Quantum Walk with Restart

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Outline

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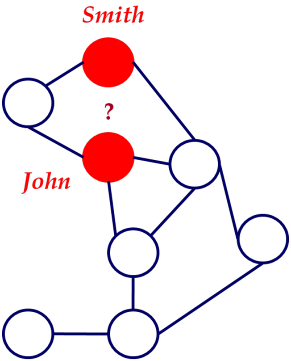
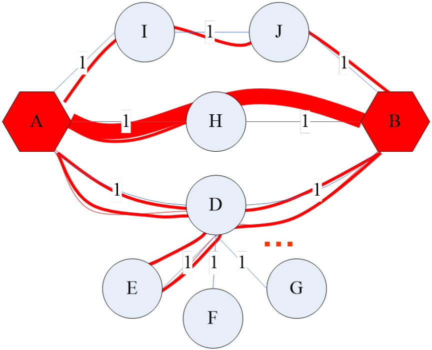
Motivation

- Should we recommend *Alice* to *Bob*?
- YES if *Alice* and *Bob* are close enough
- How to measure closeness/proximity?



How to measure closeness

- Two nodes should be close, if they have
  - many,
  - short,
  - heavy paths



Random walk with restart

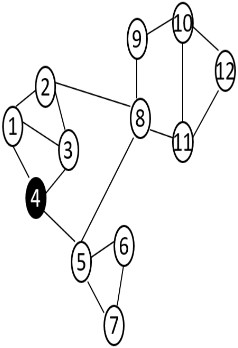
- Random walk with restart is described as

$$\underbrace{\pi}_{\textit{ranking vector}} = \underbrace{(1-c)\mathbf{P}\pi}_{\textit{keep going}} + \underbrace{c\mathbf{e}}_{\textit{restart the walk}}$$

- π is the probability distribution
- $c \in [0,1] \in \mathbb{R}$ is the restart factor
  - If $c = 0$, it is random walk on graph, may not converge
- $\mathbf{P}$ is the transition matrix
- $\mathbf{e} = (0, \cdots, 1, \cdots, 0)^T$ is the initial state. Always restart from node i.
  - If $\mathbf{e} = \frac{1}{N}(1, \cdots, 1, \cdots, 1)^T$, it is PageRank algorithm.

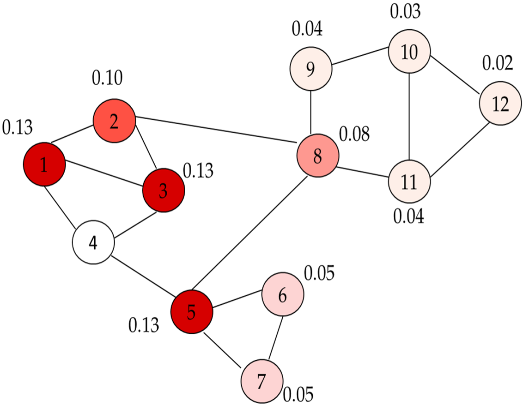
Example

$$
\underset{\pi(t+1)}{\begin{pmatrix} 0.13\\0.10\\0.13\\0.22\\0.13\\0.05\\0.05\\0.08\\0.04\\0.03\\0.04\\0.02 \end{pmatrix}}
= 0.9\times
\underset{(1\text{-}c)P}{\begin{pmatrix}
0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1/3 & 0 & 1/3 & 0 & 0 & 0 & 0 & 1/4 & 0 & 0 & 0 & 0\\
1/3 & 1/3 & 0 & 1/3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1/3 & 0 & 1/3 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 1/3 & 0 & 1/2 & 1/2 & 1/4 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 1/4 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 1/4 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 1/3 & 0 & 0 & 1/4 & 0 & 0 & 0 & 1/2 & 0 & 1/3 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 1/3 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 & 0 & 1/3 & 1/2\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/4 & 0 & 1/3 & 0 & 1/2\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/3 & 1/3 & 0
\end{pmatrix}}
\underset{\pi(t)}{\begin{pmatrix} 0.13\\0.10\\0.13\\0.22\\0.13\\0.05\\0.05\\0.08\\0.04\\0.03\\0.04\\0.02 \end{pmatrix}}
+ 0.1\times
\underset{ce}{\begin{pmatrix} 0\\0\\0\\\color{red}{1}\\0\\0\\0\\0\\0\\0\\0\\0 \end{pmatrix}}
$$



Example (cont.)

- *Click here for animation*
- Nearer nodes, higher scores. More red, more relevant.



	Node 4
Node 1	0.13
Node 2	0.10
Node 3	0.13
Node 4	0.22
Node 5	0.13
Node 6	0.05
Node 7	0.05
Node 8	0.08
Node 9	0.04
Node 10	0.03
Node 11	0.04
Node 12	0.02

Applications and variances

- *rwr* is good at measuring the closeness between nodes
- Basic *rwr*
  - Haweliwala@02, Pan@04, Sun@06, Tong@06
  - ***Fast Random Walk with Restart and Its Applications***, Tong@ICDM06. Ten year's best paper in ICDM (2006-2015).
- *rwr* for image segmentation ...
- *rwr* for recommendation systems ...
- *rwr* for clustering ...
- *rwr* in big data ...
- ...

Outline

Graph denotation

- Consider only **undirected regular** graphs $G = (V, E), V(G) = N, D(G) = D$
- Label each vertex with a distinct integer between 1 to N
- For each vertex, label its outgoing edges with distinct integers between 1 and D
- For each vertex $v \in \{1, \cdots, N\}$, let $N(v, c)$ denote the c-th neighbour of v

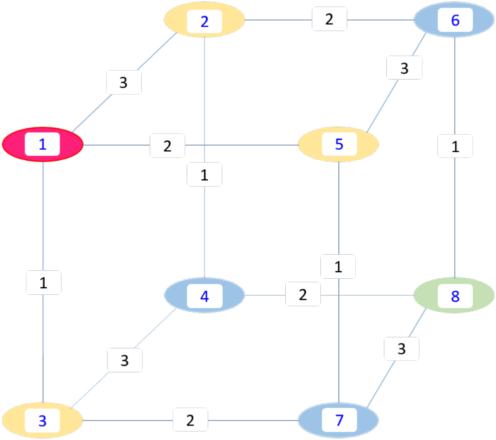


Figure: Cube, $V(G) = 8, D(G) = 3$. Vertices and edges are labeled

Quantum walk on graphs

- Coin operator C is Grover operator: $(I \otimes C)|v\rangle|c\rangle = |v\rangle C|c\rangle$
- Shift operator S: $S|v\rangle|c\rangle = |N(v,c)\rangle|c\rangle$
- Evolution operator U: $U = S \cdot (I \otimes C)$
- Quantum walk on graph:

$$\begin{aligned} \text{one step} &: \quad |\psi(t+1)\rangle = U|\psi(t)\rangle = S \cdot (I \otimes C)|\psi(t)\rangle \\ t \text{ steps} &: \quad |\psi(t)\rangle = U^t|\psi(0)\rangle \end{aligned}$$

  where $|\psi(0)\rangle = |1\rangle \otimes \sum_{c=1}^{D} \psi_c(0,1)|c\rangle$ is the initial state.
- Probability distribution after walking t steps:

$$P(t) = (P(t,1), P(t,2), \cdots, P(t,N))^T$$

  where $P(t,i)$ is the probability at vertex i after t steps

Limiting distribution

- Quantum walk consists only of unitary operations,

$$\lim_{t\to\infty} P(t)$$

  dose not converge, the walk has no limit distribution.
- **Averaged Probability Distribution**

$$\overline{P(T)} = \frac{1}{T}\sum_{t=0}^{T} P(t)$$

- $\lim_{T\to\infty} \overline{P(T)}$ has a limit distribution.

Quantum walk with restart

- Currently, quantum walk with restart is described as

$$|\widetilde{\psi(t+1)}\rangle = \underbrace{(1-\rho)U|\widetilde{\psi(t)}\rangle}_{\textit{keep going}} + \underbrace{\rho|\psi(0)\rangle}_{\textit{restart the walk}}$$

- $\widetilde{|\psi(t)\rangle}$ is the probability distribution at step t
- $\rho \in [0,1] \in \mathbb{C}$ is the restart factor
  - If $\rho = 0$, it is quantum walk on graph.
- $|\psi(0)\rangle$ is the initial state

$$|\psi(0)\rangle = \underbrace{|1\rangle}_{\text{restart from node 1}} \otimes \underbrace{\left[\frac{1}{\sqrt{D}}\sum_{c=1}^{D}|c\rangle\right]}_{\text{uniform superposition}}$$

Limiting distribution

- Relationship between $\widetilde{|\psi(t)\rangle}$ and $|\psi(t)\rangle$

$$\begin{aligned}\widetilde{|\psi(t)\rangle} &= \underbrace{(1-\rho)^t|\psi(t)\rangle}_{\text{walking } t \text{ steps}} + \underbrace{(1-\rho)^{t-1}\rho|\psi(t-1)\rangle}_{\text{walking } t-1 \text{ steps}} \\ &\quad + \cdots + \underbrace{(1-\rho)\rho|\psi(1)\rangle}_{\text{walking } 1 \text{ step}} + \underbrace{\rho|\psi(0)\rangle}_{\text{walking } 0 \text{ step}}\end{aligned}$$

- Limit form

$$\begin{aligned}\lim_{t\to\infty} \widetilde{|\psi(t)\rangle} &= \sum_{i=0}^{t}(1-\rho)^i\rho|\psi(i)\rangle \\ &= \sum_{i=0}^{t}\rho(1-\rho)^i U^i|\psi(0)\rangle \\ &= \rho\Big[I-(1-\rho)U\Big]^{-1}|\psi(0)\rangle\end{aligned}$$

Difference from *averaged probability distribution*

- Averaged probability distribution

$$\overline{P(T)} = \sum_{t=0}^{T} \frac{1}{T} \cdot P(t)$$

  Sum over equally weighted probabilities of T quantum walks.

- Quantum walk with restart

$$\widetilde{|\psi(T)\rangle} = \sum_{t=0}^{T} \rho(1-\rho)^t \cdot |\psi(t)\rangle$$

  Sum over unequally weighted probability amplitudes of T quantum walks.

Decoherence by pure dephasing

- Decoherence by pure dephasing (**PRL 104.153602, 2010**)

$$\rho_{t+1} = (1-\rho)U\rho_t U^\dagger + \rho \sum_i K_i U \rho_t U^\dagger K_i^\dagger$$

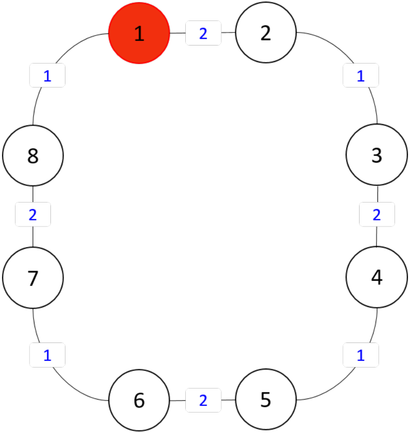
  where $K_i = |i\rangle\langle i|$ corresponds to pure dephasing
- Quantum walk with restart in density operator form

$$\widetilde{\rho_{t+1}} = (1-\rho)U\widetilde{\rho}_t U^\dagger + \rho\widetilde{\rho_0}$$

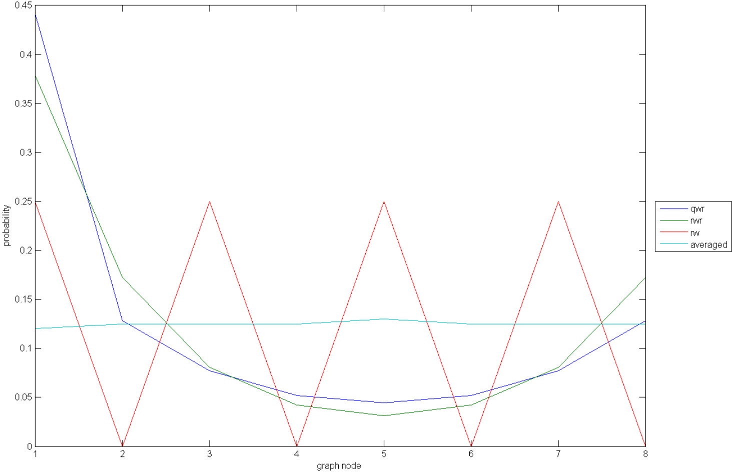
- From decoherence by pure dephasing to *qwr*

$$\rho_{t+1} = (1-\rho)U\rho_t U^\dagger + \underbrace{\rho K_1 U \rho_t U^\dagger K_1^\dagger}_{\neq \rho\widetilde{\rho_0},\ \text{varies in time}}$$

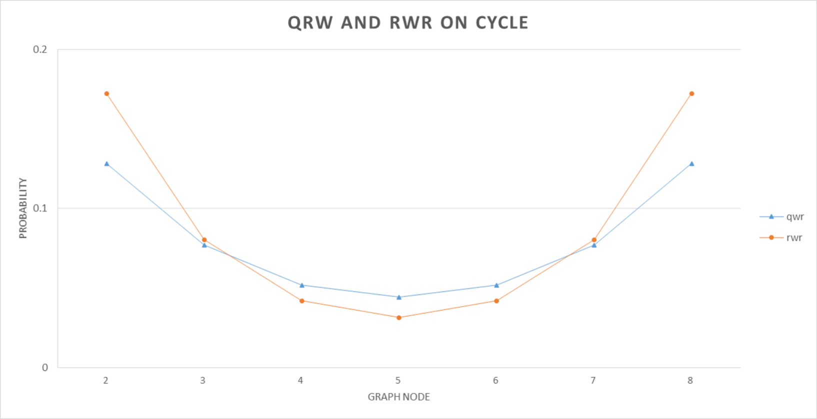
Cycle



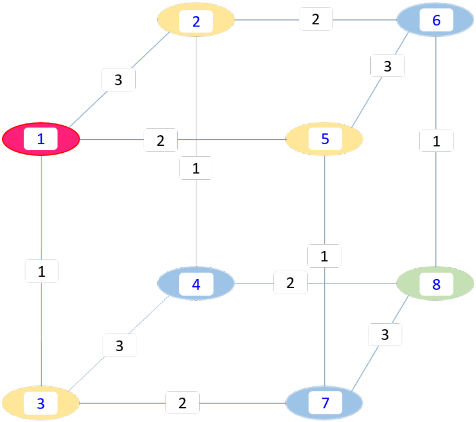
Four distributions in cycle ($T = 100, \rho = 0.25$)



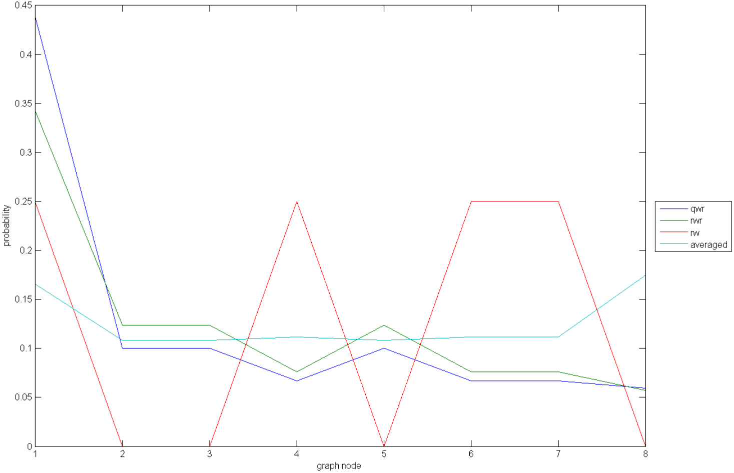
QWR and RWR in cycle ($T = 100, \rho = 0.25$)



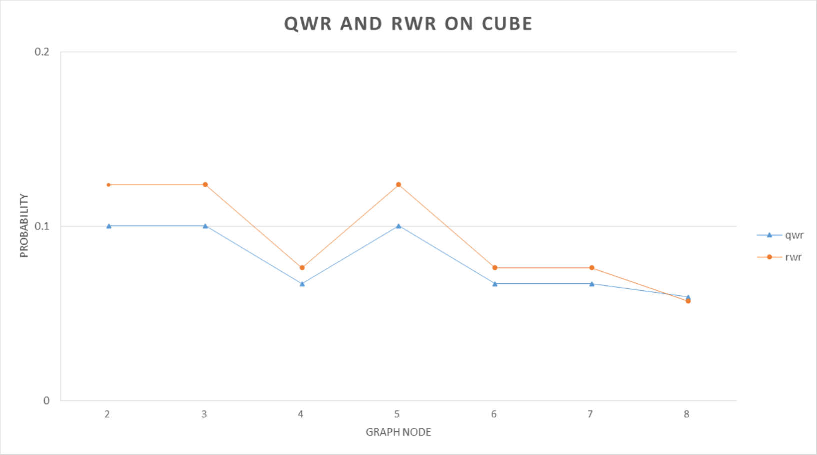
Cube



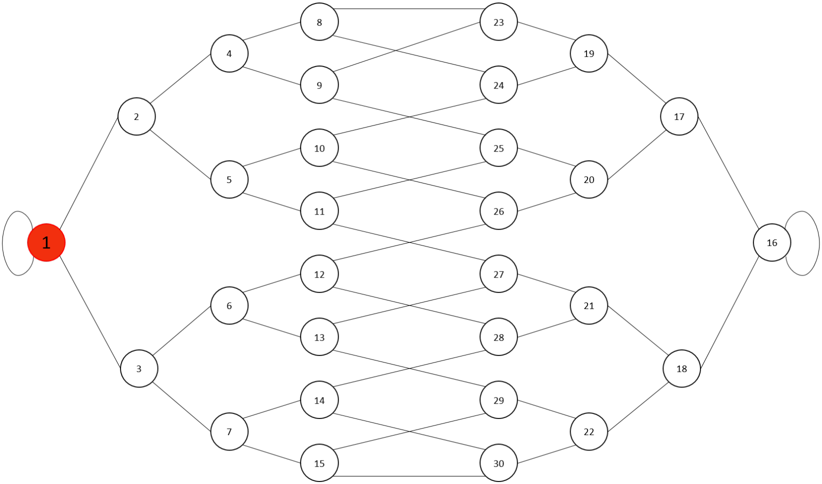
Four distributions in cube ($T = 100, \rho = 0.25$)



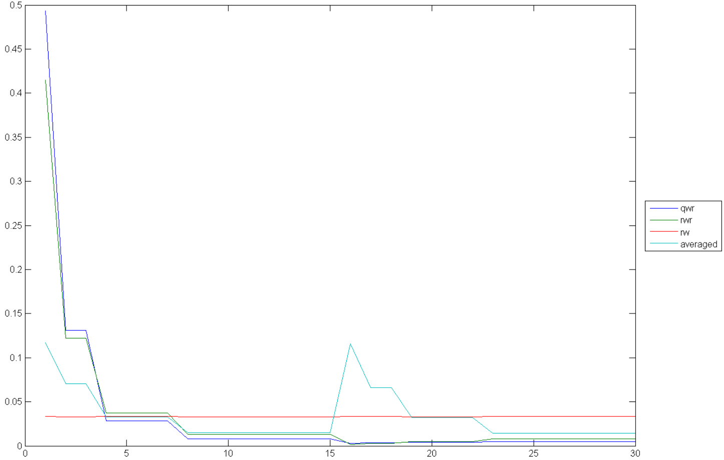
QWR and RWR in cube ($T = 100$, $\rho = 0.25$)



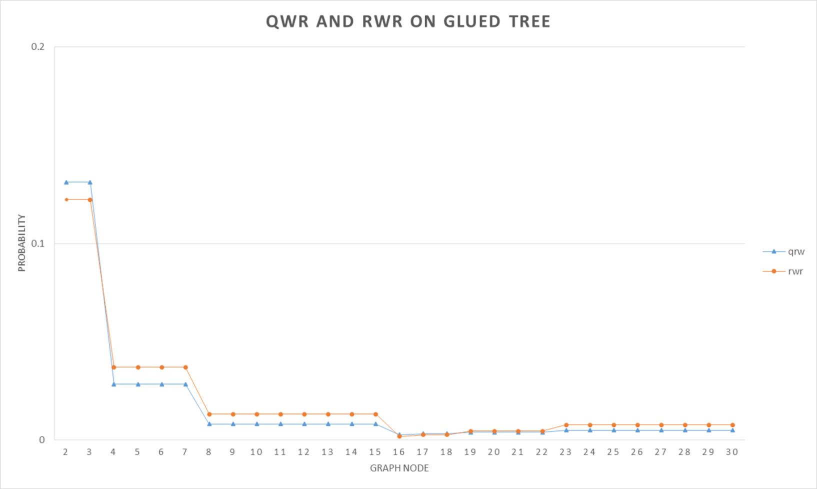
Glued tree ($G4$)



Four distributions in glued tree ($T = 100, \rho = 0.25$)



QWR and RWR in glued tree ($T = 100, \rho = 0.25$)



Outline

QWR vs. RWR

- Why random walk with restart?
  - Offers a good measure on the closeness of graph nodes
  - Many useful applications and variances
- Why quantum walk with restart?
  - More precise measure than its classical counterpart?
  - A new model of quantum walk
  - There are more parameters in *qwr* than in *rwr*, which give us more control on the distribution

There are so many to do

1. On what kind of graphs will the quantum walk with restart will converge?
2. Analytical form for the limit distribution
   - From the method of *Aharonvo@STOC01*, express the limit distribution with the evolution operator's eigenvalues and eigenstates
3. Convergence speed
4. How will coin initial state and coin operator effect the limit distribution?
5. Can we get the same distribution of *rwr* by setting the parameters of *qwr*? i.e., Can we simulate *rwr* by *qwr*?

Different measures

- Averaged probability distribution

$$\overline{P(T)} = \sum_{t=0}^{T} \frac{1}{T} \cdot P(t)$$

- Quantum walk with restart: type 1

$$|\widetilde{\psi(T)}\rangle = \sum_{t=0}^{T} \rho(1-\rho)^t \cdot |\psi(t)\rangle$$

- Quantum walk with restart: type 2

$$\overline{P(T)} = \sum_{t=0}^{T} \rho(1-\rho)^t \cdot P(t)$$

Different measures (cont')

- Decoherence by pure dephasing

$$|\widetilde{\psi(t+1)\rangle} = (1-\rho)U|\widetilde{\psi(t)\rangle} + \rho K_1 U|\widetilde{\psi(t)\rangle}$$

where $K_1 = \sum_{c=1}^{D} |1,c\rangle\langle 1,c|$

Different measures (cont')

- $$\mu_X = E[X] = \sum_{x=-N}^{N} xP(x)$$

  $$\mu_X = E[Y] = \sum_{y=-N}^{N} yP(y)$$

$$\begin{aligned} cov(X,Y) &= E[(X-\mu_X)(Y-\mu_Y)] \\ &= E[XY] - E[X]E[Y] \\ &= \sum_{x=-N}^{N} \sum_{y=-N}^{N} (x-\mu_X)(y-\mu_Y)P(x,y) \end{aligned}$$

$$cov(X,Y) = \sum_{x=-N}^{N} \sum_{y=-N}^{N} (x-\mu_X)(y-\mu_Y)P(x,y)$$

Different measures (cont')

- $$cov(X,Y) > 0$$
  $$cov(X,Y) = 0$$
  $$cov(X,Y) < 0$$

- $$|0,L\rangle|0,L\rangle + |0,R\rangle|0,R\rangle$$
  $$|0,L\rangle|0,L\rangle + |0,S\rangle|0,S\rangle + |0,R\rangle|0,R\rangle$$
  $$|-1,S\rangle|-1,S\rangle + |1,S\rangle|1,S\rangle$$
  $$|-1,S\rangle|-1,S\rangle + |0,S\rangle|0,S\rangle + |1,S\rangle|1,S\rangle$$
  $$|-1,L\rangle|-1,L\rangle + |1,R\rangle|1,R\rangle$$
  $$|-1,L\rangle|-1,L\rangle + |0,S\rangle|0,S\rangle + |1,R\rangle|1,R\rangle$$

Different measures (cont')

- $$|0,L\rangle|0,R\rangle$$
$$|0,L\rangle|0,L\rangle \pm |0,R\rangle|0,R\rangle$$
$$|0,L\rangle|0,R\rangle \pm |0,R\rangle|0,L\rangle$$
$$|0,L\rangle|0,L\rangle + |0,S\rangle|0,S\rangle + |0,R\rangle|0,R\rangle$$
$$|0,L\rangle|0,L\rangle - |0,S\rangle|0,S\rangle + |0,R\rangle|0,R\rangle$$
$$|-1,S\rangle|-1,S\rangle \pm |1,S\rangle|1,S\rangle$$
$$|-1,S\rangle|1,S\rangle \pm |1,S\rangle|-1,S\rangle$$
$$|-1,S\rangle|-1,S\rangle + |0,S\rangle|0,S\rangle + |1,S\rangle|1,S\rangle$$
$$|-1,S\rangle|-1,S\rangle - |0,S\rangle|0,S\rangle + |1,S\rangle|1,S\rangle$$

Different measures (cont')

- $$\frac{1}{3}|0,L\rangle|0,L\rangle \pm \frac{\sqrt{8}}{3}|0,R\rangle|0,R\rangle$$
  $$\frac{1}{3}|0,L\rangle|0,L\rangle + \frac{2}{3}|0,S\rangle|0,S\rangle + \frac{2}{3}|0,R\rangle|0,R\rangle$$
  $$\frac{1}{3}|0,L\rangle|0,L\rangle - \frac{2}{3}|0,S\rangle|0,S\rangle + \frac{2}{3}|0,R\rangle|0,R\rangle$$
  $$\frac{1}{3}|-1,S\rangle|-1,S\rangle \pm \frac{\sqrt{8}}{3}|1,S\rangle|1,S\rangle$$
  $$\frac{1}{3}|-1,S\rangle|-1,S\rangle + \frac{2}{3}|0,S\rangle|0,S\rangle + \frac{2}{3}|1,S\rangle|1,S\rangle$$
  $$\frac{1}{3}|-1,S\rangle|-1,S\rangle - \frac{2}{3}|0,S\rangle|0,S\rangle + \frac{2}{3}|1,S\rangle|1,S\rangle$$

Different measures (cont')

- $$|-1,L\rangle|-1,L\rangle \pm |1,R\rangle|1,R\rangle$$
  $$|-1,R\rangle|1,L\rangle \pm |1,L\rangle|-1,R\rangle$$
  $$|-1,L\rangle|-1,L\rangle + |0,S\rangle|0,S\rangle + |1,R\rangle|1,R\rangle$$
  $$|-1,L\rangle|-1,L\rangle - |0,S\rangle|0,S\rangle + |1,R\rangle|1,R\rangle$$
  $$\frac{1}{3}|-1,L\rangle|-1,L\rangle \pm \frac{\sqrt{8}}{3}|1,R\rangle|1,R\rangle$$
  $$\frac{1}{3}|-1,L\rangle|-1,L\rangle + \frac{2}{3}|0,S\rangle|0,S\rangle + \frac{2}{3}|1,R\rangle|1,R\rangle$$
  $$\frac{1}{3}|-1,L\rangle|-1,L\rangle - \frac{2}{3}|0,S\rangle|0,S\rangle + \frac{2}{3}|1,R\rangle|1,R\rangle$$

Thank you !

Any questions ?