Quantum Physics and Graph Spectra

Chris Godsil

Bristol, July 2009

Outline

Summary

Quote

Hydrogen is a colorless, odorless gas which given sufficient time,

Summary

Quote

Hydrogen is a colorless, odorless gas which given sufficient time, turns into people. (Henry Hiebert)

Outline

Unitary Operators

Suppose X is a graph with adjacency matrix A.

Definition

We define the operator $H_X(t)$ by

$$H_X(t) := \exp(iAt).$$

An Example

We have

$$H_{K_2}(t) = \begin{pmatrix} \cos(t) & i\sin(t) \\ i\sin(t) & \cos(t) \end{pmatrix}$$

Note that $H_X(t)$ is symmetric, because A is, and unitary because

$$H_X(t)^* = \exp(-iAt) = H_X(t)^{-1}.$$

Probability Distributions

If H is unitary, the Schur product

$$H \circ \overline{H}$$

is doubly stochastic. Hence each row determines a probability density. (It determines a continuous quantum walk.)

State Transfer

Definition

We say that perfect state transfer from the vertex u to the vertex v occurs at time τ if

$$|(H_X(\tau))_{u,v}| = 1.$$

Example:

$$H_{K_2}(\pi/2) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix},$$

thus we have perfect state transfer between the end vertices of K_2 at time $\pi/2$.

More Examples

Since

$$H_{X \square Y}(t) = H_X(t) \otimes H_Y(t)$$

it follows that if perfect state transfer from u to v in X occurs at time τ, then we also have perfect state transfer from (u, u) to (v, v) in $X \square X$ at time τ.

So we get perfect state transfer between antipodal vertices in the d-cube Q_d at time $\pi/2$.

Outline

Squaring

If perfect state transfer from 1 to 2 occurs at time τ, then

$$H_X(\tau) = \begin{pmatrix} 0 & \gamma & 0 & \dots & 0 \\ ? & 0 & ? & \dots & ? \\ \vdots & \vdots & & Q & \\ ? & 0 & & & \end{pmatrix}$$

where $|\gamma| = 1$. Consequently $|(H_X(\tau))_{2,1}| = 1$ and

$$H_X(2\tau) = \begin{pmatrix} \gamma^2 & 0 & 0 & \dots & 0 \\ 0 & \gamma^2 & 0 & \dots & 0 \\ \vdots & \vdots & & Q & \\ 0 & 0 & & & \end{pmatrix}$$

Periodicity

Definition

We say that X is periodic at the vertex u with period τ if $|(H_X(\tau))_{u,u}| = 1$. We say X is *periodic* if it is periodic at each vertex (with the same period).

Lemma (Godsil)

If perfect state transfer from u to v occurs at time τ, then X is periodic at u and v with period 2τ.

Spectral Decomposition

We have

$$A = \sum_{\theta} \theta E_{\theta}$$

where θ runs over the distinct eigenvalues of A and the matrices E_{θ} represent orthogonal projection onto the eigenspaces of A.

Spectral Decomposition

We have

$$A = \sum_{\theta} \theta E_{\theta}$$

where θ runs over the distinct eigenvalues of A and the matrices E_{θ} represent orthogonal projection onto the eigenspaces of A. Further if f is a function on the eigenvalues of A, then

$$f(A) = \sum_{\theta} f(\theta) E_{\theta}$$

and therefore

$$H_X(t) = \sum_{\theta} \exp(i\theta t) E_{\theta}.$$

Integer Eigenvalues

Lemma

If the eigenvalues of X are integers, it is periodic with period 2π.

Proof.

$$H_X(\pi) = \sum_\theta E_\theta = I.$$

□

A Converse

Theorem (Godsil)

If X is a connected regular graph, then it is periodic if and only if its eigenvalues are integers.

Paths

The graph P_3 has perfect state transfer between its end-vertices. It eigenvalues are

$$-\sqrt{2}, \quad 0, \quad \sqrt{2}.$$

We do not get perfect state transfer between end-vertices on P_n when $n \geq 4$. We do get perfect state transfer in the Cartesian powers of P_3. (Christandl et al)

Outline

An Involution

Theorem (Godsil)

If X is vertex transitive and perfect state transfer occurs at time τ, then

$$H_X(\tau) = \gamma \begin{pmatrix} 0 & 1 & & & & & \\ 1 & 0 & & & & & \\ & & 0 & 1 & & & \\ & & 1 & 0 & & & \\ & & & & \ddots & & \\ & & & & & 0 & 1 \\ & & & & & 1 & 0 \end{pmatrix} = \gamma T$$

A Central Automorphism

The involution T must be an automorphism in the center of $\mathrm{Aut}(X)$. Hence

A Central Automorphism

The involution T must be an automorphism in the center of $\mathrm{Aut}(X)$. Hence

Corollary

If perfect state transfer takes place on the vertex-transitive graph X, then $|V(X)|$ must be even.

The Multiplicity Polynomial

Definition

Assume X is vertex transitive with integer eigenvalues and let m_θ denote the multiplicity of θ as an eigenvalue. Let μ be the polynomial defined by

$$\mu(z) := \sum_\theta m_\theta z^\theta.$$

A Necessary Condition

Lemma (Godsil)

If X is vertex transitive and perfect state transfer takes place at time τ, then $\exp(i\tau)$ is a root of $\mu(z)$.

Proof.

$\operatorname{tr}(T) = 0.$ □

(And $\exp(ri\tau)$ will be a root for each odd integer r.)

Cubelike Graphs

If X is cubelike, then

$$A(X) = P_1 + \cdots + P_k$$

where $P_1, \ldots, P_k$ are commuting involutions. So

$$H_X(t) = \prod_{r=1}^{k} \exp(itP_k) = \prod_{r=1}^{k} (\cos(t)I + i\sin(t)P_r)$$

Cubelike Graphs

If X is cubelike, then

$$A(X) = P_1 + \cdots + P_k$$

where $P_1, \ldots, P_k$ are commuting involutions. So

$$H_X(t) = \prod_{r=1}^{k} \exp(itP_k) = \prod_{r=1}^{k} (\cos(t)I + i\sin(t)P_r)$$

Corollary (Bernasconi, Severini, Godsil)

We have perfect state transfer on X at time $\pi/2$ if and only if $P_1 \cdots P_k \neq I$.

Severini

Outline

Antipodal Vertices

If X has diameter d, we say that vertices at distance d are antipodal. In all examples we have where perfect state transfer takes place, the vertices involved are antipodal.

Question

Is antipodality necessary? (It is if X is distance-regular.)

Antipodal Vertices

If X has diameter d, we say that vertices at distance d are antipodal. In all examples we have where perfect state transfer takes place, the vertices involved are antipodal.

Question

Is antipodality necessary? (It is if X is distance-regular.)

I suspect antipodality is not necessary. In fact

Question

If $|V(X)| \geq 3$, can we get perfect state transfer between two adjacent vertices?

Efficiency

Question

What is the minimum number of edges in a graph where perfect state transfer takes place between two vertices at distance d?

Mixing

We say that perfect mixing occurs at time τ if, for all vertices u and v in X,

$$|(H_X(\tau))_{u,v}| = \frac{1}{\sqrt{|V(X)|}}.$$

(For example Q_d at time $\pi/4$.

Question

What can we usefully say about graphs where perfect mixing occurs?

Outline

Walk Matrices

Definition

Let A be the adjacency matrix of the graph X on n vertices and let $\mathbf{1}$ denote the all-ones vector of length n. The walk matrix of X is the $n \times n$ matrix

$$\begin{pmatrix} \mathbf{1} & A\mathbf{1} & \dots & A^{n-1}\mathbf{1} \end{pmatrix}.$$

Automorphisms

The automorphism group of X is (isomorphic to) the group of permutation matrices P that commute with A.

Lemma

If $P \in \mathrm{Aut}(X)$ then P fixes each column of W. $\square$

Automorphisms

The automorphism group of X is (isomorphic to) the group of permutation matrices P that commute with A.

Lemma

If $P \in \mathrm{Aut}(X)$ then P fixes each column of W. □

Proof.

$P\mathbf{1} = \mathbf{1}$ and therefore:

$$PA^r\mathbf{1} = A^rP\mathbf{1} = A^r\mathbf{1}.$$

□

Asymmetric Graphs

Corollary

If $\mathrm{rk}(W) = n$ *then* X *is asymmetric.* □

Awfulness

Definition

A graph X is awful if its walk matrix is invertible.

Awfulness

Definition

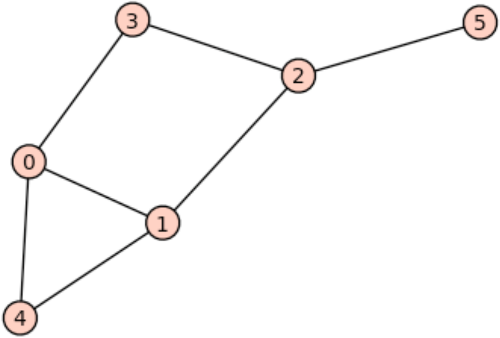
A graph X is awful if its walk matrix is invertible.

Exercise

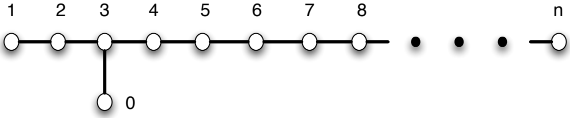
A graph is awful if and only if its complement is.

The Scapegoat

An Example



More Examples



A Sequence

6	7	9	10	15	19	21	22	25	27	30	31
34	37	39	42	45	46	49	51	54	55	57	61
66	67	69	70	75	79	81	82	85	87	90	91
94	97	99	102	105	106	109	111	114	115	117	121

Awful Algebra

Theorem (Godsil)

Let X be a graph with adjacency matrix A. The following claims are equivalent:

- *X is awful.*

Awful Algebra

Theorem (Godsil)

Let X be a graph with adjacency matrix A. The following claims are equivalent:

- *X is awful.*
- *The matrices A and J generate the algebra of all $n \times n$ matrices.*

Awful Algebra

Theorem (Godsil)

Let X be a graph with adjacency matrix A. The following claims are equivalent:

- *X is awful.*
- *The matrices A and J generate the algebra of all $n \times n$ matrices.*
- *The matrices $A^i J A^j$ $(0 \leq i, j < n)$ are a basis for the space of $n \times n$ matrices.*

A Conjecture

Conjecture

Almost all graphs are awful.

Outline

Walk Equivalence

Definition

Let X and Y be graphs with walk matrices W_X and W_Y respectively. We say that X and Y are walk equivalent if

$$W_X^T W_X = W_Y^T W_Y.$$

Walk Equivalence

Definition

Let X and Y be graphs with walk matrices W_X and W_Y respectively. We say that X and Y are walk equivalent if

$$W_X^T W_X = W_Y^T W_Y.$$

Note that

$$(W^T W)_{i,j} = \mathbf{1}^T A^{i+j} \mathbf{1}.$$

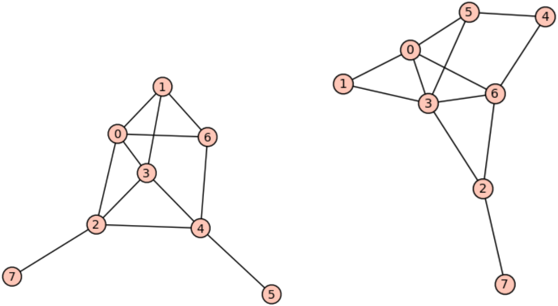
Hence any two k-regular graphs on n vertices are walk equivalent.

Cospectral Graphs

Lemma

If two graphs X and Y are cospectral with cospectral complements, they are walk equivalent.

Two Walk-Equivalent Awful Graphs



Walk-Equivalent Awful Graphs

Theorem (Wang & Xu)

If X and Y are walk-equivalent awful graphs, then $Q = W_X W_Y^{-1}$ is orthogonal, $Q^T A_X Q = A_Y$ and $Q\mathbf{1} = \mathbf{1}$.

Example

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

Rationality

The matrix Q is clearly rational. The experimental evidence seems to indicate that usually $2Q$ is integral. If $2Q$ is integral, the structure of Q is known (Wang & Xu). Up to permutation equivalence we have:

Structure I

If

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

then we may have one of the matrices

$$\frac{1}{2}\begin{pmatrix} A & B \\ B & A \end{pmatrix}, \quad \frac{1}{2}\begin{pmatrix} A & B & 0 \\ B & 0 & A \\ 0 & A & B \end{pmatrix}, \quad \frac{1}{2}\begin{pmatrix} A & B & 0 & 0 \\ B & 0 & A & 0 \\ 0 & A & 0 & B \\ 0 & 0 & B & A \end{pmatrix}, \ldots$$

Structure IIa

Otherwise we have one of

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

$$I + P^2 + P^3 - P^4, \quad P^7 = I.$$

Structure IIb

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

$$I + Q_1 + Q_2 + Q_3 - Q_1Q_2Q_3, \quad Q_i^2 = I,\ Q_iQ_j = Q_jQ_i.$$

Outline

Generation

Theorem (Godsil)

If X is awful and A is its adjacency matrix, then the matrices

$$\exp(iAt), \quad \exp(iJt) \qquad (t \geq 0)$$

generate a dense subgroup of the unitary group.

Generation

Theorem (Godsil)

If X is awful and A is its adjacency matrix, then the matrices

$$\exp(iAt), \quad \exp(iJt) \qquad (t \geq 0)$$

generate a dense subgroup of the unitary group.

Proof.

Play with Lie algebras. □

Sparser Generators?

Let D denote the diagonal matrix of valencies of X. If X is connected then $\ker(A-D)$ is spanned by $\mathbf{1}$. By spectral decomposition, it follows that $J=\mathbf{1}\mathbf{1}^T$ is a polynomial in $A-D$.

Lemma

If X is awful, then A and D generate the algebra of all $n\times n$ matrices. □