

Graph Laplacian Matrices as Quantum State Density Matrices and their Entanglement Properties

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ACM Poughkeepsie Chapter Talk

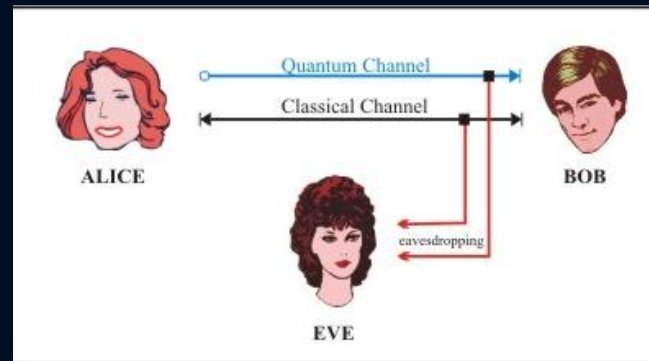
May 22, 2017

Quantum information processing

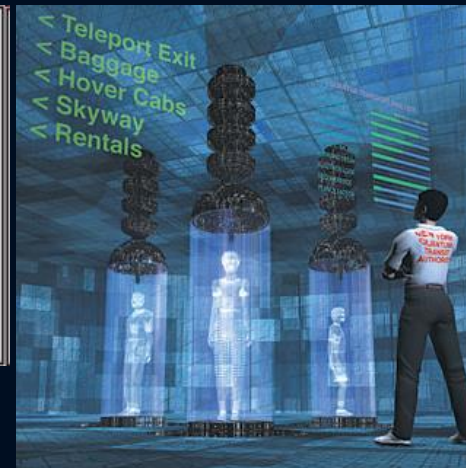
- The peculiarities of quantum physics promise to deliver revolutionary applications.
- ***Quantum computing***: superposition of states allow many computations to be performed in parallel. Can solve “hard” problems such as integer factorization in polynomial time.
- This could render well known cryptographic algorithms such as RSA obsolete.
- Fortunately, quantum cryptography can provide unbreakable crypto-systems. Relies on the fact that observation modifies the state and thus can detect eavesdropping/tampering.

Entanglement in quantum mechanics

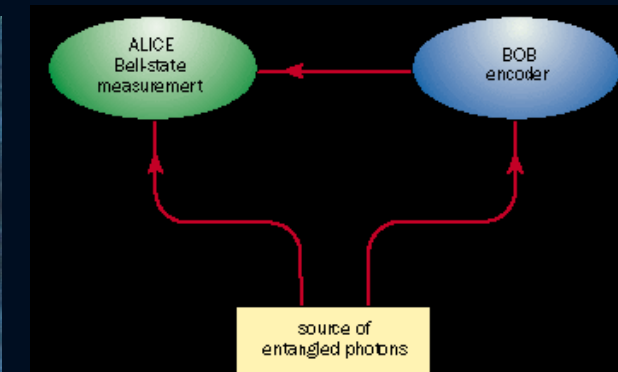
- An important ingredient in creating the myriad of nonintuitive phenomena in quantum physics is *entanglement of quantum states*.
- Entanglement has emerged as a crucial resource in applications of quantum mechanics such as
 1. Quantum computation
 2. Quantum teleportation
 3. Quantum cryptography
 4. Quantum dense coding
 5. and many others



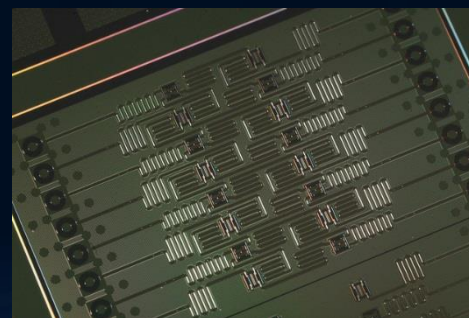
<http://www.acm.org/crossroads/xrds11-3/qcrypto.html>



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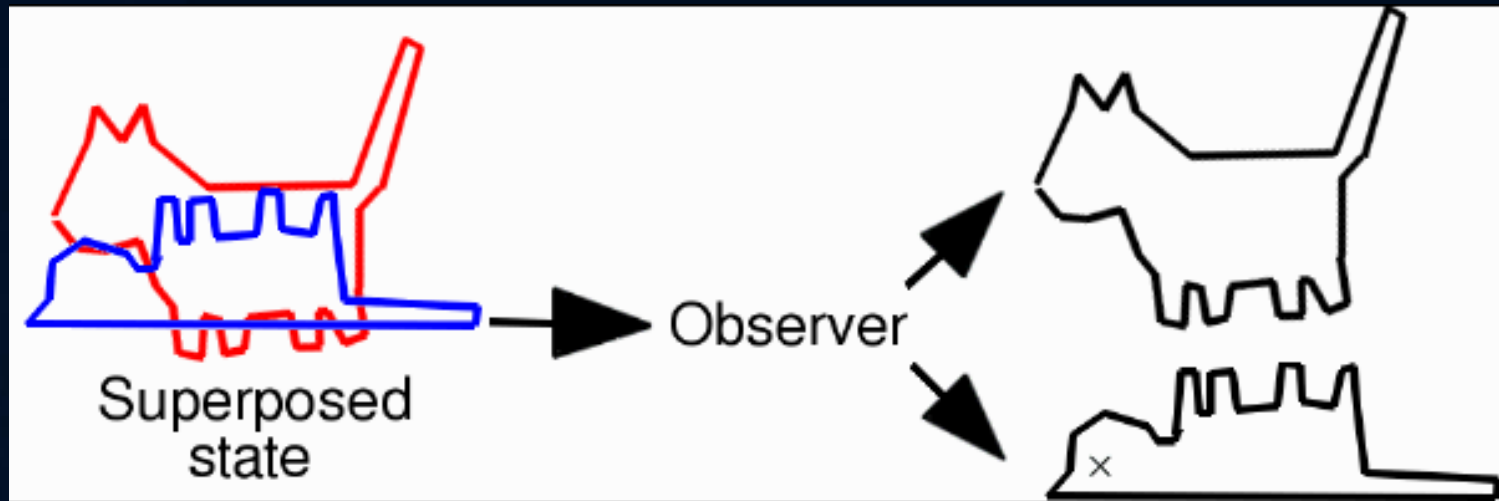
<http://physicsworld.com/cws/article/print/1658>



IBM's 16 qubit processor

Entanglement in quantum mechanics

- On the other hand, entanglement with the *environment* is undesirable in quantum computing as it leads to *decoherence*, causing a collapse of the superimposed state.

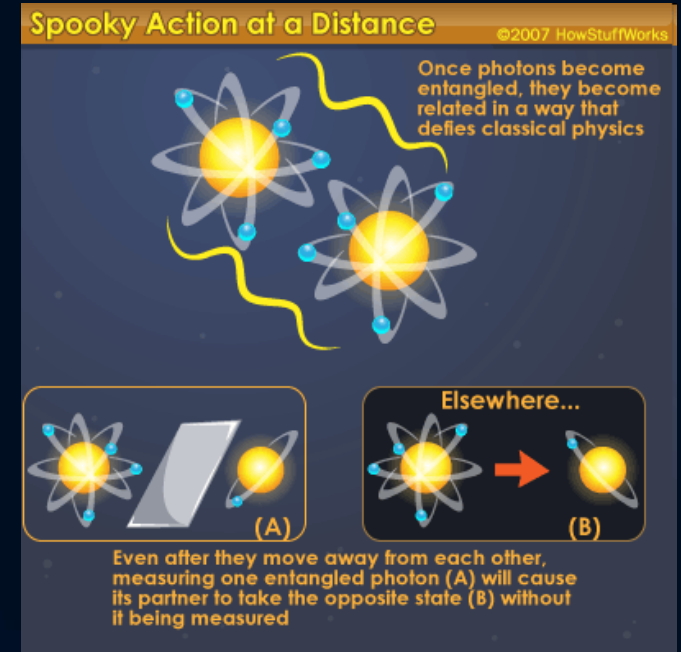
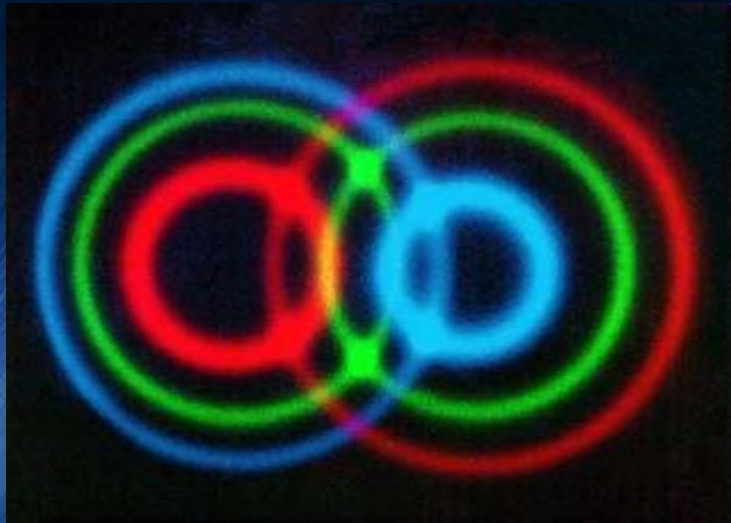


<http://brneurosci.org/subjectivity.html>

What is entanglement?

- Roughly speaking, entanglement is when two subsystems can not be described independently.
- This is responsible for the phenomenon whereby two subsystems can influence each other even though they are spatially separated.

Entangled photons



<http://science.howstuffworks.com/quantum-cryptology6.htm>

<http://physicsworld.com/cws/article/indepth/11360/1/smallphotons>

Quantum states

- A *pure* state can be described by a state vector (e.g. $\langle 0|$ or $|1\rangle$).
- In matrix algebra terms, the **bra** notation $\langle r|$ is identified with a row vector and the **ket** notation $|r\rangle$ is identified with a column vector.
- A mixture of pure states is a *mixed* state. A *mixed* state can be viewed as
 1. a statistical mixture of a number of pure states (i.e. experiments where the parameters are random)
 2. an ensemble of pure states (a large number of pure states with different proportions for each pure state).
- A mixed state cannot be expressed as a state vector.
- We need another structure to capture the properties of a mixed state.

Density matrix formulation of quantum mechanics (Von Neumann, 1927)

- The state of a quantum mechanical systems is associated with a *density* matrix: a complex matrix A that:
 1. Is Hermitian (i.e. $A = A^H$),
 2. Is positive semidefinite (i.e. all eigenvalues ≥ 0),
 3. Has unit trace (i.e. sum of diagonal elements = sum of eigenvalues = 1).
- A pure state is represented as a rank one density matrix $|r\rangle\langle r|$.
- This formulation allows for mixed states to be described as a weighted sum of pure states.

Tensor product

- Given two state vectors $|x\rangle$ and $|y\rangle$, the combined system is described by the tensor product $|x\rangle \otimes |y\rangle$
- A *qubit* is described by a 2 dimensional complex vector. n qubits are described by a 2^n dimensional complex vector.
- In the density matrix formulation, the combined state of two systems with density matrix A and B is

$$A \otimes B$$

Kronecker product of matrices

- In matrix notation, tensor product of 2 matrices can be expressed as a Kronecker product of matrices.

$$A \otimes B = \begin{bmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{bmatrix}$$

Density matrix formulation: separability and entanglement

- We say a density matrix of order $n=pq$ is bipartite *separable* if it can be written as:

$$A = \sum_i c_i B_i \otimes C_i, c_i \geq 0, \sum_i c_i = 1$$

where B_i and C_i are density matrices of order p and q resp.

- A density matrix is bipartite *entangled* if it is not bipartite separable.
- Determining whether a density matrix is entangled or not is NP-hard [Gurvits, 2003].
- Of interest are simple criteria for entanglement and separability.

Partial transpose

- Decompose a density matrix A into p^2 submatrices of order q

$$A = \begin{pmatrix} A^{1,1} & A^{1,2} & \dots & A^{1,p} \\ A^{2,1} & A^{2,2} & \dots & A^{2,p} \\ \vdots & \vdots & & \vdots \\ A^{p,1} & A^{p,2} & \dots & A^{p,p} \end{pmatrix}$$

- The *partial transpose* A^{T_B} is defined as:

$$A^{T_B} = \begin{pmatrix} (A^{1,1})^T & (A^{1,2})^T & \dots & (A^{1,p})^T \\ (A^{2,1})^T & (A^{2,2})^T & \dots & (A^{2,p})^T \\ \vdots & \vdots & & \vdots \\ (A^{p,1})^T & (A^{p,2})^T & \dots & (A^{p,p})^T \end{pmatrix}$$

Peres-Horodecki necessary condition for separability

- [Peres, 1996]: If the density matrix is separable, then its partial transpose is positive semidefinite, i.e. all its eigenvalues are nonnegative.
- Definition: a density matrix satisfies the PPT condition if its partial transpose is positive semidefinite.
- The PPT condition is also sufficient for separability in the cases of $(p=2, q=2)$ and $(p=2, q=3)$ [Horodecki et al, 1996]
- But not a sufficient condition in general for larger values of p, q .

Laplacian matrices of graphs

- The Laplacian matrix of a graph is defined as $L = D - A$, where D is the diagonal matrix of vertex degrees and A is the adjacency matrix.

Labeled graph	Degree matrix	Adjacency matrix	Laplacian matrix
	$\begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$

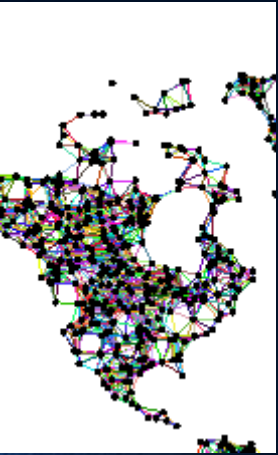
https://en.wikipedia.org/wiki/Laplacian_matrix

Laplacian matrices of graphs

- Properties of Laplacian matrices:
 1. Singular
 2. Positive semidefinite (all eigenvalues are nonnegative).
 3. Symmetric
 4. Trace is positive (for nonempty graphs)
- This means that a Laplacian matrix with its trace normalized to 1 can be considered as a density matrix.
- In 2006, *Braunstein et al.* first considered Laplacian matrices of graph as density matrices and studied the relationship between the graph and the corresponding quantum mechanical state expressed by the density matrix.

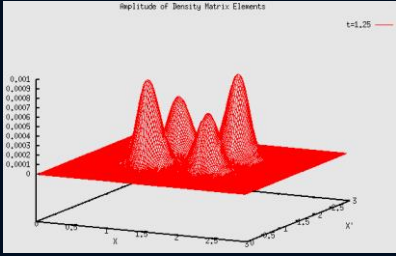
Laplacian matrices of graphs as density matrices

- Graph ↔ Laplacian matrix ↔ Density matrix ↔ state of quantum system

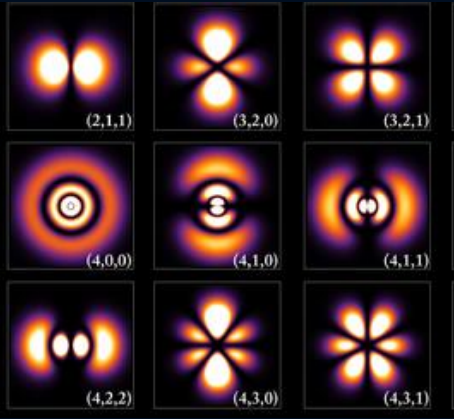


$$\begin{pmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$$

http://en.wikipedia.org/wiki/Laplacian_matrix



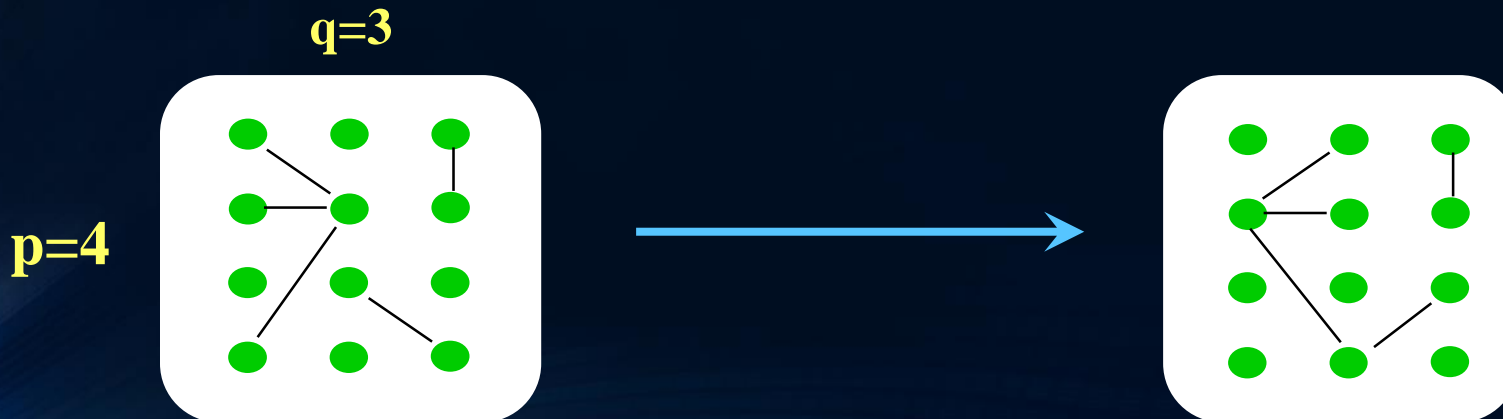
<http://www.personal.psu.edu/axt236/decoherence/>



http://en.wikipedia.org/wiki/Quantum_state

Partial transpose graph

- Arrange vertices on a p by q grid
- Each vertex has a label (u,v) , $u \in \{1, \dots, p\}$, $v \in \{1, \dots, q\}$.
- The *partial transpose graph* has the same vertex set and $((u,v),(w,t))$ is an edge of the partial transpose graph if and only if $((u,t),(w,v))$ is an edge of the original graph.
- Graphically, this corresponds to mirroring each edge around a horizontal axis through its middle.

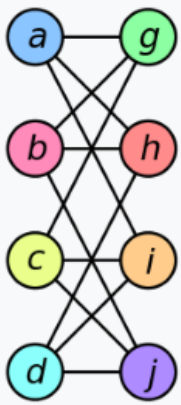
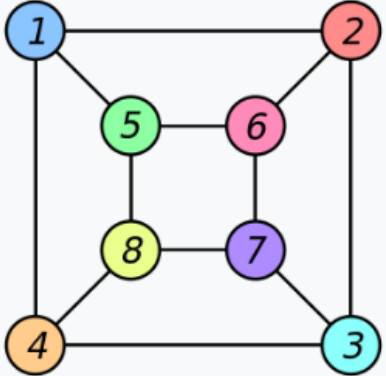


Partial transpose graph

- It is easy to show that the adjacency matrix of partial transpose graph is partial transpose of adjacency matrix.
- [Braunstein et al., 2006] introduced the vertex degree criterion:
 - *Each vertex has the same degree as its counterpart in the partial transpose graph*and showed that it is a necessary condition for separability
- It turns out this condition is as strong as the PPT condition.
- For Laplacian matrices of graphs it was shown that [Wu, 2006],
 - Vertex degree condition \leftrightarrow Peres-Horodecki PPT condition \leftrightarrow partial transpose of Laplacian has zero row sums.

Graph isomorphism

- Two graphs are isomorphic if they have the same number of vertices connected in the same way.

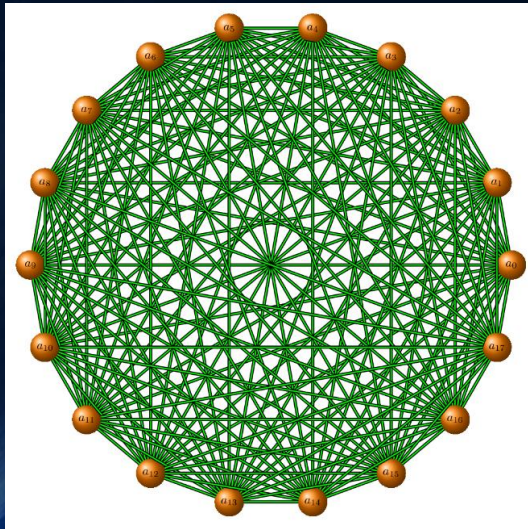
Graph G	Graph H	An isomorphism between G and H
		$f(a) = 1$ $f(b) = 6$ $f(c) = 8$ $f(d) = 3$ $f(g) = 5$ $f(h) = 2$ $f(i) = 4$ $f(j) = 7$

https://en.wikipedia.org/wiki/Graph_isomorphism

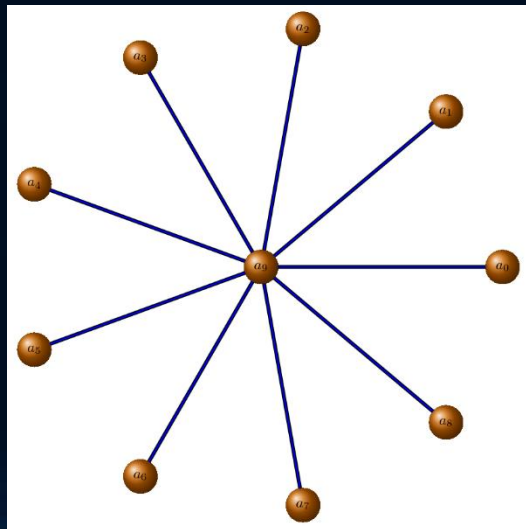
- Equivalently, two graph are isomorphic if their adjacency matrices are permutation-similar (i.e. mapped to each other via simultaneous row and column permutations.)

Separability of Laplacian matrices

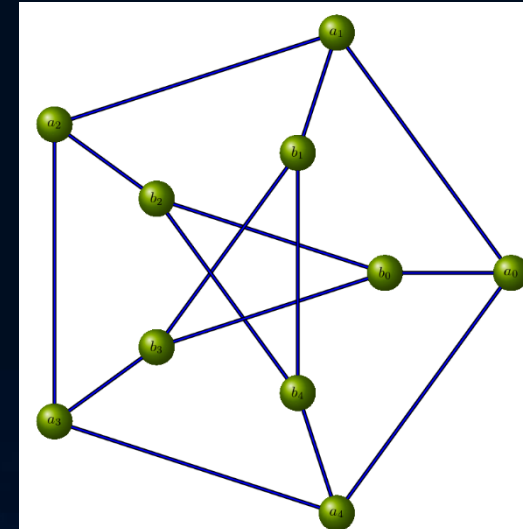
- Separability is *not* invariant under graph isomorphism. Vertex labelling is important.
- In [Braunstein et al, 2006] it was shown that:
 1. The complete graph is *separable* under all vertex labellings.
 2. The star graph is *entangled* under all vertex labellings.
 3. The Petersen graph is separable or entangled depending on the vertex labelling.



Complete graph



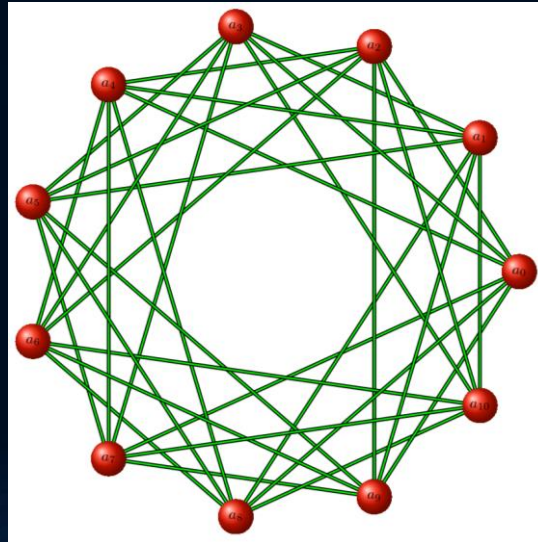
Star graph



Petersen graph

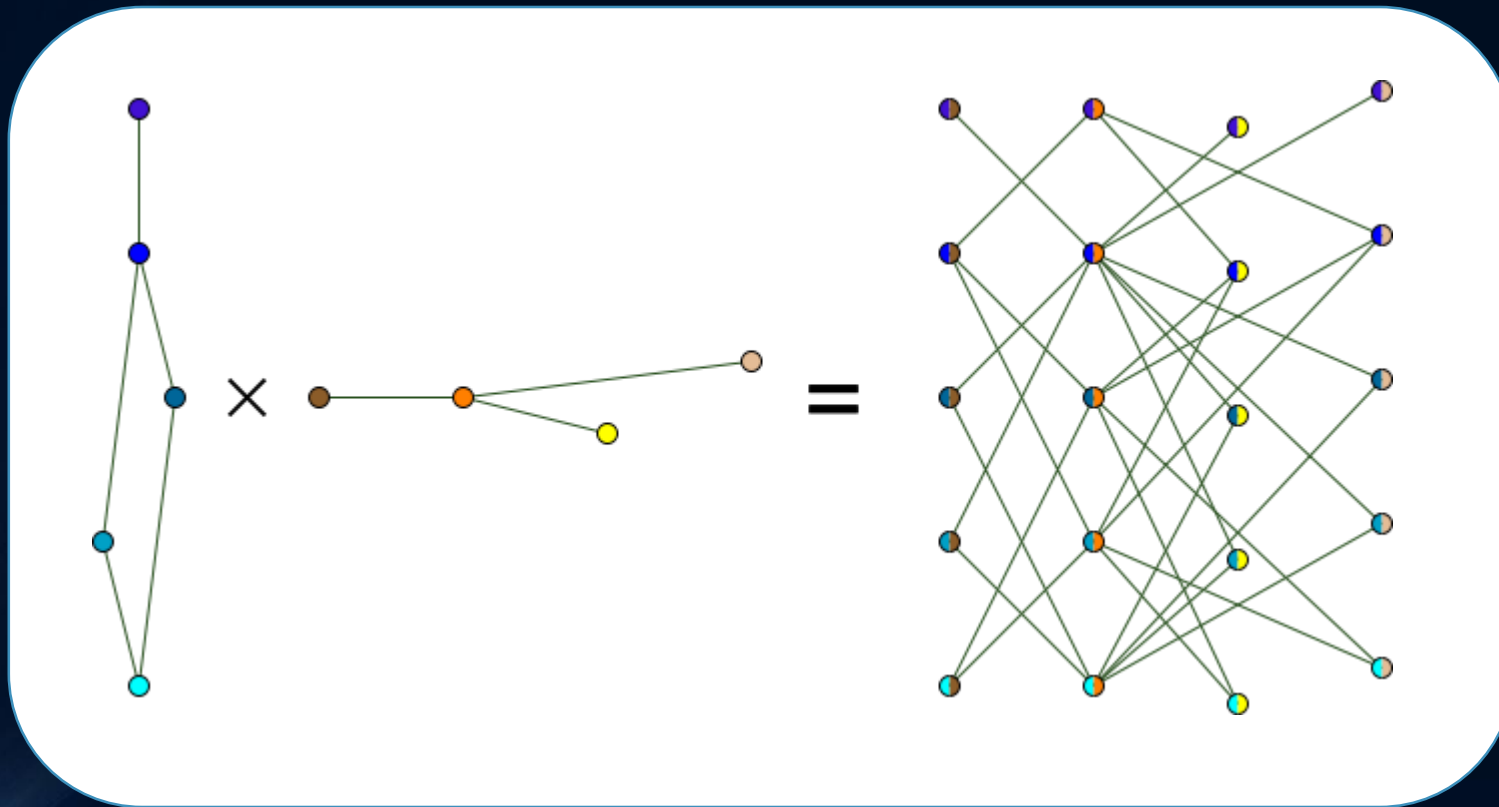
Separability of Laplacian matrices

- Vertex degree condition is *not* a sufficient condition for separability of Laplacian matrices [Hildebrand et al., 2008].
- However, vertex degree condition (and thus also PPT) is *necessary and sufficient* for separability when $p=2$ [Wu, 2006].
- Circulant graphs with canonical vertex labelling are separable [Braunstein et al., 2006].



Effect of graph operations on separability

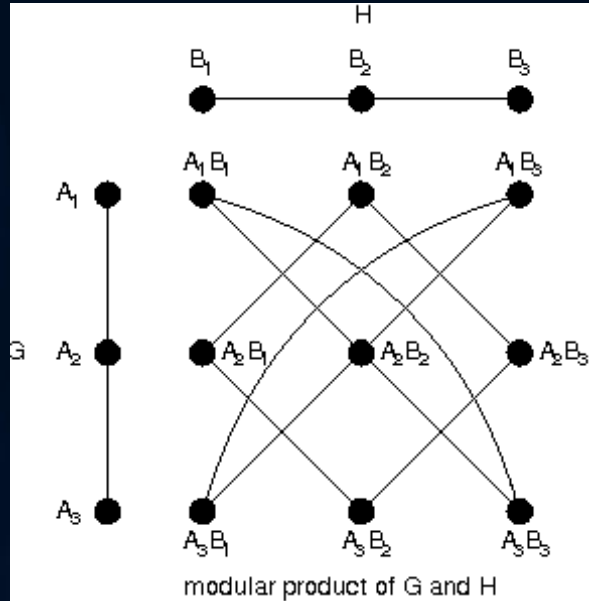
- Tensor products of graphs result in a separable Laplacian matrix [Braunstein et al., 2006].



https://en.wikipedia.org/wiki/Tensor_product_of_graphs

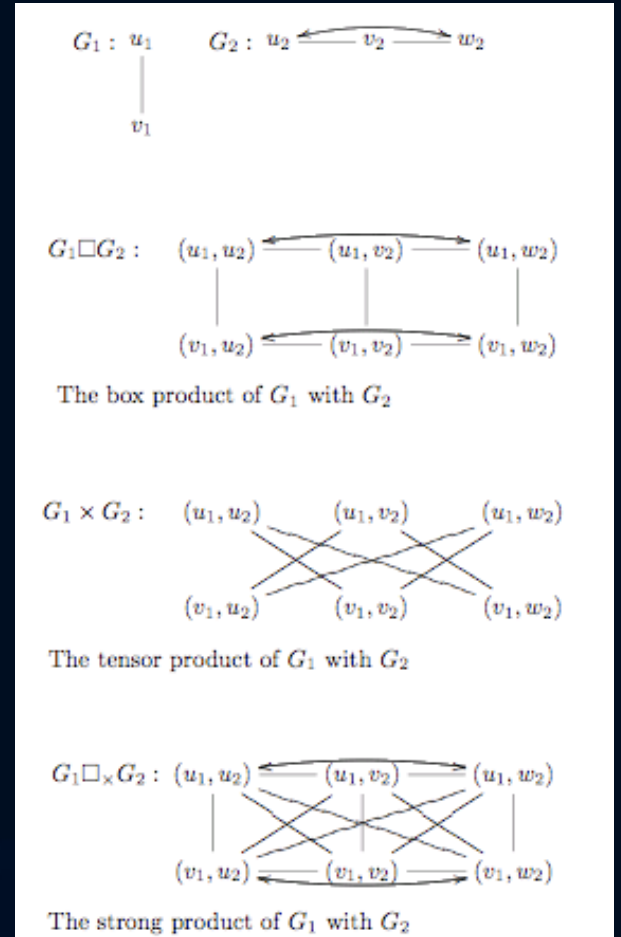
Effect of graph operations on separability

- Any type of products of graphs (Cartesian, lexicographical, tensor, strong, modular, etc.) results in a separable Laplacian matrix [Wu, 2009].



http://en.wikipedia.org/wiki/Modular_product_of_graphs

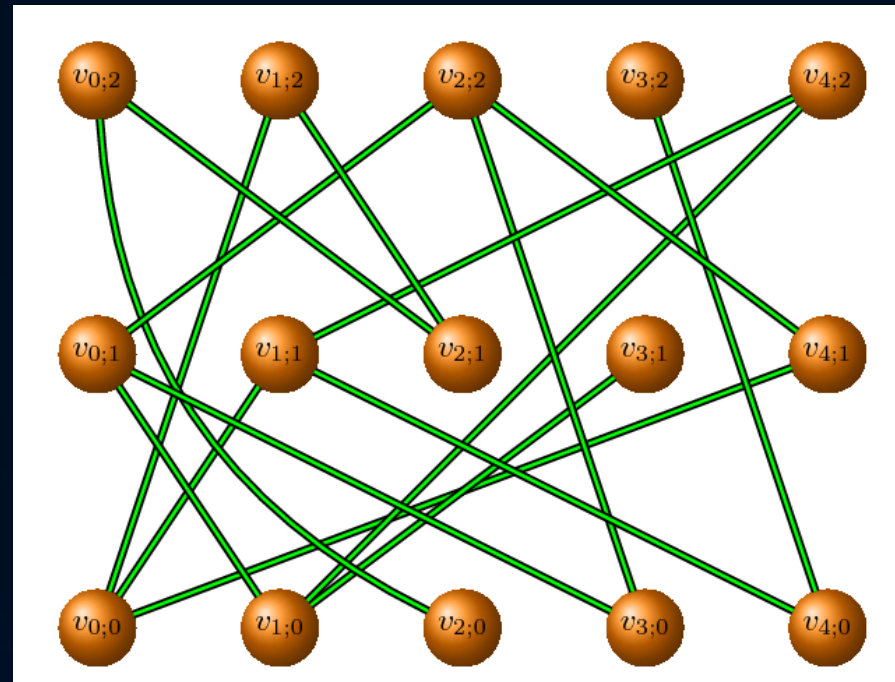
- Corollary: complete graphs are separable since complete graphs are strong products of complete graphs.
- Sums of graphs preserve separability but union of graphs does not preserve separability [Wu, 2009].



http://wiki.csisusmath.net/index.php?title=A_Reference_to_Some_Common_Binary_Operations_on_Graphs

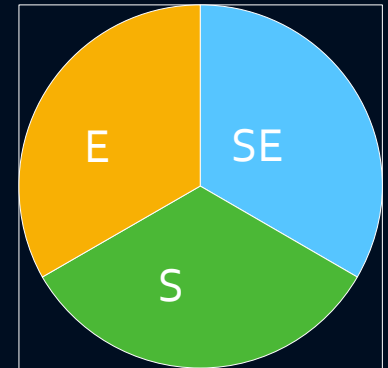
A sufficient condition for separability

- *Theorem:* If the number of edges from vertex (u,v) to vertices of the form (w,\bullet) is the same as the number of edges from (w,v) to vertices of the form (u,\bullet) , then the density matrix is separable [Wu, 2006].

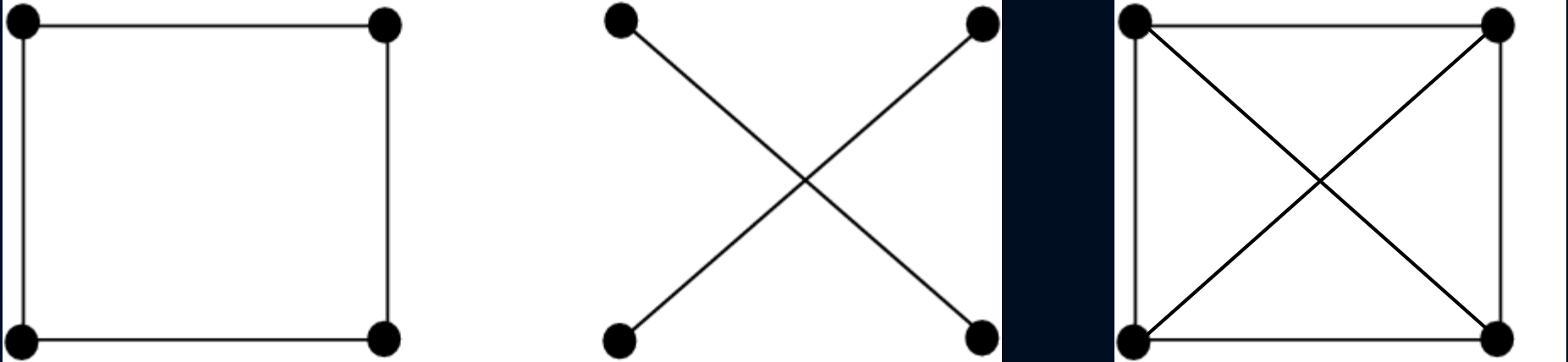


Invariance of separability under graph isomorphism

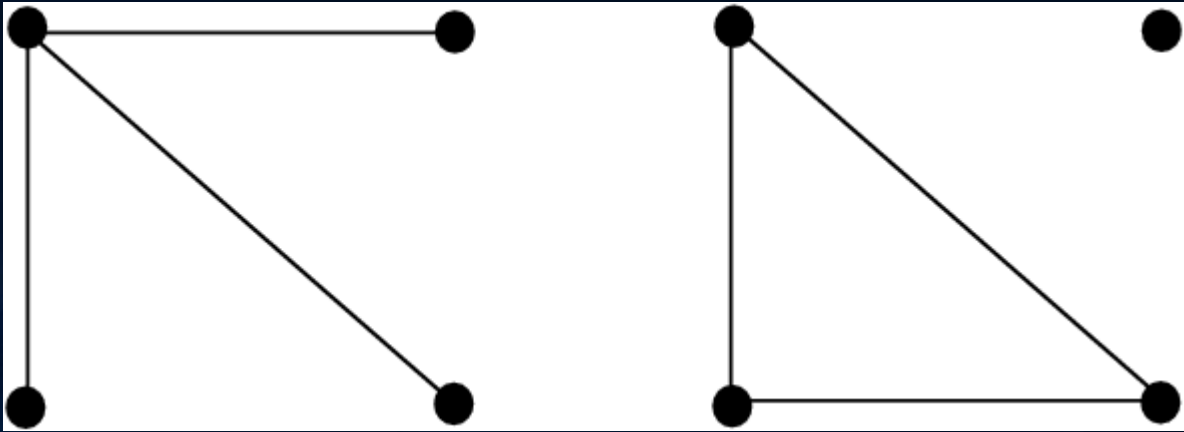
- Separability and entanglement are not invariant under graph isomorphism in general.
- Braunstein et al. ask the question: For which graphs are these properties invariant under graph isomorphism?
- Partition graphs into 3 classes:
 1. **E**: normalized Laplacian matrix is entangled under all vertex labellings
 2. **S**: normalized Laplacian matrix is separable under all vertex labellings
 3. **SE**: normalized Laplacian matrix is entangled for some vertex labellings and separable for others.
- It turns out that each of these 3 classes are nonempty for each n .
- For $p=2$, vertex degree condition can be used to determine E, S, and SE.



Partitions for 2 x 2



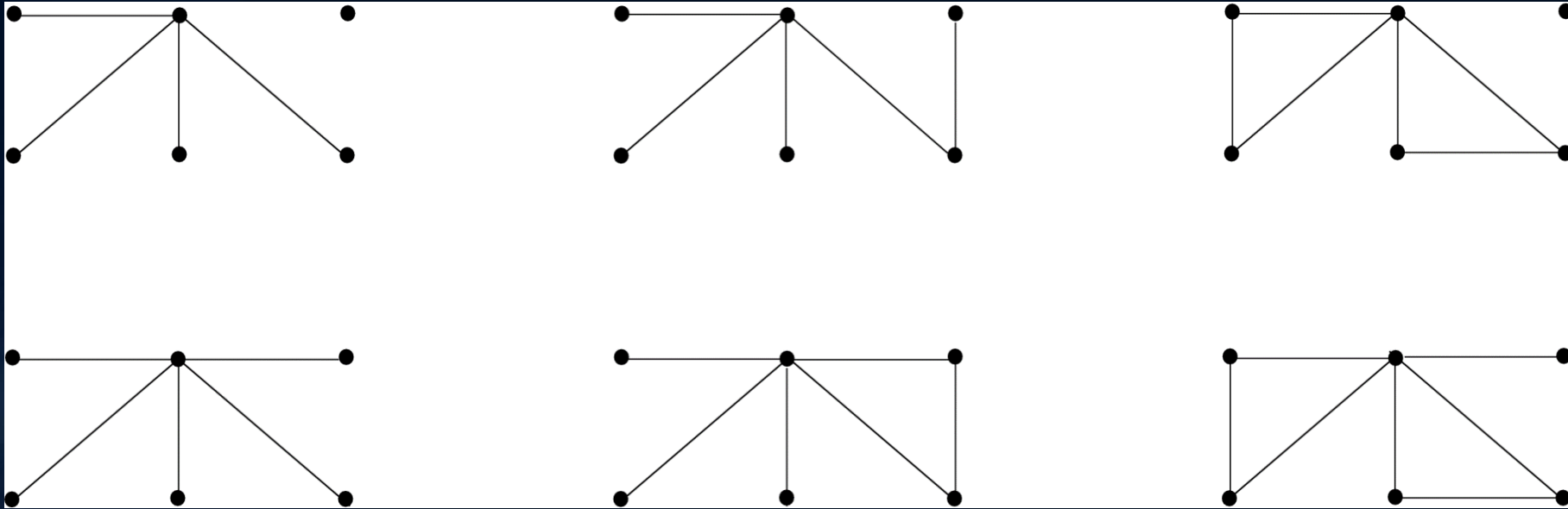
S



E

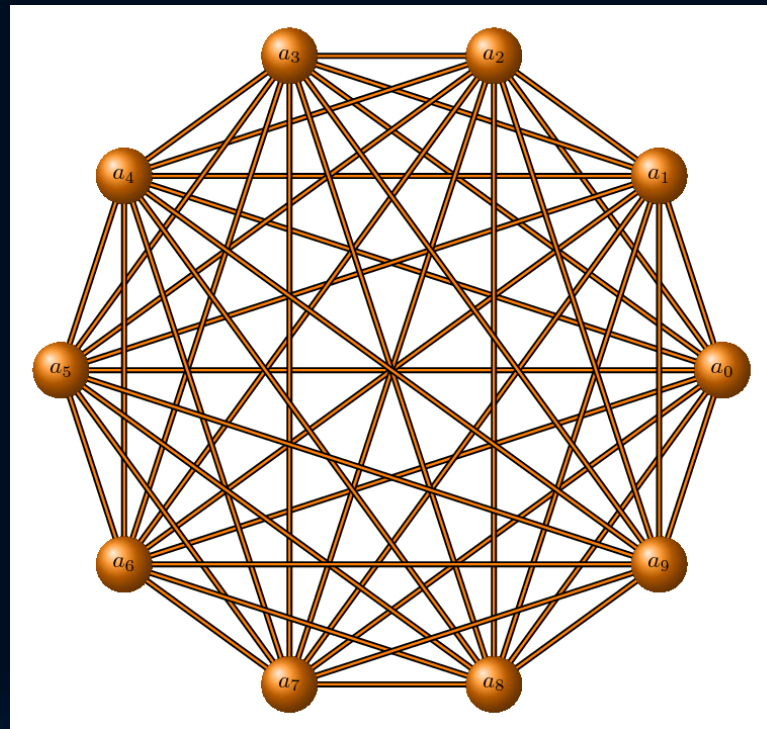
Partition for 2×3

- S is the complete graph K_6
- These following 6 graphs and their complements form E



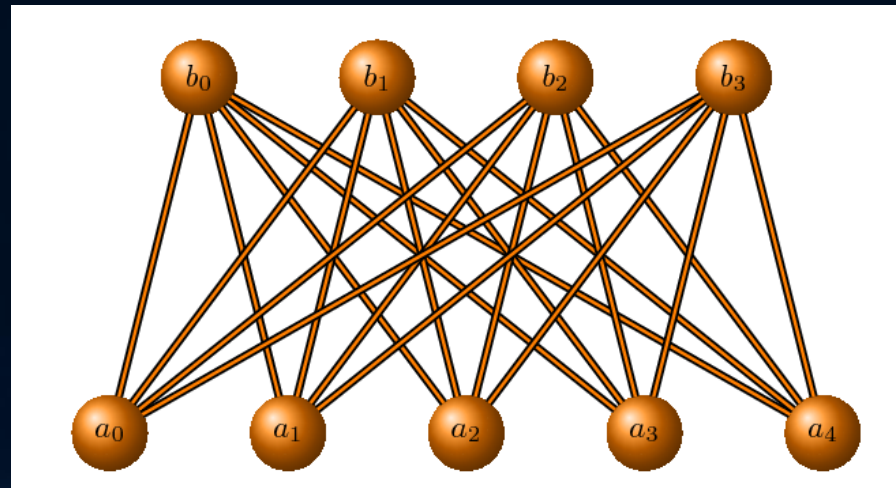
Characterization of the set S

- For $n > 4$, S consists of the complete graph K_n [Wu, 2009].
- For all non-complete graphs, there exists a vertex labelling such that the resulting density matrix is entangled.



Characterization of the set SE and E

- For $n > 4$ and $p \mid r$, complete bipartite graphs $K_{r,n-r}$ and their complements belong to class SE.
- For $r < q$ and $p \mid r$, complete bipartite graphs $K_{r,n-r}$ and their complements belong to class E [Wu, 2008].
- Complete characterization of SE and E is still an open problem.



Counting the number of separable and entangled Laplacian matrices and labeled graphs

- How many labeled graphs correspond to separable or entangled density matrices?
- We can ignore the empty graph since it has trace 0.
- Number of nonempty labeled graphs of n vertices is

$$L(n) = 2^{\frac{n(n-1)}{2}} - 1$$

- Definition: a square matrix is *line sum symmetric* if the sum of the i -th row is equal the sum of the the i -th column for all i .
- Theorem [Wu, 2006]: A normalized Laplacian matrix A is separable if $A^{i,j}$ is line sum symmetric for all i,j .

Number of separable and entangled graphs

- Definition: $L_s(p,q)$ and $L_e(p,q)$ are the number of nonempty labeled graphs corresponding to separable and entangled density matrices of $n = pq$ vertices.

$$L_s(p,q) + L_e(p,q) = L(n) = 2^{n(n-1)/2} - 1$$

- Definition: Let $N_s(n)$ denote the number of n by n 0-1 matrices that are line sum symmetric and $N_e(n)$ denote the number of n by n 0-1 matrices that are not line sum symmetric.
- $N_s(n) + N_e(n) = 2^{n^2}$
- The first few values of $N_s(n)$ are: 2, 8, 80, 2432, 247552, 88060928, 112371410944, 523858015518720, 9041009511609073664, 583447777113052431515648 (OEIS sequence A229865).

Number of labeled graphs with at least one pendant vertex

- Definition: Let $M_n(i)$ denote the number of symmetric n by n 0-1 matrices such that
 - There is at least one row with a single 1
 - The diagonal entries are 0
 - There are $2i$ nonzero elements in the matrix.
- These matrices are the set of adjacency matrices of labeled graphs of n vertices and i edges with at least one vertex of degree 1 (i.e. has at least one pendant vertex).

n	$M_n(1)$	$M_n(2)$	$M_n(3)$	$M_n(4)$	$M_n(5)$	$M_n(6)$	$M_n(7)$	$M_n(8)$
1	0							
2	1							
3	3	3						
4	6	15	16	12				
5	10	45	110	195	210	120	20	
6	15	105	435	1320	2841	4410	4845	3360
7	21	210	1295	5880	19887	51954	106785	171360
8	28	378	3220	20265	97188	369950	1147000	2931138

OEIS A245796

<https://oeis.org/A245796>

Some properties of $M_n(i)$

- Theorem: $M_n(i) = 0$ if $i > (n-1)(n-2)/2 + 1$. For $j \geq 0, n \geq 4 + j$,

$$M_n\left(\frac{(n-1)(n-2)}{2} - j + 1\right) = n(n-1) \binom{\frac{(n-1)(n-2)}{2}}{j}$$

- For $i \leq 3$, $M_n(i)$ is equal to the number of labeled bipartite graphs with n vertices and i edges.

$$M_n(1) = \frac{n(n-1)}{2}, M_n(2) = \frac{(n+1)n(n-1)(n-2)}{8}, M_n(3) = \frac{((n+1)(n+2)+2)n(n-1)(n-2)(n-3)}{48}$$

Lower bound for $L_S(p, q)$

- L is separable if q by q submatrices $A^{i,j}$ are all line sum symmetric.
- In upper triangular part of L , there are $p(p-1)/2$ of them, resulting in $N_S(q)^{\frac{p(p-1)}{2}}$ combinations.
- There are $pq(q-1)/2$ remaining entries (edges) which form $2^{\frac{pq(q-1)}{2}}$ combinations.

$$L_S(p, q) \geq 2^{\frac{pq(q-1)}{2}} N_S(q)^{\frac{p(p-1)}{2}} - 1$$

Lower bound for $L_e(p, q)$

- L is entangled if the partial transpose does not have zero row sums.
- Replace each A^{ij} with 0 if it is line sum symmetric and 1 otherwise. This results in a p by p 0-1 matrix B . If B is the adjacency matrix of a graph with i edges and at least one pendant vertex, then the partial transpose of L does not have zero sums. There are $M_p(i)N_e(q)^i N_s(q)^{\frac{p(p-1)}{2}-i}$ such combinations.
- As before, there are $pq(q-1)/2$ remaining entries which form $2^{\frac{pq(q-1)}{2}}$ combinations.

$$L_e(p, q) \geq \sum_{i=1}^{\frac{(p-1)(p-2)+1}{2}} M_p(i)N_e(q)^i N_s(q)^{\frac{p(p-1)}{2}-i} 2^{\frac{pq(q-1)}{2}}$$

Upper and lower bounds for numbers of separable and entangled graphs

- Theorem [Wu, 2016]:

$$L_s(p, q) \geq 2^{\frac{pq(q-1)}{2}} N_s(q)^{\frac{p(p-1)}{2}} - 1$$

$$L_s(p, q) \leq L(pq) - \sum_{i=1}^2 \frac{(p-1)(p-2)+1}{2} M_p(i) N_e(q)^i N_s(q)^{\frac{p(p-1)}{2}-i} 2^{\frac{pq(q-1)}{2}}$$
$$L_e(p, q) \leq L(pq) - 2^{\frac{pq(q-1)}{2}} N_s(q)^{\frac{p(p-1)}{2}} - 1$$

$$L_e(p, q) \geq \sum_{i=1}^2 \frac{(p-1)(p-2)+1}{2} M_p(i) N_e(q)^i N_s(q)^{\frac{p(p-1)}{2}-i} 2^{\frac{pq(q-1)}{2}}$$

Upper and lower bounds for numbers of separable graphs

- When $p = 2$, the upper and lower bounds coincide and we have exact values for $L_s(2, q)$ and $L_e(2, q)$

$$L_s(2, q) = 2^{q(q-1)} N_s(q) - 1$$

$$L_e(2, q) = 2^{q(q-1)} N_e(q)$$

- This is a consequence of the fact that the line sum symmetry condition for entanglement and separability is both necessary and sufficient when $p = 2$.

References

- S. L. Braunstein, S. Ghosh, and S. Severini, "The Laplacian of a graph as a density matrix: a basic combinatorial approach to separability of mixed states," *Annals of Combinatorics*, vol. 10, pp. 291-317, 2006.
- S. L. Braunstein, S. Ghosh, T. Mansour, S. Severini, and R. C. Wilson, "Some families of density matrices for which separability is easily tested," *Physical Review A*, vol. 73, p. 012320, 2006.
- L. Gurvits, "Classical deterministic complexity of Edmonds' Problem and quantum entanglement," *Proceedings of the thirty-fifth ACM Symposium on Theory of Computing*, pp. 10-19, 2003.
- R. Hildebrand, S. Mancini, S. Severini, "Combinatorial laplacians and positivity under partial transpose," *Math. Struct. in Comp. Sci.* vol.18, pp. 205-219, 2008.
- M. Horodecki, P. Horodecki, and R. Horodecki, "Separability of mixed states: necessary and sufficient conditions," *Physics Letters A*, vol. 223 pp. 1-8, 1996.
- M. Nielsen and I. Chuang, *Quantum computation and quantum information*, Cambridge University Press, 2000.
- A. Peres, "Separability criterion for density matrices," *Physical Review Letters*, vol. 77, no. 8, pp 1413-1415, 1996
- Z. Wang and Z. Wang, "The tripartite separability of density matrices of graphs," *The Electronic Journal of Combinatorics*, vol. 14, p. R40, 2007.
- C. W. Wu, "Conditions for separability in generalized Laplacian matrices and diagonally dominant matrices as density matrices," *Physics Letters A*, vol. 351, no. 1-2, pp. 18-22, 2006.
- C. W. Wu, "Multipartite separability of laplacian matrices of graphs," *The Electronic Journal of Combinatorics*, vol. 16, no. 1, p. R61, 2009.
- C. W. Wu, "On graphs whose Laplacian matrix's multipartite separability is invariant under graph isomorphism," *Discrete Mathematics*, vol. 310, no. 21, pp. 2811-2814, 2010.
- C. W. Wu, "Graphs whose normalized Laplacian matrices are separable as density matrices in quantum mechanics," *Discrete Mathematics*, vol. 339, no. 4, pp. 1377-1381, 2016.