
New Graph Invariants from Quantum Physics



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Quantum Information at
Imperial College
London

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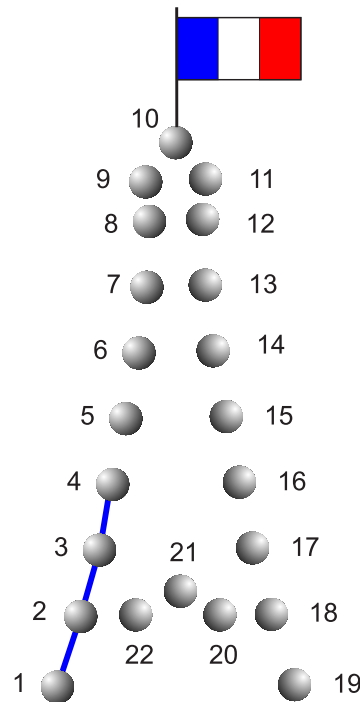
Impressum

- This talk is about the paper: “Symmetric Squares of Graphs”,
- Joint work of KA, Terry Rudolph (Imperial), Chris Godsil (Uni of Waterloo) and Gordon Royle (Uni of Western Australia).
- Accepted for Journal of Combinatorial Theory, Series B
- Sneak preview at [Math.CO/0507251](https://math.com/0507251)



Graphs

- **Graph Theory** is that branch of Mathematics that has found its way into Kindergarten.





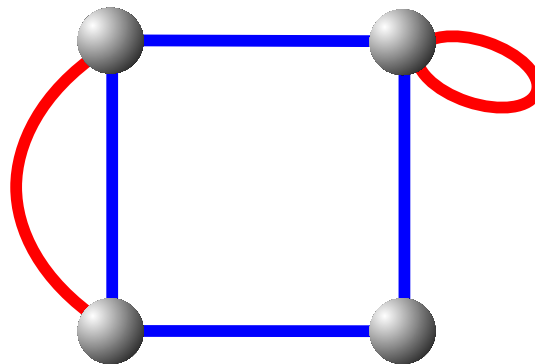
Graphs

- Graph theory has many applications, in many areas of science.
 - Computer Science: representation of networks, relations,...
 - Chemistry: representation of chemical compounds
 - Printing Industry: 4-colour problem
 - Quantum Information: graph states (cf D. Gross' talk this morning)
 - Present talk has nothing to do whatsoever with graph states



Graph Terminology

- A **Graph** is a collection of **vertices** V (dots), connected by **edges** E (lines). Vertices are commonly labelled $1, 2, \dots, v$.
- In a **simple** graph, no vertex is connected with itself (no loops), and any two vertices are connected by at most one edge.

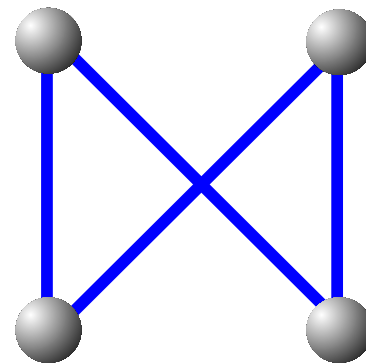
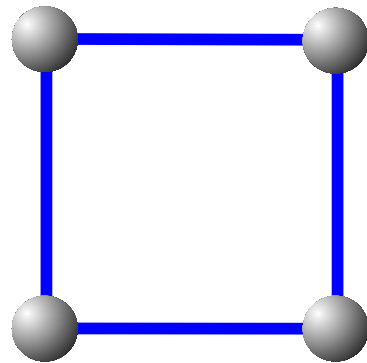


- Vertices that are connected are called **adjacent**; notation: $a \sim b$
- If $a \sim b$ we call b a **neighbour** of a (and a of b)
- Vertex **degree** = number of neighbours of a vertex



Graph Isomorphism (GI)

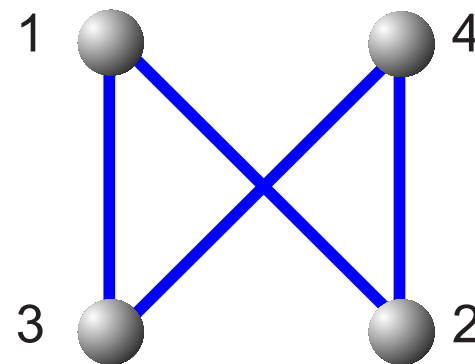
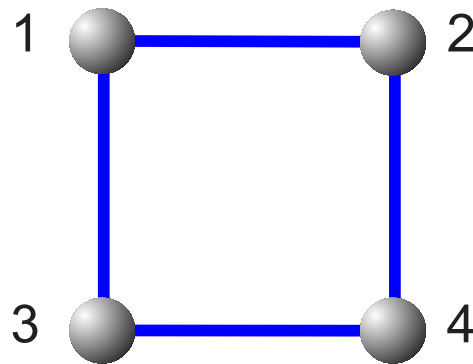
- Two graphs are **isomorphic** if they are identical up to relabelling of the vertices.





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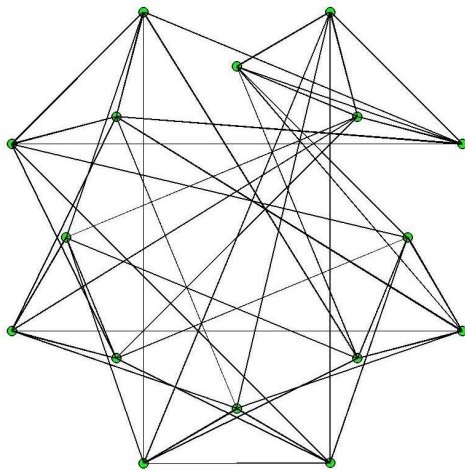
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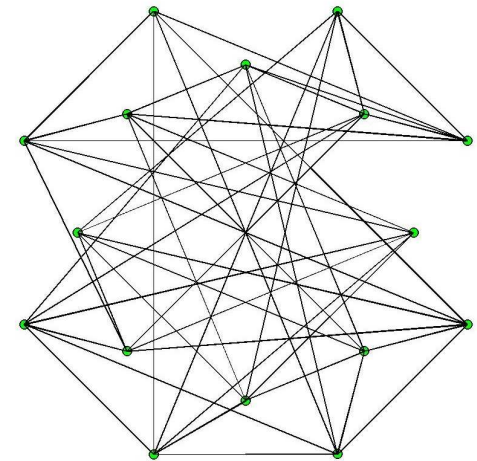


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Isomorphic?





Graph Isomorphism (GI)

- Determination of graph isomorphism has been annoying computer scientists for ages.
- Easy as it looks, its complexity class is unknown.
- Not believed to be NP complete.
- Polynomial for typical graphs. Efficient for, e.g. trees.
- General case is very hard: no known polynomial algorithm.
- Best existing upper bound: $\exp \sqrt{cv \log v}$
- Graph Isomorphism problem: is GI in P?



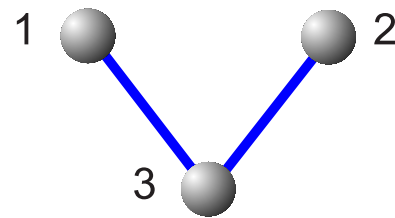
Overview

- There are various approaches to graph theory, and to GI in particular
- Purpose of this talk: Present a physically inspired approach to GI
 - “Hard-core Bosons on a Graph”
 - Implementable on a Quantum Computer
 - Strong interplay with the algebraic approach (in both directions)
 - new graph operation: Symmetric Power
 - new graph invariants: spectrum of symmetric power
- First: algebraic approach



Algebraic Approach

- Graph theory has an algebraic counterpart: Algebraic graph theory
- Represent graph by a matrix
- For G a graph with v vertices, its **Adjacency matrix** $A(G)$ is a $v \times v$ symmetric matrix
- $A_{ij} = 1$ if vertices i and j are neighbours, 0 if not.
- Example:



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



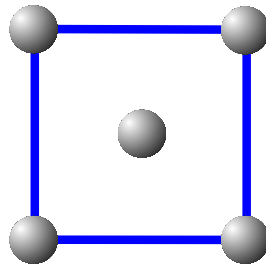
Algebraic Approach to GI

- Graphs G_1 and G_2 are isomorphic iff there exists a permutation matrix P such that $A(G_1) = P A(G_2) P^T$.
- Permutation matrices are orthogonal: $PP^T = P^T P = \mathbf{I}$
- The adjacency matrices of isomorphic graphs are thus orthogonally equivalent, and therefore have the same eigenvalues: such graphs are called **cospectral**
- GI algorithm #1: check spectra of adjacency matrices.
If the spectra are different, the graphs cannot be isomorphic.
- Works fine for generic graphs.

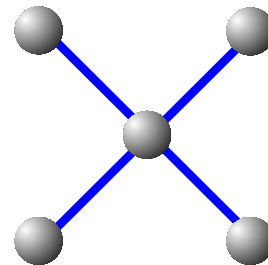


Algebraic Approach to GI

- If the spectra are equal, we can't say anything
- Happens for specific classes of graphs: one can find cospectral non-isomorphic graphs.
- Example: box5 and star5 both have eigenvalues $-2, 0, 0, 0, 2$.



Box5



Star5

- **Strongly regular graphs** are notorious counterexamples, and hence form a good testbed for any GI algorithm.



Regular Graphs

- A **Regular** graph is one in which all vertices have the same degree k .
- Algebraic criterion: let

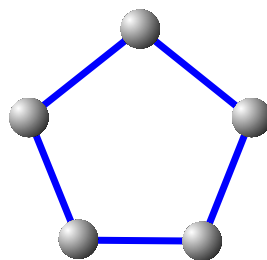
$$J = \begin{pmatrix} 1 & 1 & \dots & 1 \\ 1 & 1 & \dots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \dots & 1 \end{pmatrix},$$

then G is regular iff $A(G)$ commutes with J .

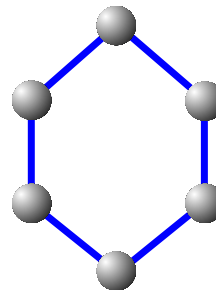


Strongly Regular Graphs

- A degree- k regular graph is **strongly** regular with parameters a and c iff
 - any pair of adjacent vertices have a common neighbours
 - any pair of non-adjacent vertices have c common neighbours
- Smallest regular graph that is not strongly regular: cycle6



Cycle5



Cycle6

- Algebraic criterion: $A^2 - (a - c)A - (k - c)I = cJ$.



A Quantum-Physical Approach to GI

- One can tailor quantum systems such that the interaction Hamiltonian is the adjacency matrix of a graph
- Exchange Hamiltonian of system with v sites: $H_{int} = g \sum_{i < j} A_{ij} S^{ij}$, where $S^{ij} = |i\rangle\langle j| + |j\rangle\langle i|$ flips particle position between sites i and j
- We use a position basis: $\langle x|i\rangle$ is amplitude that particle is in site i ; with $|i\rangle = e^i$, $H_{int} = gA$
- The spectrum of the system yields the eigenvalues of A
 - Two-level atoms in a molecule with dipole-dipole interaction
 - Spins on a lattice with XY interaction
 - Boson hopping around a lattice (Bose-Hubbard model)



Multiple particles

- As we already know, just looking at the spectrum does not work in general
- New Idea: look at spectrum of a *multi-particle* system
- Motto: more complex system, hence more complex behaviour, and, hopefully, more information
- Specifically: Bose-Hubbard hopping model for N particles.
- Sum of one-particle hops

$$H_N = \sum_{k=1}^N H_k = \sum_{k=1}^N \mathbf{I}^{\otimes k-1} \otimes H \otimes \mathbf{I}^{\otimes N-k}.$$

- Here, the k -th tensor factor H_k operates on the k -th particle.



Multiple particles

- That's for distinguishable particles only. To be “symmetrised” for indistinguishable particles.
- We keep working in the position basis; no creation/annihilation operators
- I will first consider the case of ordinary bosons or fermions, and explain why increasing N gives no further information on the underlying graph.
- To make the idea work we will use N **hard-core bosons**: by including a strong repulsive (Coulomb) force, at most one boson can occupy a site.



Multiple particles

- All three cases (Bosons, Fermions, Hard-Core Bosons) will be treated in the same way:
 - Start from single-particle states in position basis $x \in \mathbb{C}^v$ (amplitudes of being in vertex $1, 2, \dots, v$)
 - Form N -particle states by taking the tensor product $x_1 \otimes \dots \otimes x_N$
 - Symmetrise by projecting on appropriate subspace of $(\mathbb{C}^v)^{\otimes N}$



Bosonic States

- The quantum state of N v -level bosons “lives” in the **totally symmetric subspace** of $(\mathbb{C}^v)^{\otimes N}$: interchanging two bosons should not change the state.
- This subspace, $(\mathbb{C}^v)^{\vee N}$, is the linear span of all symmetric tensor products
- For $N = 2$, these are $x_1 \vee x_2 := \frac{1}{\sqrt{2!}} (x_1 \otimes x_2 + x_2 \otimes x_1)$.
- For general N ,

$$x_1 \vee \dots \vee x_N := \frac{1}{\sqrt{N!}} \sum_{\pi} x_{\pi(1)} \otimes \dots \otimes x_{\pi(N)},$$

where π runs over all index permutations, x_k vectors in \mathbb{C}^v .

- Basis states are $|i_1\rangle \vee \dots \vee |i_N\rangle / \sqrt{m_1! \dots m_v!}$, for $1 \leq i_1 \leq i_2 \leq \dots \leq i_N \leq v$, where m_j is the number of indices having value j .



Bosonic States

- Bosons: project tensor product of single-particle states onto $(\mathbb{C}^v)^{\vee N}$.
- Define projector $P_{\vee} : (\mathbb{C}^v)^{\otimes N} \mapsto (\mathbb{C}^v)^{\vee N}$:

$$P_{\vee}(x_1 \otimes \dots \otimes x_N) = \frac{1}{\sqrt{N!}} x_1 \vee \dots \vee x_N$$

- Corresponding inclusion map from $(\mathbb{C}^v)^{\vee N}$ into $(\mathbb{C}^v)^{\otimes N}$: $Q_{\vee} = P_{\vee}^{\dagger}$.
- Columns of Q_{\vee} are coordinates of basis vectors of $(\mathbb{C}^v)^{\vee N}$ in $(\mathbb{C}^v)^{\otimes N}$.
- Example: $v = 2$, $N = 2$, basis states $(1, 1)$, $(1, 2)$, and $(2, 2)$.

$$P_{\vee} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$



Fermionic States

- Fermions: project on totally **antisymmetric** subspace $(\mathbb{C}^v)^{\wedge N}$.
- Antisymmetric tensor product:

$$x_1 \wedge \dots \wedge x_N := \frac{1}{\sqrt{N!}} \sum_{\pi} \epsilon_{\pi} x_{\pi(1)} \otimes \dots \otimes x_{\pi(N)},$$

where $\epsilon_{\pi} = \pm 1$ is the signature of π .

- Basis states: $|i_1\rangle \wedge \dots \wedge |i_N\rangle$, for $1 \leq i_1 < i_2 < \dots < i_N \leq v$.
This is only possible for $N \leq v$.



Fermionic States

- Projector $P_\wedge : (\mathbb{C}^v)^{\otimes N} \mapsto (\mathbb{C}^v)^{\wedge N}$:

$$P_\wedge(x_1 \otimes \dots \otimes x_N) = \frac{1}{\sqrt{N!}} x_1 \wedge \dots \wedge x_N$$

- Example: $v = 3$, $N = 2$, basis states: $(1, 2)$, $(1, 3)$, and $(2, 3)$.

$$P_\wedge = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 \end{pmatrix}.$$



Bosonic Hopping

- We now combine the Hopping Hamiltonian for distinguishable particles with the bosonic symmetriser, yielding the bosonic hopping Hamiltonian:

$$\begin{aligned} H_{boson,N} &= P_{\vee} H_N P_{\vee}^{\dagger} \\ &= P_{\vee} \left(\sum_{k=1}^N \mathbf{I}^{\otimes k-1} \otimes H \otimes \mathbf{I}^{\otimes N-k} \right) P_{\vee}^{\dagger} \\ &= N P_{\vee} (H \otimes \mathbf{I}^{\otimes N-1}) P_{\vee}^{\dagger}. \end{aligned}$$

- Burning question: does spectrum of $H_{boson,N}$ yield more information than H ?
- Alas, no!



Bosonic Hopping

- Alternative expression:

$$\begin{aligned} H_{boson,N} &= P_{\vee} \left(\sum_{k=1}^N \mathbf{I}^{\otimes k-1} \otimes H \otimes \mathbf{I}^{\otimes N-k} \right) P_{\vee}^{\dagger} \\ &= \left. \frac{\partial}{\partial t} \right|_{t=0} P_{\vee} (\mathbf{I} + tH)^{\otimes N} P_{\vee}^{\dagger}. \end{aligned}$$

- $P_{\vee} (\mathbf{I} + tH)^{\otimes N} P_{\vee}^{\dagger}$ is the totally symmetric irreducible representation (irrep) of $\mathbf{I} + tH$ on N copies of \mathbb{C}^v .
- Eigenvalues of an irrep of a matrix A depend only on the eigenvalues of A itself.
- Therefore, spectrum of $H_{boson,N}$ depends on the spectrum of H only.
- A similar reasoning applies when using fermions (P_{\wedge} instead of P_{\vee}).



Hard-Core Bosons: a marriage of reason

- By including a strong repulsive force in the Hamiltonian, we enforce that at most one boson can occupy a site.
- Most easily described by a symmetriser that is a hybrid of the bosonic and fermionic symmetrisers.
- We take the totally symmetric subspace but drop any basis state in which more than one boson occupies the same site.
- We get basis $|i_1\rangle \vee \dots \vee |i_N\rangle$, but with $1 \leq i_1 < i_2 < \dots < i_N \leq v$. Again $N \leq v$.
- Named, in jest, the “Fermi-Bose” subspace
- Projector P_{FB} is elementwise absolute value of fermionic projector P_{\wedge} .



Hard-Core Bosons: a marriage of reason

- Example: $v = 3$, $N = 2$, basis states: $(1, 2)$, $(1, 3)$, and $(2, 3)$.

$$P_{FB} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}.$$

- Corresponding Hamiltonian:

$$H_{FB,N} = N P_{FB} (H \otimes \mathbf{I}^{\otimes N-1}) P_{FB}^\dagger.$$

- This has nothing to do with irreps anymore, and typically “screws up” H so much that the spectrum of H_{FB} is no longer completely determined by the spectrum of H .
- Which is what we need!



Symmetric Powers of Graphs

- “Fermi-Bose” symmetrisation can be translated into a graph-theoretical notion.
- We define the **symmetric N -th power** of a graph G (with Hamiltonian H), denoted $G^{\{N\}}$, as the graph for which the exchange Hamiltonian is

$$H_{FB,N} = N P_{FB} (H \otimes \mathbf{I}^{\otimes N-1}) P_{FB}^\dagger.$$

- This can be defined in purely graph-theoretical terms.
- Classical trajectory of a particle corresponds to a **walk** on the graph.
- Define an **N -walk** on G as a walk of N particles, each occupying a different site, where at every step a single particle moves to an unoccupied adjacent site.
- Vertices of $G^{\{N\}}$: the different configurations of N particles on G .
- Edges of $G^{\{N\}}$: N -walk on G = simple walk on $G^{\{N\}}$.



Symmetric Powers of Graphs

- Constructive definition of symmetric square of G
- Create **Cartesian Product** $G \square G$:
 - Vertices are pairs (x, y) where x and y are vertices of G
 - $(x, y) \sim (x', y')$ if either $x \sim x'$ and $y = y'$ or $x = x'$ and $y \sim y'$. Thus

$$A(G \square G) = A(G) \otimes \mathbf{I} + \mathbf{I} \otimes A(G)$$

- **Remove “diagonal”**: all vertices (x, x) , and all edges incident with them
- **Quotienting**: identify vertices (x, y) and (y, x) .



Main Results of the Paper

- Introduction of Symmetric Power concept



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- Numerical study, including all SRG's on up to 30 vertices: in all cases, symmetric cube determines original graph.
- Algebraic study of relation between spectra of A and $A^{\{2\}}$ for Hermitian A .



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- On a quantum computer, tractability only requires $k = O(v)$. An efficient quantum circuit simulating evolution under H_{int} is guaranteed to exist by various standard results in the theory of quantum computation.



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- On a quantum computer, tractability only requires $k = O(v)$. An efficient quantum circuit simulating evolution under H_{int} is guaranteed to exist by various standard results in the theory of quantum computation.
- Fruitful interplay: graph theory + algebra + physics