SPIN CHAINS, GRAPHS AND STATE REVIVAL

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1. Introduction

The transfer of quantum state and the generation of entangled states are two important tasks

Set of sites labelled by integers $n = 0, 1, \ldots, N$

$|n\rangle$ characteristic vector in $\mathbb{C}^{N+1}$ which has entry 1 at position n and represents our state at location n

$U(t) = e^{-itH}$ evolution operator for some Hamiltonian H

Pick a reference site, say 0

We wish to have dynamics such that for some $t = T$

$$U(T)|0\rangle = \alpha|0\rangle + \beta|N\rangle \qquad |\alpha|^2 + |\beta|^2 = 1$$

one has then Fractional Revival (FR) at two sites.

Special cases

- Perfect State Transfer (PST) $\alpha = 0, \quad \beta = e^{i\phi}$

  State is transferred from 0 to N

- Maximally entangled state $|\alpha| = |\beta| = \frac{1}{\sqrt{2}}$

These tasks can be achieved in properly engineered spin chains, focusing on one-excitation dynamics

Also modelled in photonic waveguide lattices

This dynamics can be viewed as Quantum Walks on weighted paths

Prompted study of PST on more general graphs with the Hamiltonian taken to be the adjacency matrix (or the Laplacian)

QW on graphs have also been used in the design of algorithms (e.g. Grover, Ambainis, etc.)

GOALS :

Describe situations where one-excitation dynamics in spin lattices with PST correspond to quantum walks on graphs

Show that spins systems with PST can conversely be identified through correspondance

Consider graphs that belong to the Hamming and generalized Hamming scheme

Show that the "go-betweens" are orthogonal polynomials of the Krawtchouk type in one or more variables

2. OUTLINE

- FR and PST in spin chains
- Krawtchouk and para-Krawtchouk models
- Quantum Walks on the Hypercube
- Bivariate Krawtchouk Orthogonal Polynomials and SO(3)
- Generalized Hamming Scheme
- PST and FR in a 2-D spin lattice

3. FR and PST in spin chains

Consider H on $(\mathbb{C}^2)^{N+1}$ given by

$$H = \frac{1}{2}\sum_{l=0}^{N-1} J_{l+1}(\sigma_l^x\sigma_{l+1}^x + \sigma_l^y\sigma_{l+1}^y) + \frac{1}{2}\sum_{l=0}^{N} B_l(\sigma_l^z + 1)$$

J_{l+1} : coupling between site l and $l+1$

B_l : magnetic field at site l

$\sigma_l^x, \sigma_l^y, \sigma_l^z$: Pauli matrices with l indicating $\mathbb{C}^2$ factor on which they act

$\{|\uparrow\rangle, |\downarrow\rangle\}$ basis for $\mathbb{C}^2$

Focus on 1-excitation eigenspace

$|n\rangle$ represent state with one spin up at site n with all other spins down

Easy to see that H acts tridiagonally :

$$H|n\rangle = J_{n+1}|n+1\rangle + B_n|n\rangle + J_n|n-1\rangle$$

Problem : Find J_n, B_n such that FR occurs, i.e.

$$e^{-iTH}|0\rangle = \mu|0\rangle + \nu|N\rangle \qquad |\mu|^2 + |\nu|^2 = 1$$

Formulate as an inverse spectral problem

On 1-excitation subspace, let

$$H|x_s\rangle = x_s|x_s\rangle$$

(assume spectrum non-degenerate)

Let

$$|x_s\rangle = \sum_{n=0}^{N} \sqrt{w_s}\chi_n(x_s)|n\rangle$$

Since H on 1-excitation subspace is a Jacobi matrix, it is diagonalized by orthogonal polynomials χ_n

$$\sum_{s=0}^{N} w_s\chi_n(x_s)\chi_m(x_s) = \delta_{n,m}$$

Easy to see from action of H on $|n\rangle$ that the χ_n obey the 3-term recurrence relation

$$x_s\chi_n(x_s) = J_{n+1}\chi_{n+1}(x_s) + B_n\chi_n(x_s) + J_n\chi_{n-1}(x_s)$$

with J_n and B_n the recurrence coefficients

Since $(\sqrt{w_s}\chi_n(x_s))$ is an orthogonal matrix, we also have

$$|n\rangle = \sum_{s=0}^{N} \sqrt{w_s}\chi_n(x_s)|x_s\rangle$$

Using in FR condition

$$e^{-iTH}|0\rangle = \mu|0\rangle + \nu|N\rangle$$

one finds

$$e^{-iTx_s} = \mu + \nu\chi_N(x_s)$$

since $\chi_0(x_s) = 1$.

Start with PST : $\mu = 0 \quad \nu = e^{i\phi}$

$$e^{-i\phi}e^{-iTx_s} = \chi_N(x_s) \Longrightarrow \chi_N(x_s) = \pm 1$$

because the $\chi_n(x_s)$ are real.

A simple argument using interlacing properties of zeros of χ_n and that the weight w_s must be positive yields

$$\chi_N(x_s) = (-1)^{N+s}$$

as a necessary condition for PST

It can be shown that this condition is equivalent to the restriction of H being symmetric w.r.t. the antidiagonal :

$$J_{N-n+1} = J_n \qquad B_{N-n} = B_n$$

This is also referred to as mirror-symmetry

Look for chains with both FR and PST

$$e^{-iTx_s} = \mu + \nu \chi_N(x_s) \qquad |\mu|^2 + |\nu|^2 = 1$$

$$\chi_N(x_s) = (-1)^{N+s}$$

Readily seen to imply

$$e^{-iTx_s} = e^{i\phi}[\cos\theta + i(-1)^{N+s}\sin\theta]$$

Note $\theta = \frac{\pi}{2}$ corresponds to PST $(\mu = 0)$

Given a set of x_s satisfying the FR conditions above, the problem is to find the corresponding couplings and magnetic fields

Solution is obtained by constructing the monic polynomials

$$P_n(x) = x^n + \dots \qquad P_n(x) = \sqrt{J_1 J_2 \dots J_n}\chi_n(x)$$

whose recurrence coefficients will give J_n and B_n.

This can be done with the Euclidian algorithm.

Spectral data provides the characteristic polynomial

$$P_{N+1}(x) = (x - x_0)(x - x_1)\dots(x - x_N)$$

orthogonal to all other P_n.

FR conditions yield $P_N(x) \propto \chi_N(x)$ at $N+1$ points which fixes P_N by Lagrange interpolation.

Once two OPs are known, all the others are obtained by recurrence.

4. Krawtchouk and para-Krawtchouk models

Consider the following spectrum

$$x_s = \beta[s + \tfrac{1}{2}(\delta - 1)(1 - (-1)^s) - \tfrac{1}{2}(N - 1 + \delta)] \quad s = 0, \ldots, N$$

affine transformation of the superposition of 2 regular lattices of step 2 with spacing δ

Straightforward to check that FR conditions can be satisfied

$$e^{-iTx_s} = e^{i\phi}[\cos\theta + i(-1)^{N+s}\sin\theta]$$

One finds

$$T = \frac{\pi}{\beta} \qquad \theta = (-1)^N \frac{\pi}{2}\delta$$

The mixing angle is proportional to δ

In order to also have PST, there must be a $t = T_{PST}$ such that

$$e^{-iT_{PST}x_s} = e^{i\phi}(-1)^{N+s}$$

This requires $\delta = \frac{p}{q}$ with p, q coprimes and p odd

$$T_{PST} = Tq$$

To characterize the spin chain and obtain the J_n and B_n, one runs the algorithm

This leads to new OPs that we have called para-Krawtchouk because the orthogonality lattice is similar to the spectrum of parabose oscillators

FR naturally leads to those OPs

For N odd :

$$J_n = \frac{\beta}{2}\sqrt{\frac{n(N+1-n)[(N+1-2n)^2-\delta^2]}{(N-2n)(N-2n+2)}}, \qquad B_n = 0$$

(N even similar)

Observe mirror-symmetry : $J_{N+1-n} = J_n$

<u>Special case $\delta = 1$: The Krawtchouk model</u>

$x_s = \beta(s - \frac{N}{2})$ linear spectrum

$\theta = (-1)^N \frac{\pi}{2}$ only PST no FR at $T = \frac{\pi}{\beta}$

$J_n = \frac{\beta}{2}\sqrt{n(N+1-n)} \quad B_n = 0$

Recurrence coefficients of (symmetric) Krawtchouk OPs

Features of this special model can be obtained from angular momentum theory (representation theory of su(2))

We are looking for a tridiagonal (mirror-symmetric) matrix with a linear spectrum : $s - \frac{N}{2}$

Take $L_z, L_\pm$ su(2) generators, $|l,m\rangle$ angular momentum (representation) states

$$L_z|l,m\rangle = m|l,m\rangle\,, \quad L_\pm|l,m\rangle = \sqrt{(l\mp m)(l\pm m+1)}|l,m\pm 1\rangle$$

$$-l \leq m \leq l$$

Identify $|l,m\rangle = |\frac{N}{2}, n-\frac{N}{2}\rangle \equiv |n\rangle \quad n = 0,\ldots,N$

$$L_x|n\rangle = \tfrac{1}{2}(L_+ + L_-)|n\rangle = \tfrac{1}{2}\sqrt{(n+1)(N-n)}|n+1\rangle + \tfrac{1}{2}\sqrt{n(N+1-n)}|n-1\rangle$$

Since $L_x = e^{-i\frac{\pi}{2}L_y} L_z e^{i\frac{\pi}{2}L_y}$, spec L_x = spec $L_z = s - \frac{N}{2}$

We have thus found our tridiagonal matrix : βL_x

The eigenstates $|x_s\rangle$ are given by

$$|x_s\rangle = e^{-i\frac{\pi}{2}L_y}|s\rangle = \sum_{n=0}^{N} \langle n| e^{-i\frac{\pi}{2}L_y}|s\rangle \, |n\rangle = \sum_{n=0}^{N} \sqrt{w_s}\chi_n(x_s)|n\rangle$$

From knowledge of Wigner $\mathscr{D}$ functions, $\chi_n(x)$ given by normalized Krawtchouk polynomials

$$\chi_n(x) = (-1)^n \sqrt{\binom{N}{n}} {}_2F_1\left(\begin{matrix} -n, -s \\ -N \end{matrix} ; 2 \right)$$

with

$${}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix} ; z \right) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \frac{z^k}{k!} \qquad (a)_k = a(a+1)\dots(a+k-1)$$

$\chi_n(x)$ orthogonal w.r.t. binomial distribution $w_s = \binom{N}{s}\left(\frac{1}{2}\right)^N$

Observe that

$$\chi_N(s) = (-1)^N \sum_{k=0}^{N} (-s)_k \frac{2^k}{k!} = (-1)^N \sum \frac{s!}{(s-k)!} \frac{(-2)^k}{k!} = (-1)^{N+s}$$

Necessary condition for PST - mirror symmetry

5. Quantum Walks on the Hypercube

5.1 Review of the binary Hamming scheme

A graph $G = (V, E)$ is defined by

- V set of vertices
- E set of edges = 2-element subsets of V

Edges may be assigned weights

$|V|$ cardinality of V

Adjacency matrix A is $|V| \times |V|$ matrix with

$$\langle x|A|y\rangle = \text{\# of edges between vertices } x \text{ and } y$$

In binary Hamming scheme $H(N,2)$

$V = \{0,1\}^N$ i.e. N-tuples of 0 and 1

Hamming distance $d(x,y)$ between $x,y \in V$ is # of positions where N-tuples x and y differ

G_i, $i = 0,1,\dots,N$ graphs with edges connecting all pairs of vertices with Hamming distance = i

G_1 : N-dimensional hypercube

A_i : adjacency matrix of graph G_i

Intersection numbers $p^k_{ij} = p^k_{ji}$ count # $z \in V$ such that

$$d(x,z) = i \quad \text{and} \quad d(y,z) = j \quad \text{if} \quad d(x,y) = k$$

The matrices $A_0 = 1, A_1, \ldots, A_N$ verify the Bose-Mesner algebra

$$A_i A_j = \sum_{k=0}^{N} p_{ij}^k A_k$$

Moreover p_{i1}^k is a tridiagonal matrix. This is true in general (other distances). In the $H(N,2)$ case, one has

$$A_i A_1 = c_{i+1} A_{i+1} + b_{i-1} A_{i-1} \qquad 0 \le i \le N$$

with $c_{i+1} = i+1$ and $b_{i-1} = N - i + 1$.

Seen as follows : $c_{i+1} = \#$ z such that $d(x,z) = i$ and $d(y,z) = 1$ if $d(x,y) = i+1$.

Take $x = (0, \ldots, 0) \quad y = (\underbrace{1, \ldots, 1}_{i+1}, 0, \ldots, 0) \quad d(x,y) = i+1$

z's obtained by changing a 1 of y into a 0; there are $i+1$ ways. etc.

$$A_1 A_i = (i+1)A_{i+1} + (N-i+1)A_{i-1}$$

implies $A_i = p_i(A_1)$, p_i polynomial of degree i

Considering the N eigenvalues λ_s, $s = 1, \ldots, N$ which are distinct we have

$$p_i(\lambda_s) = K_i(s;2;N)$$

with

$$\lambda_s = N - 2s \quad \text{and} \quad K_i = (-1)^i \sqrt{\binom{N}{i}} \chi_i$$

Hamming scheme is a classic example of association schemes

5.2 Quantum Walks on the hypercube and the Krawtchouk model

With A_1 as the Hamiltonian, $U(t) = e^{-itA_1}$ defines a quantum walk on the hypercube

Shall see that it projects to walk on weighted path which identifies with 1-excitation dynamics of Krawtchouk model

Since the Krawtchouk model admits PST, this will hence be the case for the hypercube

Pick $(0) \equiv (0,\ldots,0)$ as reference vertex

Organize V as set of $N+1$ columns $V_n \quad n = 0,\ldots,N$ defined by

$$V_n = \{x \in V : d(0,x) = n\} \qquad k_n = \text{card}V_n = \binom{N}{n}$$

Denote by $V_{n,m} \quad m = 1,\ldots,k_n$ the vertices in column V_n

Each $V_{n,m}$ has n 1's

Each $V_{n,m}$ is connected to the $(N-n)$ elements of column V_{n+1} obtained by converting a 0 of this $V_{n,m}$ to a 1

Column space : linear span of column vectors

$$|col\ n\rangle = \frac{1}{\sqrt{k_n}} \sum_{m=1}^{k_n} |V_{n,m}\rangle \qquad n = 0, \ldots, N$$

key observation : evolution preserves column space because of regularity, i.e. each vertex in V_n is connected to same number of vertices in V_{n+1} and vice-versa

Projection on column space

$$\langle col\ n+1|A_1|col\ n\rangle = \frac{1}{\sqrt{k_{n+1}k_n}} \sum_{m'=1}^{k_{n+1}} \sum_{m=1}^{k_n} \langle V_{n+1,m'}|A_1|V_{n,m}\rangle$$

$$= \frac{k_n(N-n)}{\sqrt{k_{n+1}k_n}} = \sqrt{(n+1)(N-n)}$$

Pick first a vertex in V_n, compute matrix elements (=1) with the $(N-n)$ vertices to which it is linked in V_{n+1} and then sum over k_n vertices in V_n

By symmetry

$$\langle col\ n-1|A_1|col\ n\rangle = \langle col\ n|A_1|col\ n-1\rangle = \sqrt{n(N-n+1)}$$

Thus reach result

$$A_1|col\ n\rangle = J_{n+1}|col\ n+1\rangle + J_n|col\ n-1\rangle$$

with $\quad J_n = \sqrt{n(N-n+1)}.$

This coincides with $H|n\rangle$ in Krawtchouk model

The hypercube admits PST but no FR

6. Bivariate Krawtchouk polynomials and SO(3) – a preparatory primer

The univariate Krawtchouk polynomials

$$\mathscr{K}_n^N(x,p) = {}_2F_1\left(\begin{matrix} -n, -x \\ -N \end{matrix}; \frac{1}{p}\right)$$

are orthogonal w.r.t. the binomial distribution

$$\binom{N}{x} p^x (1-p)^{N-x}$$

R. Griffiths in 70's introduced multivariate generalizations orthogonal w.r.t. multinomial distribution

M.V. Tratnik in 90's constructed multivariate extensions of Racah polynomials and hence of Krawtchouk OPs as a special case

Focus on bivariate case

- Griffiths' OPs have 3 independent parameters
- Tratnik's Krawtchouk OPs have 2 parameters
- Both orthogonal w.r.t. trinomial distribution
- Griffiths' OPs were rediscovered by Rahman circa 2010 and bore his name for a while
- Algebraic interpretation (Vinet, Zhedanov) offers a clear picture

  Griffiths' Krawtchouk polynomials in n variables can be interpreted as matrix elements of $O(n+1)$ representations on energy eigenspaces of an isotropic n-dimensional oscillator

  Tratnik's Krawtchouk OPs then identified as special case

Sketch of interpretation

$a_i, a_i^\dagger$ $i = 1,2,3$ operators of 3 independent oscillators

$a|n\rangle = \sqrt{n}|n-1\rangle$, $a|0\rangle = 0$, $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$

$|n_1, n_2, n_3\rangle$ oscillator states

Fix $N = n_1 + n_2 + n_3$ and write

$$|m,n\rangle_N \equiv |m,n,N-m-n\rangle$$

Let $R \in SO(3)$ and define unitary representation $U(R)$ by

$$U(R) a_i U^\dagger(R) = \sum_{k=1}^{3} R_{ki} a_k$$

Consider matrix elements of $U(R)$ in the $|m,n\rangle_N$ basis cast in the form

$$_N\langle i,k|\, U(R) |m,n\rangle_N = w_{i,k;N} P_{m,n}(i,k;N)$$

with $P_{00}(i,k;N) = 1$ and $w_{i,k;N} = {}_N\langle i,k|\, U(R)|0,0\rangle_N$

Computation of $W_{i,k;N}$

Note that ${}_{N-1}\langle i,k|\, U(R)a_1|0,0\rangle_N = 0$ and also

$$
\begin{aligned}
{}_{N-1}\langle i,k|\, Ua_1|0,0\rangle_N &= {}_{N-1}\langle i,k|\, Ua_1U^\dagger U|0,0\rangle_N \\
&= R_{11}\sqrt{i+1}\;{}_N\langle i+1,k|\, U|0,0\rangle_N + R_{21}\sqrt{k+1}\;{}_N\langle i,k+1|\, U|0,0\rangle_N \\
&\quad + R_{31}\sqrt{N-i-k}\;{}_N\langle i,k|\, U|0,0\rangle_N
\end{aligned}
$$

Combining eqs and using ${}_N\langle i,k|\, U|0,0\rangle_N = w_{i,k;N}$

$$R_{11}\sqrt{i+1}w_{i+1,k;N} + R_{21}\sqrt{k+1}w_{i,k+1;N} + R_{31}\sqrt{N-i-k}w_{i,k;N} = 0$$

Similarly using ${}_{N-1}\langle i,k|\, Ua_2|0,0\rangle_N = 0$ one finds

$$R_{12}\sqrt{i+1}w_{i+1,k;N} + R_{22}\sqrt{k+1}w_{i,k+1;N} + R_{32}\sqrt{N-i-k}w_{i,k;N} = 0$$

$w_{i,k;N}$ is thus “essentially” orthogonal to 1st and 2nd column of R, one finds

$$w_{i,k;N} = C\frac{R_{13}^{i}R_{23}^{k}R_{33}^{N-i-k}}{\sqrt{i!k!(N-i-k)!}}$$

The constant C is found to be $\sqrt{N!}$ from

$$1 = {}_N\langle 0,0|\, U^\dagger U|0,0\rangle_N = \sum_{i,k\le n} {}_N\langle 0,0|\, U^\dagger |i,k\rangle_{N\,N}\langle i,k|\, U|0,0\rangle_N = \sum_{i,k} w_{i,k;N}^2$$

As a result

$$w_{i,k;N} = R_{13}^i R_{23}^k R_{33}^{N-i-k} \sqrt{\frac{N!}{i!k!(N-i-k)!}}$$

Recurrence relations

Obtained in the same fashion by exploiting the following two expansions for ${}_N\langle i,k|\, a_1^\dagger a_1 U|m,n\rangle_N$:

$$\begin{aligned} {}_N\langle i,k|\, a_1^\dagger a_1 U|m,n\rangle_N &= i\ {}_N\langle i,k|\, U|m,n\rangle_N \\ {}_N\langle i,k|\, a_1^\dagger a_1 U|m,n\rangle_N &= N\ {}_N\langle i,k|\, UU^\dagger a_1^\dagger a_1 U|m,n\rangle_N \\ &= \sum_{r,s=1}^{3} R_{r1} R_{s1\,N}\langle i,k|\, Ua_r^\dagger a_s|m,n\rangle_N \end{aligned}$$

and similarly with ${}_N\langle i,k|\, a_2^\dagger a_2 U|m,n\rangle_N$

This yields the two 7-term recurrence relations

$$
\begin{aligned}
iP_{m,n}(i,k;N) &= [R_{11}^2 m + R_{12}^2 n + R_{13}^2 (N-m-n)]P_{m,n} \\
&+ R_{11}R_{12}[\sqrt{m(n+1)}P_{m-1,n+1} + \sqrt{n(m+1)}P_{m+1,n-1}] \\
&+ R_{11}R_{13}[\sqrt{m(N-m-n+1)}P_{m-1,n} + \sqrt{(m+1)(N-m-n)}P_{m+1,n}] \\
&+ R_{12}R_{13}[\sqrt{n(N-m-n+1)}P_{m,n-1} + \sqrt{(n+1)(N-m-n)}P_{m,n+1}]
\end{aligned}
$$

$$
\begin{aligned}
kP_{m,n}(i,k;N) &= [R_{21}^2 m + R_{22}^2 n + R_{23}^2 (N-m-n)]P_{m,n} \\
&+ R_{21}R_{22}[\sqrt{m(n+1)}P_{m-1,n+1} + \sqrt{n(m+1)}P_{m+1,n-1}] \\
&+ R_{21}R_{23}[\sqrt{m(N-m-n+1)}P_{m-1,n} + \sqrt{(m+1)(N-m-n)}P_{m+1,n}] \\
&+ R_{22}R_{23}[\sqrt{n(N-m-n+1)}P_{m,n-1} + \sqrt{(n+1)(N-m-n)}P_{m,n+1}]
\end{aligned}
$$

Hence $P_{m,n}(i,k;N)$ are polynomials of degree m and n in the variables i and k

The orthogonality follows from unitarity

$$ {}_N\langle m',n'|\,U^\dagger U|m,n\rangle_N = \sum_{i+k\leq N} {}_N\langle m',n'|\,U^\dagger|i,k\rangle\,\langle i,k|\,U|m,n\rangle_N = \delta_{m,m'}\delta_{n,n'} $$

with ${}_N\langle i,k|\,U|m,n\rangle_N = w_{i,k;N}P_{m,n}(i,k;N)$

one finds

$$ \sum_{i+k\leq N} w^2_{i,k;N}P_{m,n}(i,k;N)P_{m',n'}(i,k;N) = \delta_{m,m'}\delta_{n,n'} $$

with the weight

$$ w^2_{i,k;N} = \frac{N!}{i!k!(N-i-k)!}R_{13}^{2i}R_{23}^{2k}R_{33}^{2(N-i-k)} $$

Consider the rotations $R_{yz}(\theta)$ and $R_{xz}(\chi)$ in the (yz) and (xz) planes respectively

It is found that the matrix elements

$$
\begin{aligned}
{}_N\langle i,k|\,U_{yz}(\theta)|m,n\rangle_N &= \delta_{im}(\dots)k_n(k;\sin^2\theta, N-i) \\
{}_N\langle i,k|\,U_{xz}(\chi)|m,n\rangle_N &= \delta_{kn}(\dots)k_m(i;\sin^2\chi, N-n)
\end{aligned}
$$

are expressed in terms of univariate Krawtchouk polynomials

$$
k_n(x,p;N) = (-N)_n\ {}_2F_1\left(\begin{matrix} -n, -x \\ -N \end{matrix}; \frac{1}{p}\right)
$$

Tratnik Polynomials $T^N_{m,n}(i,k)$ that depend on two parameters p and q are defined as the product of two univariate Krawtchouk polynomials

$$
T^N_{m,n}(i,k) = \frac{1}{(-N)_{m+n}} k_m(i,p;N-n)k_n(k,\tfrac{q}{1-p};N-i)
$$

The Tratnik polynomials $T^N_{m,n}(i,k)$ are found to correspond to the special rotation $R = R_{yz}(\theta)R_{xz}(\chi)$

As an indication of that note

$$\begin{aligned} {}_N\langle i,k|\,U(R)|m,n\rangle_N &= \sum_{p,q} {}_N\langle i,k|\,U_{(yz)}(\theta)|p,q\rangle_{N\,N}\langle p,q|\,U_{(xz)}(\chi)|m,n\rangle_N \\ &= \sum_{p,q}(\dots)\delta_{i,p}k_q(k,\sin^2\theta;N-i)\delta_{q,n}k_m(p,\sin^2\chi;N-n) \\ &= (\dots)k_m(i,p;N-n)k_n(k,\tfrac{q}{1-p};N-i) \end{aligned}$$

$$p = \sin^2\theta \qquad q = \sin^2\chi\cos^2\theta$$

Note that $R_{12} = 0$ for $R = R_{yz}R_{xz}$, hence one of the reccurence relations becomes a 3-term relation as is clear from definition. The other 7-term relation remains.

The precise identification is made by

$$P^N_{i,j}(x,y) = \sqrt{\binom{N}{i,j}\tilde{p}^i\tilde{q}^j(1-p-q)^{-i-j}}T^N_{i,j}(x,y)$$

with

$$R_{12} = 0 \qquad p = R_{13}^2 \qquad q = R_{23}^2$$

$$\tilde{p} = \frac{p(1-p-q)}{1-p} \qquad \tilde{q} = \frac{q}{1-p}$$

In terms of the $T^N_{i,j}(x,y)$ the recurrence relations take the form

$$\begin{aligned} xT^N_{i,j}(x,y) &= -p(N-i-j)(T^N_{i+1,j}(x,y) - T^N_{i,j}(x,y)) \\ &- (1-p)i(T^N_{i-1,j}(x,y) - T^N_{i,j}(x,y)) \end{aligned}$$

$$\begin{aligned} yT^N_{i,j}(x,y) &= \tfrac{pq}{1-p}(N-i-j)(T^N_{i+1,j}(x,y) - T^N_{i,j}(x,y)) \\ &- \tfrac{q}{1-p}(N-i-j)(T^N_{i,j+1}(x,y) - T^N_{i,j}(x,y)) \\ &+ qi \quad (T^N_{i-1,j}(x,y) - T^N_{i,j}(x,y)) \\ &- \tfrac{p(1-p-q)}{1-p}j(T^N_{i+1,j-1}(x,y) - T^N_{i,j}(x,y)) \\ &- \tfrac{q}{1-p}i(T^N_{i-1,j+1}(x,y) - T^N_{i,j}(x,y)) \end{aligned}$$

The algebraic interpretation also allows to obtain the generating function

$$(1+s+t)^{N-i-j}(1+\tfrac{p-1}{p}s+t)^{i}(1+\tfrac{p+q-1}{q}t)^{j}$$
$$= \sum_{0\leq x+y\leq N} \binom{N}{x,y} s^x t^y T_{i,j}^{N}(x,y), \qquad \binom{N}{x,y} = \frac{N!}{x!y!(N-x-y)!}$$

With $p = 1/2$, $q = 1/4$, we find in terms of the $P_{i,j}^{N}(x,y)$

$$[\alpha(N-2x)+\beta(2N-2x-4y)]P_{i,j}^{N}(x,y) = \alpha j P_{i,j}^{N}(x,y)$$
$$+\alpha\sqrt{(i+1)(N-i-j)}P_{i+1,j}^{N}(x,y)+\beta\sqrt{2(j+1)(N-i-j)}P_{i,j+1}^{N}(x,y)$$
$$+\alpha\sqrt{i(N+1-i-j)}P_{i-1,j}^{N}(x,y)+\beta\sqrt{2j(N+1-i-j)}P_{i,j-1}^{N}(x,y)$$
$$+\beta\sqrt{2i(j+1)}P_{i-1,j+1}^{N}(x,y)+\beta\sqrt{2(i+1)j}P_{i+1,j-1}^{N}(x,y)$$

7. The ordered 2-Hamming Scheme

$Q = \{0, 1\}$

V = vertices = set $Q^{(n,r)}$ of

strings $x = (\bar{x}_1, \ldots, \bar{x}_n)$ of length n

of r-binary sequences of 0 and 1s

$$\bar{x}_j = (x_{j_1}, \ldots, x_{j_r})$$

Ex. $n = 5$, $r = 3$

$$y = ((010), (111), (110), (001), (100))$$

Shape e of $x \in Q^{(n,r)}$

$$e(x) = (e_1, e_2, \ldots, e_i, \ldots, e_r)$$

e_i = # of r-sequences in x where the right-most 1 is in entry i $(i = 1, \ldots, r)$

Ex. $y = ((010), (111), (110), (001), (100))$

$$e(y) = (1, 2, 2)$$

Relations defined w.r.t. shapes

$$x, y \in V \qquad x \sim_e y \quad \text{if shape of} \quad (x - y) = e$$

Ex: $x = ((100),(001),(101),(011),(000))$

$$y = ((010),(111),(110),(001),(100))$$

$$x - y = ((110),(110),(011),(010),(100))$$

$e(x-y) = (1,3,1) \qquad x \sim_{(1,3,1)} y$

Graph G_e corresponding to shape e :

Edges between all $x, y \in V$ such that $x \sim_e y$

Adjacency matrices A_e

$$\langle x|A_e|y\rangle = \begin{cases} 1 & (x \sim_e y) \\ 0 & \text{otherwise} \end{cases}$$

Association scheme called ordered r-Hamming scheme

Consider ordered 2-Hamming scheme

$V = Q^{(N,2)} =$ set of N-strings of $(0,0),(1,0),(0,1),(1,1)$

$$e(x) = (e_1, e_2) = (i,j)$$

$e_1 = \#$ of $(1,0)$

$e_2 = \#$ of $(0,1)$ and $(1,1)$

Set of shapes $(i,j) : 0 \leq i+j \leq N$

Adjacency matrices $A_{(i,j)}$ form B.-M. algebra

$$A_{(i,j)}A_{(k,l)} = \sum_{0\leq m+n\leq N} \alpha^{(m,n)}_{(i,j),(k,l)} A_{(m,n)}$$

Intersection numbers $\alpha^{(m,n)}_{(i,j),(k,l)} = \#$ of z such that

$$e(x-z) = (i,j), \quad e(y-z) = (k,l) \quad \text{if} \quad e(x-y) = (m,n)$$

In particular it is found that

$$A_{(1,0)}A_{(i,j)} = (N+1-i-j)A_{(i-1,j)} + jA_{(i,j)} + (i+1)A_{(i+1,j)}$$

$$A_{(0,1)}A_{(i,j)} = 2(N+1-i-j)A_{(i,j-1)} + 2(i+1)A_{(i+1,j-1)} + (j+1)A_{(i-1,j+1)} + (j+1)A_{(i,j+1)}$$

Counting not difficult, for instance

$$\alpha^{(i-1,j)}_{(1,0),(i,j)} = \#\text{ of } z \text{ such that}$$

$$e(x-z) = (1,0) \quad e(y-z) = (i,j) \quad \text{if} \quad e(x-y) = (i-1,j)$$

Take $x = (\underbrace{10,\dots,10}_{i-1},\underbrace{01,\dots,01}_{j},\underbrace{00,\dots,00}_{N-i-j+1})$ and $y = (00,00,\dots,00)$

To get a z must convert a $(0,0)$ into a $(1,0)$ and there are $N-i-j+1$ ways. Etc.

Remarkably $A_{(i,j)}$ expressible in Tratnik polynomials of $A_{(1,0)}$ and $A_{(0,1)}$. More connections with Tratnik polynomials soon

8. PST and FR in a 2-D spin lattice

Take graph $G_{\alpha,\beta}$ with adjacency matrix

$$A_{\alpha,\beta} = \alpha A_{(1,0)} + \beta A_{(0,1)}$$

Consider quantum walk generated by $A_{\alpha,\beta}$

Let $(0) \equiv (00, 00, \ldots, 00)$ be reference vertex

Organize V as set of $\binom{N+1}{2}$ column V_{ij} defined by

$$V_{ij} = \{x \in V : e(x) = (i,j)\} \qquad 0 \leq i+j \leq N$$

card V_{ij} is $k_{ij} = \binom{N}{i,j} 2^j$

Pick $(\underbrace{10,\dots,10}_{i},\underbrace{01,\dots,01}_{j},00,\dots,00)$ in V_{ij}

For relation corresponding to $(1,0)$, each $V_{(i,j),k}$ in V_{ij}

Connected to	$(N-i-j)$	vertices in	$V_{i+1,j}$	$[(00)\to(10)]$
to	j	vertices in	$V_{i,j}$	$[(01)\to(11)]$

For relation corresponding to $(0,1)$, each $V_{(i,j),k}$ in V_{ij}

Connected to	$2(N-i-j)$	vertices in	$V_{i,j+1}$	$[(00)\to(01),(11)]$
to	j	vertices in	$V_{i+1,j-1}$	$[(01)\to(10)]$

Easy to see that number of connections does not depend on vertex picked

Consider span of column vectors

$$|col\ i,j\rangle = \frac{1}{\sqrt{k_{i,j}}} \sum_k |V_{(i,j),k}\rangle$$

$V_{(i,j),k}$ denotes vertices in column $V_{(i,j)}$

Regularity assures that $A_{(1,0)}$ and $A_{(0,1)}$ preserve column space and allows to project

Have all info needed. Same method as for hypercube.

$$\langle col\ i+1,j|A_{(10)}|col\ i,j\rangle = \sqrt{(i+1)(N-1-j)}$$

$$\langle col\ i,j|A_{(10)}|col\ i,j\rangle = j$$

$$\langle col\ i,j+1|A_{(01)}|col\ i,j\rangle = \sqrt{2(j+1)(N-1-j)}$$

$$\langle col\ i+1,j-1|A_{(01)}|col\ i,j\rangle = \sqrt{2(i+1)j}$$

Observation : Quantum walk on $G_{\alpha,\beta}$ projects to 1-excitation dynamics of spin lattice of triangular shape with Hamiltonian

$$H = \sum_{0\le i+j\le N} \alpha\sqrt{(i+1)(N-i-j)}\,\tfrac{1}{2}(\sigma^x_{i,j}\sigma^x_{i+1,j}+\sigma^y_{i,j}\sigma^y_{i+1,j})$$
$$+\beta\sqrt{2(j+1)(N-i-j)}\,\tfrac{1}{2}(\sigma^x_{i,j}\sigma^x_{i,j+1}+\sigma^y_{i,j}\sigma^y_{i,j+1})$$
$$+\beta\sqrt{2(i+1)j}\,\tfrac{1}{2}(\sigma^x_{i,j}\sigma^x_{i+1,j-1}+\sigma^y_{i,j}\sigma^y_{i-1,j+1})+\alpha j\tfrac{1}{2}(1+\sigma^z_{i,j})$$

in 1-excitation basis $|e_{i,j}\rangle = E_{i,j}$
($E_{i,j}$ matrix with 1 at i,j entry and 0 elsewhere)

$$H|e_{i,j}\rangle = \alpha\sqrt{(i+1)(N-i-j)}|e_{i+1,j}\rangle + \beta\sqrt{2(j+1)(N-i-j)}|e_{i,j+1}\rangle$$
$$+\alpha j|e_{i,j}\rangle + \alpha\sqrt{i(N+1-i-j)}|e_{i-1,j}\rangle + \beta\sqrt{2j(N+1-i-j)}|e_{i,j-1}\rangle$$
$$+\beta\sqrt{2(i+1)j}|e_{i+1,j-1}\rangle + \beta\sqrt{2i(j+1)}|e_{i-1,j+1}\rangle$$

which corresponds to $[\alpha A_{(1,0)} + \beta A_{(0,1)}]|col\ i,j\rangle$

Transport properties

Comparison with recurrence relations of the Tratnik polynomials shows that

$$\langle e_{i,j}|x,y\rangle = w_{x,y;N} P_{i,j}^{N}(x,y) \qquad w_{x,y;N} = \binom{N}{x,y} p^x q^y (1-p-q)^{N-x-y}$$

with $p = 1/2$, $q = 1/4$ are eigenfunctions of H with eigenvalues

$$\lambda_{x,y} = \alpha(N-2x) + \beta(2N-2x-4y)$$

We wish to compute transition amplitude

$$f_{(i,j)}(t) = \langle e_{i,j}|\, e^{-itH} |e_{0,0}\rangle$$

between site $(0,0)$ and (i,j)

$$
\begin{aligned}
f_{(i,j)}(t) &= \langle e_{i,j}|\, e^{-itH}\,|e_{0,0}\rangle \\
&= \sum_{0\le x+y\le N} \langle e_{i,j}|x,y\rangle\, e^{-it\lambda_{x,y}}\,\langle x,y|0,0\rangle \\
&= \sum_{0\le x+y\le N} \binom{N}{x,y} \left(\tfrac{1}{2}\right)^x \left(\tfrac{1}{4}\right)^y \left(\tfrac{1}{4}\right)^{N-x-y} P^N_{0,0}(x,y) P^N_{i,j}(x,y) e^{-it\lambda_{x,y}}
\end{aligned}
$$

$$
P^N_{0,0} = 1 \qquad \lambda_{x,y} = \alpha(N-2x) + \beta(2N-2x-4y)
$$

Generating function gives expression for

$$
\sum_{0\le x+y\le N} \binom{N}{x,y} u^x v^y P^N_{i,j}(x,y)
$$

This is form we have with $u = 2z_1$, $v = z_2$

$$
z_1 = e^{2i(\alpha+\beta)t} \qquad z_2 = e^{i4\beta t}
$$

One finds

$$f_{(i,j)}(t) = e^{-iN(\alpha+2\beta)t} \frac{\sqrt{2^j}}{4^N} \sqrt{\binom{N}{i,j}} (1+2z_1+z_2)^{N-i-j}(1-2z_1+z_2)^i(1-z_2)^j$$

$$z_1 = e^{2i(\alpha+\beta)t} \qquad z_2 = e^{i4\beta t}$$

To have transfer only to site s with $i+j=N$ must have <u>for some $t=T$</u>

$$1+2z_1+z_2 = 0 \qquad (*)$$

Since $|z_1| = |z_2| = 1$, (*) implies

$$z_2 = 1 \qquad \text{and} \qquad z_1 = -1$$

and thus, since $1-z_2 = 0$ we must have $j=0$ and hence

$$|f_{(N,0)}(T)| = 1 \qquad |f_{(i,j)}(T)| = 0 \quad (i,j) \neq (N,0)$$

meaning that PST occurs between $(0,0)$ and $(N,0)$

$$z_1 = e^{2i(\alpha+\beta)t} = -1 \qquad z_2 = e^{i4\beta t} = 1$$

can be realized in different ways

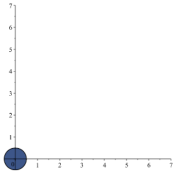
$\alpha = 1, \beta = 2$ and $T = \frac{\pi}{2}$ is one such instance

Note that for $\alpha = 1, \beta = 2$ and $T = \frac{\pi}{4}$:

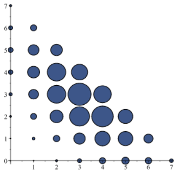
$$z_2 = 1$$

implies the $|f_{(i,j)}(T)| = 0$ for $j \neq 0$, we then have FR on the sites $(i,0)$, $i = 0,\ldots,N$

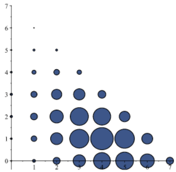
This is depicted on the following figure where $N = 7$



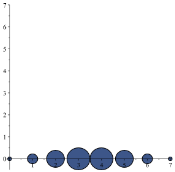
$t = 0$



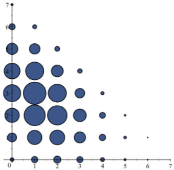
$t = \frac{\pi}{6}$



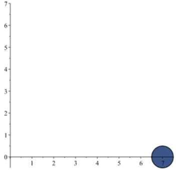
$t = \frac{\pi}{5}$



$t = \frac{\pi}{4}$



$t = \frac{\pi}{3}$



$t = \frac{\pi}{2}$

9. CONCLUDING REMARKS

- QW on graphs are useful and deserve explorations
- We have focused on PST and FR
- We have indicated how PST and FR can occur on weighted paths associated to spin chains with non-uniform couplings prescribed by orthogonal polynomials
- We have discussed correspondance between such weighted paths and also graphs from 2 association schemes
- We have reviewed the correspondance between QW on hypercube and Krawtchouk spin chain
- The occurence of Krawtchouk polynomials as eigen-wavefunctions and as matrix eigenvalues of the scheme underscored the connection

- We have reviewed the algebraic interpretation of multivariable generalizations of the Krawtchouk polynomials
- We have discussed the much less known ordered r- Hamming scheme which features the Krawtchouk polynomials of Tratnik type
- By projecting the QW on a graph of the generalized Hamming scheme we have identified a 2D spin lattice with PST and FR
- These observations raise many issues that should be pursued

THANK YOU FOR THE ATTENTION