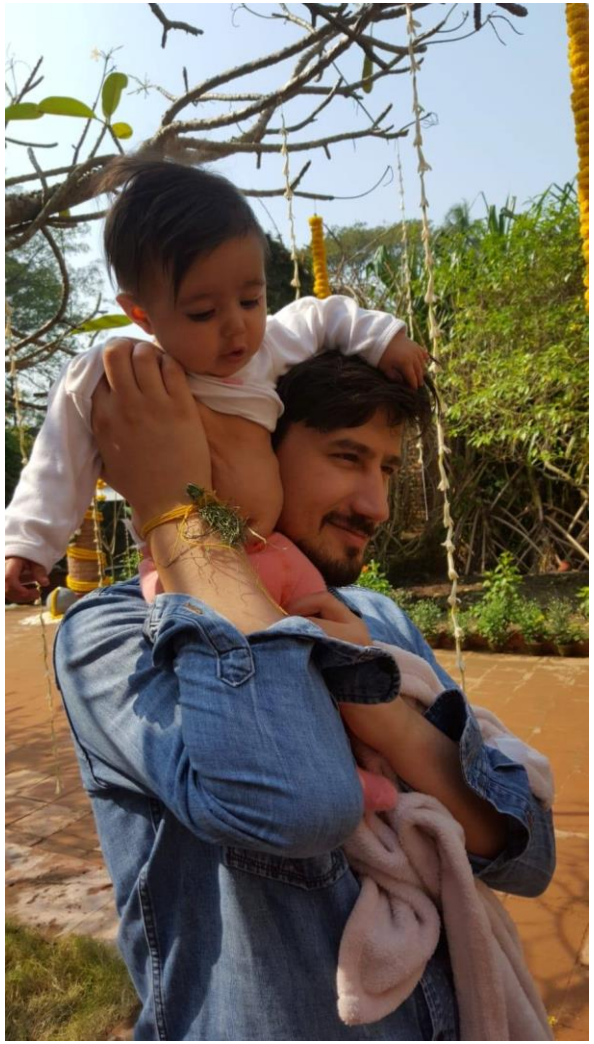
$$\omega^d = 1$$

- “Free parafermion” models [16]

$$H = \sum_{jk} h_{jk} \gamma_j \gamma_k^\dagger$$

- Quadratics fail to commute if indices are ***interleaved***

  i.e. $\left[\gamma_j \gamma_k^\dagger, \gamma_l \gamma_m^\dagger\right] \neq 0$ when $j < l < k < m$



[16] P. Fendley, J. Phys. A **47** 075001 (2014).

Future work - Free parafermions and circle graphs

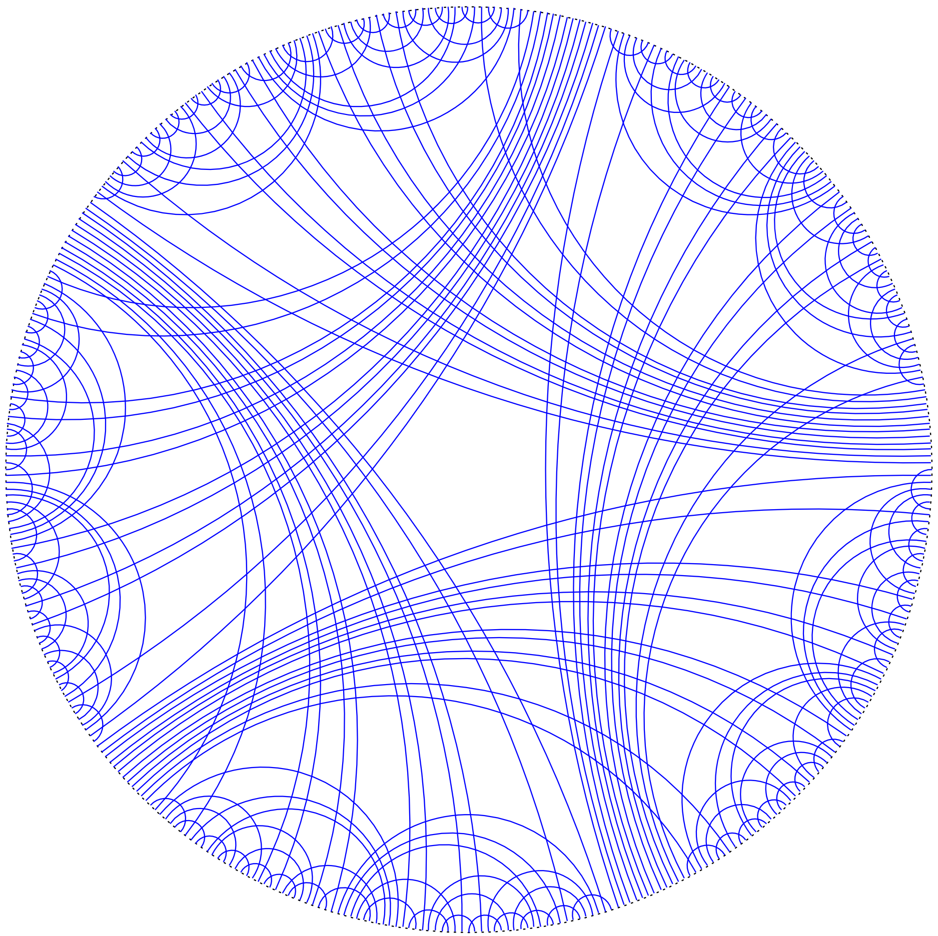
- Free parafermion models for $d = 3$ are described by (oriented) circle graphs.

- Vertices of are chords on a circle, which are neighboring if the corresponding chords intersect.

- Forbidden subgraph characterization defined up to equivalence by local complementation [17].

- Line and circle graphs intersect, but do not properly contain one another.

- Though free parafermions lack nice Lie-theoretic properties, they still admit a graph theoretic characterization.



[17] A. Bouchet, J Combin. Theory Ser. B **60**(1) (1994), 107–144.

Outlook

- We give a graph theoretic characterization of a wide class of fermion-solvable models.

- Cases where the solvability depends on Hamiltonian coefficients are still uncharacterized.

- Some applications for finding line subgraphs dynamically
  - Quantum impurity models.
  - Fermion-Gaussian “rank” for Hamiltonians.

Thanks!

Photo Credit: Anirban Chowdhury