Constructing physically intuitive graph invariants

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In this brief note, I try to give a simple example of where physical intuition about a collection of interacting qubits can lead to the construction of "natural" versions of what are, generically, quite abstract mathematical objects - in this case, graph invariants.

By a graph, a mathematician generally means a collection of points (vertices) and a list indicating how they are connected (a collection of edges). The study of graphs and their properties is a huge industry, with applications from the completely abstract (e.g., classification of algebras) to the very applied (e.g., network routing). The simplest type of graph, and the only type which I'll consider here, is one that has either zero or one (no multiple) undirected connections between any two vertices.

Given two graphs, such as in Fig. 1., one of the simplest questions to ask is whether they are actually the same graph; this is known as the graph isomorphism problem. If the two graphs are different, the question is often simple to decide. For example, the two graphs may have different numbers of vertices, although these two do not. If they have the same number of vertices they may have a different number of edges, although again these two do not. If they have the same number of vertices and edges, it may be, as in Fig. 1., that only one of the graphs has a vertex which is connected to exactly four other vertices, indicating clearly the graphs cannot be isomorphic. More generally, we can list the degrees of each graph's vertices and check if the lists are identical. (Note that we are only interested in the underlying connectivity of the graph, and so the distances between vertices are not important; the same graph can be drawn many different ways.)

Once we have performed these few simple checks, which I should emphasize are capable only of telling us whether the graphs are different, things get a little trickier. To be convinced that two graphs are the same, we need to find a map of the vertices of graph 2 to those of graph 1. That is, we try and find a relabelling of the second graph's vertices such that it is now manifestly clear that it is the same as the first graph. The problem is that the number of ways we can re-label the N vertices of a graph is N! - the number of permutations of N items. This amounts to a very large number of possible relabellings, and for modest values of N searching through them all becomes computationally infeasible. (Of course if someone magically hands us the correct relabelling it is very easy to check that the two graphs are the same!)

Fig. 1. Two non-isomorphic ten vertex graphs

In this note I'll be considering graph invariants. These are properties of the graph, such as number of vertices, number of edges or degrees of vertices mentioned above, which are relatively easy to compute and which must be the same if the two graphs are the same. That is, if we compute the graph invariants for two graphs and they are different we know for sure that the graphs are different; if they're the same we have learned nothing.

A common way of encoding a graph is through its adjacency matrix - a real symmetric matrix with a 1 at position (i, j) if vertex i is connected to vertex j and a zero otherwise. For example, the adjacency matrices of the two graphs in Fig. 2. are

$$A = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$ (1)
Given the adjacency matrices $G_1$, $G_2$ of two graphs, we rephrase the problem of deciding whether the two graphs are isomorphic, as the question as to whether there exists a permutation matrix $\sigma$ such that $\sigma^T G_2 \sigma = G_1$. A more sophisticated graph invariant than those mentioned above consists of the eigenvalues of the adjacency matrix. That is, if the eigenvalues of $G_2$ are different from those of $G_1$, then $G_1$ and $G_2$ are definitely not isomorphic. This is because the eigenvalues of $\sigma^T G_2 \sigma$ are solutions to the equation $\det(\sigma^T G_2 \sigma - \lambda I) = 0$. Since $\sigma^T \sigma = I$, and $\det(AB) = \det(BA)$, this becomes $\det(\sigma^T (G_2 - \lambda I)\sigma) = \det(\sigma \sigma^T (G_2 - \lambda I)) = \det(G_2 - \lambda I)$; the latter is the eigenvalue equation for $G_2$. Hence applying a permutation to a matrix doesn’t change its eigenvalue equation.

Spectral graph theory is the area of mathematics devoted to analyzing graphs through the eigenvalue spectra of their adjacency matrix; whole books have been written on the subject [1]. As with any graph invariants however, there exist annoying non-isomorphic graphs which are not distinguished by them. The two 5-vertex graphs $A$ and $B$ of Fig. 2 and Eq. (1), are an example, they both have the eigenvalues $\{-2, [0]^3, 2\}$. (Obviously these two graphs could be distinguished by other means!) What I will explain later on, is that if we have a 5-dimensional adjacency matrix $G$, and from its elements we construct the 10-dimensional symmetric matrix

$$
G^{(2)} = \begin{pmatrix}
0 & G_{23} & G_{24} & G_{25} & G_{13} & G_{14} & G_{15} & 0 & 0 & 0 \\
G_{23} & 0 & G_{34} & G_{35} & G_{12} & 0 & 0 & G_{14} & G_{15} & 0 \\
G_{24} & G_{34} & 0 & G_{45} & 0 & G_{12} & 0 & G_{13} & 0 & G_{15} \\
G_{25} & G_{35} & G_{45} & 0 & 0 & 0 & G_{12} & 0 & G_{13} & G_{14} \\
G_{13} & G_{12} & 0 & 0 & 0 & G_{34} & G_{35} & G_{24} & G_{25} & 0 \\
G_{14} & 0 & G_{12} & 0 & G_{34} & 0 & G_{45} & G_{23} & 0 & G_{25} \\
G_{15} & 0 & 0 & G_{12} & G_{35} & G_{45} & 0 & 0 & G_{23} & G_{24} \\
0 & G_{14} & G_{13} & 0 & G_{24} & G_{23} & 0 & 0 & G_{45} & G_{35} \\
0 & G_{15} & 0 & G_{13} & G_{25} & 0 & G_{23} & G_{45} & 0 & G_{34} \\
0 & 0 & G_{15} & G_{14} & 0 & G_{25} & G_{24} & G_{35} & G_{34} & 0
\end{pmatrix},
$$

(2)

then the eigenvalues of this larger matrix are a graph invariant, and in fact are more powerful invariant than those of the original matrix $G$. If we take the two adjacency matrices $A, B$ of Eq. (1) and use Eq. (2) to construct $A^{(2)}$ and $B^{(2)}$, what I will call their level 2 matrices, then we find that the eigenvalues of $A^{(2)}$ are $\{-\sqrt{6}, [-\sqrt{2}]^3, [0]^3, [\sqrt{2}]^3, \sqrt{6}\}$ while those of $B^{(2)}$ are $\{-2\sqrt{2}, -2, [0]^6, 2, 2\sqrt{2}\}$. The fact these eigenvalues are different proves the non-isomorphism of the two graphs.

All this is not particularly useful unless we know how to find level 2 matrices for graphs with more than 5 vertices! It turns out we can, and they are always $\binom{N}{2} \times \binom{N}{2}$ dimensional. To construct a level 2 matrix for a graph of an arbitrary number of vertices we follow this procedure. We first define an $(N - 1) \times N$ dimensional indexing matrix $I_N$ which contains the entries $1, 2, \ldots, \binom{N}{2}$ arranged as this example for $N = 6$ indicates:

$$
I_6 = \begin{pmatrix}
0 & 1 & 2 & 3 & 4 & 5 \\
0 & 0 & 6 & 7 & 8 & 9 \\
0 & 0 & 0 & 10 & 11 & 12 \\
0 & 0 & 0 & 0 & 13 & 14 \\
0 & 0 & 0 & 0 & 0 & 15
\end{pmatrix},
$$

(3)

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1 It is interesting to note that, since the $G_{ij}$’s are all equal to 1 or 0, the level 2 matrix of Eq. (2) is itself the adjacency matrix of a graph. The graphs of Fig. 1. are in fact the graphs of $A^{(2)}$ and $B^{(2)}$. Note that this means we can use the whole machinery already developed for the spectral graph theory of adjacency matrices for analysing these higher level matrices.
Using this indexing matrix we define two functions: \( \alpha(i) \) is the row of \( \mathcal{I}_N \) which contains the integer \( i \), while \( \beta(i) \) is the column of \( \mathcal{I}_N \) which contains \( i \). The \( (i,j) \)th element of the level 2 matrix for a graph \( G \) is then given by

\[
G^{(2)}_{ij} = \delta_{\alpha(i)\alpha(j)}G_{\beta(i)\beta(j)} + \delta_{\alpha(i)\beta(j)}G_{\beta(i)\alpha(j)} + \bar{\delta}_{\beta(i)\alpha(j)}G_{\alpha(i)\beta(j)} + \bar{\delta}_{\beta(i)\beta(j)}G_{\beta(i)\beta(j)},
\]

where \( \delta \) denotes the usual kronecker delta function.

This all seems, on the face of it, a little unlikely. So now for the physics which underlies the construction of the \( G^{(2)} \) matrices, and which in fact shows us how to construct level \( n \) matrices \( G^{(n)} \) (with each value of \( n \) giving a stronger invariant than the preceding one) up to level \( n = \lfloor \frac{N}{2} \rfloor \).

We begin by considering \( N \) interacting qubits (two-level atoms say), each of ground state \( |0\rangle \) and excited state \( |1\rangle \) with transition frequency \( \omega_0 \). Assume they are interacting via an (excitation-)exchange Hamiltonian, but that qubit \( i \) only interacts with qubit \( j \) if vertices \( i \) and \( j \) are connected in the graph \( G \). The generic interaction Hamiltonian is of the form:

\[
H_{\text{int}}(G) = g \sum_{i,j} (S_i^+S_j^- + S_i^-S_j^+),
\]

Here \( S_i^+ = |1\rangle\langle 0| \) \( (S_i^- = |0\rangle\langle 1|) \) is the raising(lowering) operator for qubit \( i \), and \( i \sim j \) means vertex \( i \) is connected to vertex \( j \) in \( G \). \( g \) is a coupling constant, which we take to be equal for all interacting qubits (the “small sample” or “long wavelength” limit for atomic spectrosocists), and we normalize it to 1.

The number of possible states of the \( N \) qubits is \( 2^N \). For our purposes we will label the states by which qubits are excited (in the state \(|1\rangle \)). For example the 5 qubit state \(|0\rangle \otimes |1\rangle \otimes |0\rangle \otimes |0\rangle \otimes |1\rangle \) will be labelled simply as \(|25\rangle \), which is a “bi-exciton” state. The nature of the Hamiltonian \( H_{\text{int}}(G) \) is such that its matrix elements between states with a different number of excited qubits are always 0; e.g. \( \langle 23|H_{\text{int}}(G)|134 \rangle = 0 \) regardless of \( N \). This is because the interaction conserves excitation - if one qubit goes “up”, the other must come “down”. Furthermore, it is clear from the form of \( G^{(2)} \), that even if the two states have the same number of excited qubits, the matrix element of \( H_{\text{int}}(G) \) can only be non-zero if the two states have a different amount of excitation in one, and only one, pair of qubits.\(^2\)

Consider the subset of states which contain only one excited qubit: \(|1\rangle, |2\rangle, \ldots, |N\rangle \). If we write the matrix for \( H_{\text{int}}(G) \) using this subset of states, we find precisely the adjacency matrix of \( G \). The eigenvalues of this matrix tell us at which energies we would see absorption lines if we shone appropriate light at our qubit cluster. (Since we have considered just the interaction Hamiltonian, these eigenvalues are strictly speaking the shifts from \( \omega_0 \) of the energy levels). Now, thinking physically, its obvious that the order in which some human experimenter chooses to label the atoms is irrelevant to the energy shifts she will see. In other words, these energy shifts form a graph invariant (as we know).

The level 2 matrices discussed above are simply the matrices for what a spectroscopist would call the “bi-exciton” energy manifold. That is, we look at the subset of states for which two atoms are excited: \(|12\rangle, |13\rangle, \ldots, |1N\rangle, |23\rangle, \ldots, |2N\rangle, \ldots, |(N-1)N\rangle \). These form the second submatrix of \( H_{\text{int}}(G) \). Once again it is physically obvious that the way we relabel the atoms cannot affect the physical properties we observe, and thus the eigenvalues of this matrix also form a graph invariant.

The main purpose of this short note is to point out that any physical quantity we can compute for this hypothetical cluster of qubits, for which its intuitively obvious the labelling order is irrelevant, forms a graph invariant. This includes the emission spectrum, the absorption spectrum, total transition rates from a given exciton manifold to the one below it, the average amount of pairwise entanglement when the atoms sit in a thermal bath, and so on. What is interesting about these other possibilities, is that they naturally incorporate the eigenvectors of the adjacency matrix, something which from my (admittedly very brief) reading of the graph theory literature appear to be somewhat underexploited.

Finally I should mention that graph theorists sometimes use a slightly different matrix for encoding graphs, known as the Laplacian matrix. This is essentially the adjacency matrix on the off-diagonal elements, but now with non-zero

\(^2\) In general \( H_{\text{int}}(G) \) is block diagonal, with each block corresponding to a different exciton level (number of excited qubits) \( n \). Each block is a \( \binom{N}{n} \times \binom{N}{n} \) matrix whose eigenvalues form a graph invariant. In abstract terms, the level \( n \) matrix \( G^{(n)} \) can be constructed by indexing each row and each column of the matrix by an \( n \)-tuple of integers chosen from 1, \ldots, \( N \). Denote the \( n \)-tuple corresponding to row/column \( i \) by \( S_i \). The element \( G^{(n)}_{i,j} \) can be nonzero only if the set \( S_i \cup S_j \setminus S_i \cap S_j \) contains exactly 2 integers, say \( a, b \). If it does, then \( G^{(n)}_{i,j} = G_{a,b} \).
diagonal elements whose magnitudes reflect the degree of that vertex. Studying the eigenvalues and other properties of these matrices seems to also be quite popular. In the quantum mechanical picture I’m advocating here, the Laplacian matrix arises when we use not just the interaction Hamiltonian, but an appropriately chosen “free” Hamiltonian as well. Similar constructions to those above yield “higher level” Laplacian matrices, and once again they can form stronger invariants than the simple, level one, standard Laplacian matrix.

I expect that in fact physicists stand to gain more from learning some spectral graph theory, than mathematicians stand gain from learning some physics. For example, the automorphism groups of a graph, which are much studied by mathematicians, would seem to be directly related to certain optical properties of the emission spectra. However the purpose of this note is to give physicists some feeling of how physical intuition can lead to natural invariants of abstract mathematical structures. The most famous (but vastly more complicated) example of this is of course Ed Witten’s construction of knot invariants by considering an appropriate conformal field theory.

References

[1] The two resources I have used are: Chapter 1 of Edwin van Dam’s thesis at [http://cwis.kub.nl/~few5/center/staff/dam/pub.htm](http://cwis.kub.nl/~few5/center/staff/dam/pub.htm); and Chapter 1 of the book *Spectral Graph Theory* by Fan Chung, which is available at: [http://math.ucsd.edu/~fan/cbms.pdf](http://math.ucsd.edu/~fan/cbms.pdf)

An afterword for graph theorists

To test the ideas discussed above I chose two “very similar” 24 vertex, strongly regular graphs with identical adjacency (and Laplace) matrix spectra. They are contained in a list available at [http://www.maths.gla.ac.uk/~es/reggraph.html](http://www.maths.gla.ac.uk/~es/reggraph.html) in the file “I.graphs.24.gz”. The two graphs I chose have four distinct eigenvalues of their adjacency matrices. The graphs are:

\[
\text{Spectrum} = \{[8]^1, [2]^{11}, [-2]^9, [-4]^3\}
\]

1. FF0001E3800003F000030F001998019FC03A30C21E1E01CC303C1542A892610A45292
   \[|\text{Aut}| = 384 \begin{pmatrix} 1,2,7,8,9,10,11,12 \end{pmatrix}(3,4,5,6,13,14,15,16,17,18,19,20,21,22,23,24)\]

2. FF0001E3800003F000030F001998019FC03A30C21E1E01CC303C1542A862911231692
   \[|\text{Aut}| = 384 \begin{pmatrix} 1,2,7,8,9,10,11,12 \end{pmatrix}(3,4,5,6,13,14,15,16,17,18,19,20,21,22,23,24)\]

(The adjacency matrix is found by converting the hexadecimal number to binary, this binary string is a concatenation of the upper triangular part of the adjacency matrix. I have no idea about the notation used for the automorphism group.)

It turns out that the level two matrices of these graphs still have identical spectra, however at level three the spectra are different, showing the graphs to not be isomorphic. Note that in general the level k matrix is \(O(N^k \times N^k)\), which according to complexity theorists is not too bad. However, I assure you it means programming skills far exceeding mine are required to play around with any much larger examples.