From Continuous Time Random Walks to Continuous Time Quantum Walks

- Motivation: fundamental aspects of transport
- Coherent and incoherent energy transfer
- From Continuous Time Random Walks (CTRW) to Continuous Time Quantum Walks (CTQW)
- Regular structures; rings, tori, fractals
- Dendrimers, Husimi cacti, small-world-networks
- Transmission probabilities
- Efficiency of the CTQW transport
- Trapping in the CTQW framework
- Conclusions and outlook

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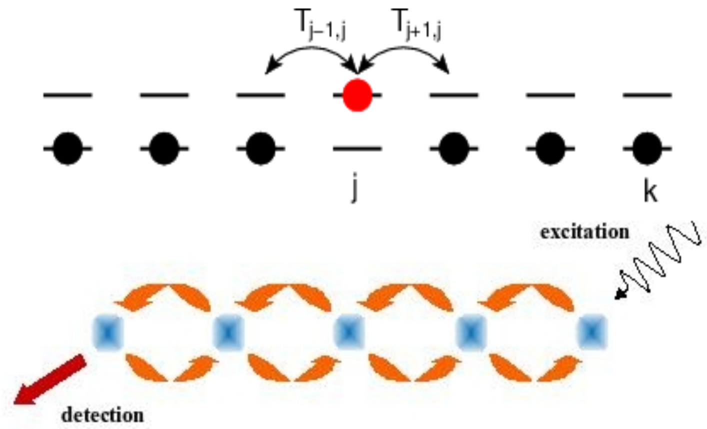
Motivation

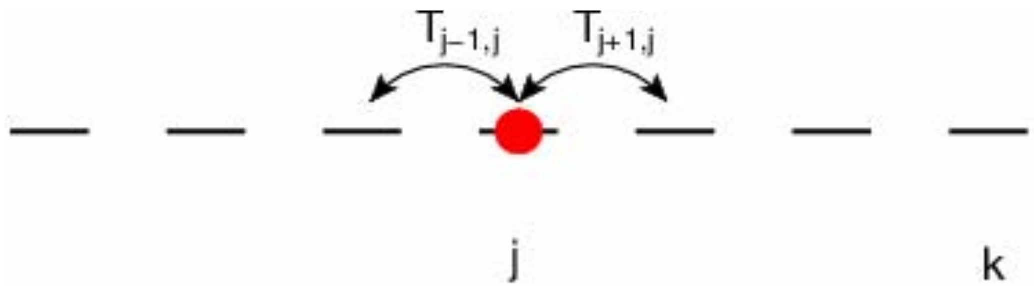
Various types of transport occur in Physics, Chemistry and Biology:

- Motion of defects in crystals
- Exciton dynamics in molecular systems (light-harvesting complexes in photosynthesis)
- Energy transfer between Rydberg atoms
- Electronic conductivity in condensed matter
- Light propagation in wave guide arrays



Fundamental aspects of transport

Dynamics over networks (discrete sets) in continuous time.



Two limiting pictures appear:

A) Classical motion (incoherent)

- Stepwise transfer over a set of sites (network of participating centers)
- Model: Continuous-Time Random Walk (CTRW)

B) Quantum mechanical motion (coherent)

- Wavelike motion over the network. Assumptions here (phenomenological): „two-level“ systems, tight binding picture
- One model: Continuous-Time Quantum Walk (CTQW)

Basic questions

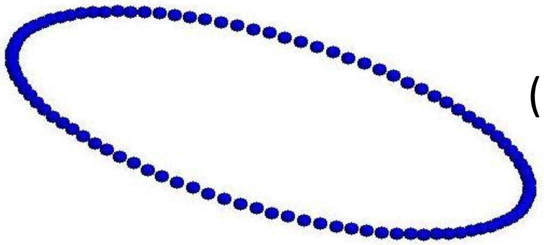
How does the topology of the network
influence the classical or the quantum transfer?

How do classical or quantum dynamics influence
reaction kinetics?

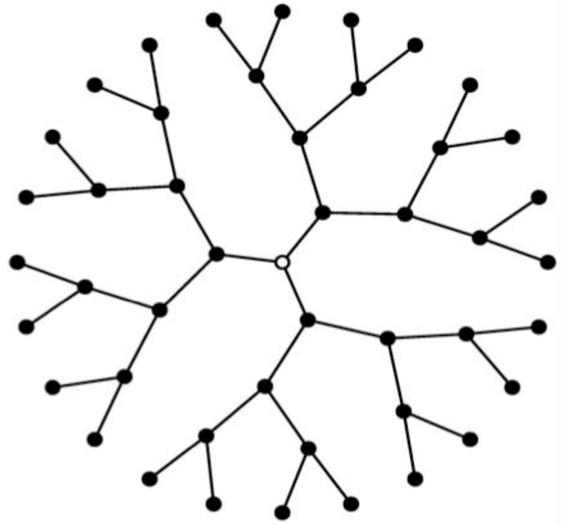
Recent review on quantum transfer and on simple reactions
O. Mülken and A.B., Physics Reports **502**, 37 (2011)

Networks

- **Network**: Set of N connected sites (nodes)



(ring)



(dendrimer)

- The nodes span a N-**dimensional vector space** with a complete orthonormal basis, e.g.,

$$\boldsymbol{n}_1 \equiv \left|1\right\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix};\ \boldsymbol{n}_2 \equiv \left|2\right\rangle = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix};\ \ldots;\boldsymbol{n}_N \equiv \left|N\right\rangle = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

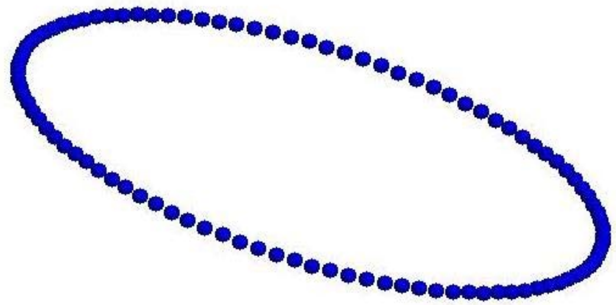
- The topology is given by the connectivity matrix **A** = (A_{kj})

$$A_{kj} = \left\{ \begin{array}{ll} f_j & \text{for } k = j \\ -1 & \text{if } k \text{ and } j \quad \text{are connected} \\ 0 & \text{else} \end{array} \right\} \text{Thus } A_{kj} = A_{jk}.$$

Here f_j is the number of bonds stemming from node j

Example: Connectivity matrix A for a ring of N nodes

$$\mathbf{A} = \begin{pmatrix} 2 & -1 & 0 & \cdots & & -1 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \cdots \\ \vdots & & & & & \\ & & & -1 & 2 & -1 \\ -1 & 0 & \cdots & & -1 & 2 \end{pmatrix}$$



Or, in operator form:

$$\mathbf{A} = \sum_m \left(2|m\rangle\langle m| - |m-1\rangle\langle m| - |m+1\rangle\langle m| \right), \text{ where } |N+1\rangle = |1\rangle.$$

Question: What is the probability $p_{kj}(t)$ (classical) or $\pi_{kj}(t)$ (quantum mechanical) to be at node k after time t when starting at node j at time 0?

Here the initial condition is either $p_{kj}(0) = \delta_{kj}$ or $\pi_{kj}(0) = \delta_{kj}$.

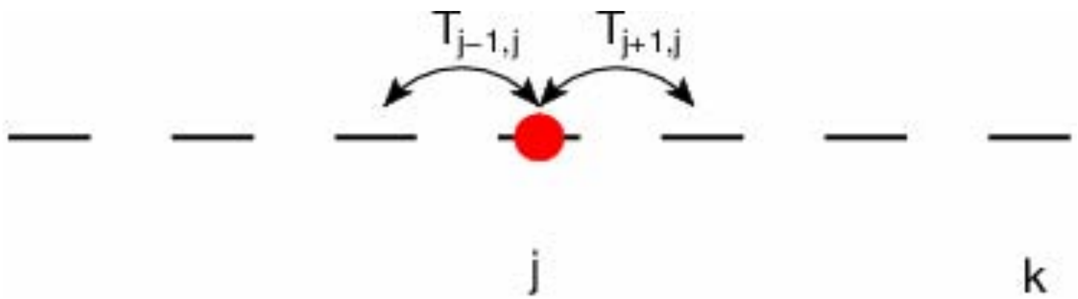
Transition rates

- Classical transition probabilities

Initial node j: $\left| j,0 \right\rangle \equiv \left| j \right\rangle$ $\qquad$ $\left\langle j \middle| j \right\rangle \equiv p_{jj}(0) = 1$

State after time t: $\left| j,t \right\rangle$

Probability of being at node k at time t: $\left\langle k \middle| j;t \right\rangle \equiv p_{kj}(t)$



- The transition rates per unit time between two nodes are given by the transfer matrix **T** with elements $T_{kj} \equiv \left\langle k \middle| \mathbf{T} \middle| j \right\rangle$

- In the simplest case the transfer matrix is $\mathbf{T} = -\gamma \mathbf{A}$ (having equal transition rates γ between all bonds)

Master Equation (CTRW)

- The classical motion over the network is determined by the transfer matrix **T**. The CTRW dynamics obeys the Master Equation (ME)

$$\frac{d}{dt} p_{kj}(t) = \sum_m T_{km} p_{mj}(t)$$

In the simplest case $\mathbf{T} = -\gamma \mathbf{A}$ (γ the same for all nodes)

- The ME is similar to the diffusion equation; **A** acts as Laplacian
- The complete solution of the ME (a linear equation) is obtained by determining the eigenvalues λ_n and the eigenstates $|\Psi_n\rangle$ of **T**
- Formally, the ME solution can be written (akin to quantum mechanics) as

$$p_{kj}(t) = \langle k | e^{\mathbf{T}t} | j \rangle = \langle k | e^{-\gamma \mathbf{A} t} | j \rangle,$$

$e^{-\gamma \mathbf{A} t}$ being the time-evolution operator

CTRW dynamics at long times

As in the case of diffusion, the CTRW are irreversible.

Using the time evolution operator and the completeness of the set $\left|\Psi_n\right\rangle$:

$$p_{kj}(t) = \left\langle k \left| e^{-\gamma A t} \right| j \right\rangle = \sum_n e^{-\lambda_n \gamma t} \left\langle k \middle| \Psi_n \right\rangle \left\langle \Psi_n \middle| j \right\rangle$$

For a finite, connected network, **A** has a single vanishing eigenvalue.

The other eigenvalues are all positive.

We set $\lambda_1 = 0$ and $\lambda_n > 0$ for $n > 1$.

At long times, in $p_{kj}(t)$ only the term corresponding to $n = 1$ survives.

One has ground state dominance for $t >> 1$, $\lim_{t \to \infty} p_{kj}(t) = 1/N$

Hence the $p_{kj}(t)$ attain equipartition.

The way to the Continuous Time Quantum Walks (CTQW)

Farhi and Gutmann, Phys. Rev. A **58**, 915 (1998)

Quantum mechanically, the states $\left| j \right\rangle$ (representing the nodes) span the accessible Hilbert space. Furthermore, they obey:

$$\left\langle k \middle| j \right\rangle = \delta_{kj}; \quad \sum_j \left| j \right\rangle \left\langle j \right| = 1$$

The transition amplitudes and the transition probabilities are given by

$$\alpha_{kj}(t) = \left\langle k \middle| e^{-i\mathbf{H}t} \middle| j \right\rangle \equiv \left\langle k \middle| j;t \right\rangle \qquad \pi_{kj}(t) \equiv \left| \alpha_{kj}(t) \right|^2$$

The Schrödinger equation (SE) reads (setting $\hbar \equiv 1$)

$$i \frac{d}{dt} \alpha_{kj}(t) = \sum_m H_{km} \alpha_{mj}(t)$$

<u>The introduction of CTQWs</u>

Taking **H** = −**T** leads to identical right-hand-side expressions of the SE and of the Master Equation. Hence the solution of the SE again requires determining the E_n and the $\left| \Psi_n \right\rangle$.

The fundamental difference between SE and ME is „*i*“, the imaginary unit multiplying $\frac{d}{dt}$.

Dynamics over networks − CTQWs

- The CTRW are irreversible and reach equipartition over the network
- The CTQW are unitary and thus reversible: there exists no definite limiting value ($t \longrightarrow \infty$) for

$$\pi_{kj}(t) = \left| \sum_n e^{iE_n t} \langle k | \Psi_n \rangle \langle \Psi_n | j \rangle \right|^2$$

- In order to compare to CTRW one has to use long time averages

$$\chi_{kj} \equiv \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \pi_{kj}(t)$$

$$= \sum_{n,m} \delta_{E_n, E_m} \langle k | \Psi_n \rangle \langle \Psi_n | j \rangle \langle j | \Psi_m \rangle \langle \Psi_m | k \rangle$$

- Here χ_{kj} depends both on k and on j
- χ_{kj} reflects the connectivity of the network
- δ_{E_n, E_m} equals 1 if $E_n = E_m$ and is zero otherwise

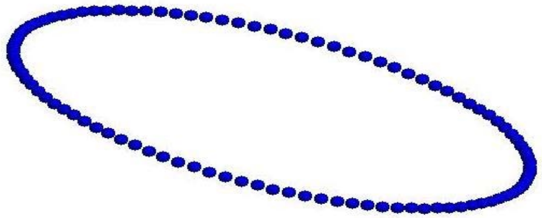
An example: CTQWs over a ring (a 1D regular network)

O. Mülken and A.B., Phys. Rev. E **71**, 036128 (2005)

- Consider a quantum particle on a discrete ring $(\hbar = 1, \ \gamma = 1)$

$$\mathbf{H} = \mathbf{A} = \sum_m \left(2|m\rangle\langle m| - |m-1\rangle\langle m| - |m+1\rangle\langle m|\right)$$

$$i\frac{d}{dt}|j\rangle = \mathbf{H}|j\rangle = 2|j\rangle - |j-1\rangle - |j+1\rangle$$



- Bloch ansatz: The time independent SE reads $\mathbf{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$, with

$$E_n = 2 - 2\cos(2\pi n/N) \text{ and } |\Psi_n\rangle = \frac{1}{\sqrt{N}}\sum_j e^{-i2\pi nj/N}|j\rangle$$

- The time evolution of state $|j\rangle$ is given by

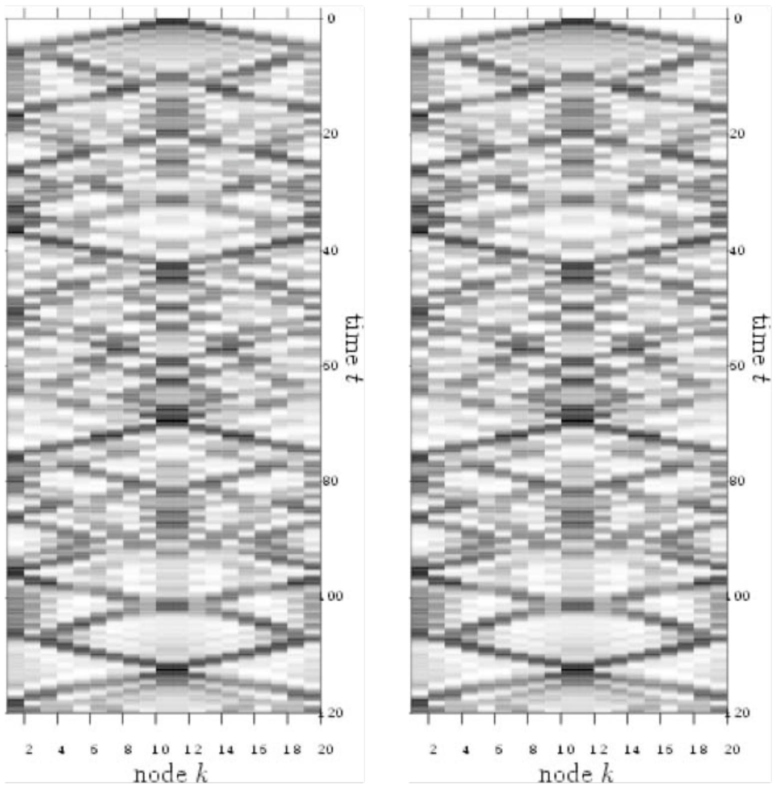
$$e^{-i\mathbf{H}t}|j\rangle = \sum_n e^{-iE_nt}|\Psi_n\rangle\langle\Psi_n|j\rangle = \frac{1}{\sqrt{N}}\sum_n e^{-iE_nt}e^{i2\pi nj/N}|\Psi_n\rangle$$

Hence $\langle k|e^{-i\mathbf{H}t}|j\rangle = \dfrac{1}{N}\sum_n e^{-iE_nt}e^{i2\pi n(j-k)/N}$

1D regular networks – Dynamics; Results

O. Mülken and A.B., Phys. Rev. E **71**, 036128 (2005)

N=21 *N*=20



$\pi_{kj}(t)$ with $j = 11$

Dark= high, bright = low probability

- There appear characteristic regular patterns in space-time
- One observes almost complete revivals at times τ at which

$$\alpha_{kj}(\tau) = \alpha_{kj}(0)$$

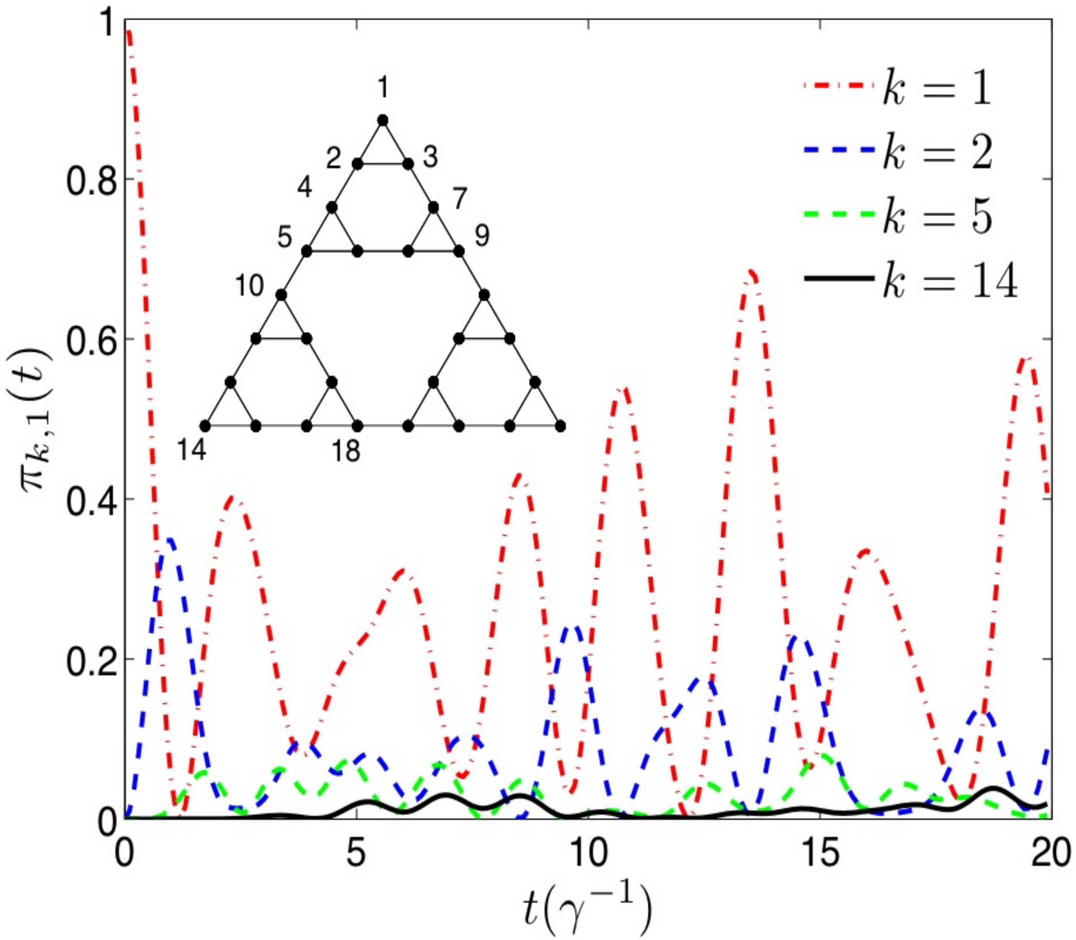
- One observes wave interferences
- The results are discrete analogs of quantum carpets and of Talbot revivals

Grossmann, Rost, Schleich, J. Phys. A **30**, L 277 (1997)
Berry, Marzoli, Schleich, Phys. Today, June 2001
Iwanow et al., Phys. Rev. Lett. **95**, 053902 (2005)

The discreteness diminishes the probability of finding perfect revivals

$\pi_{kj}(t)$ for finite dual Sierpinski gaskets; here $\pi_{k1}(t)$

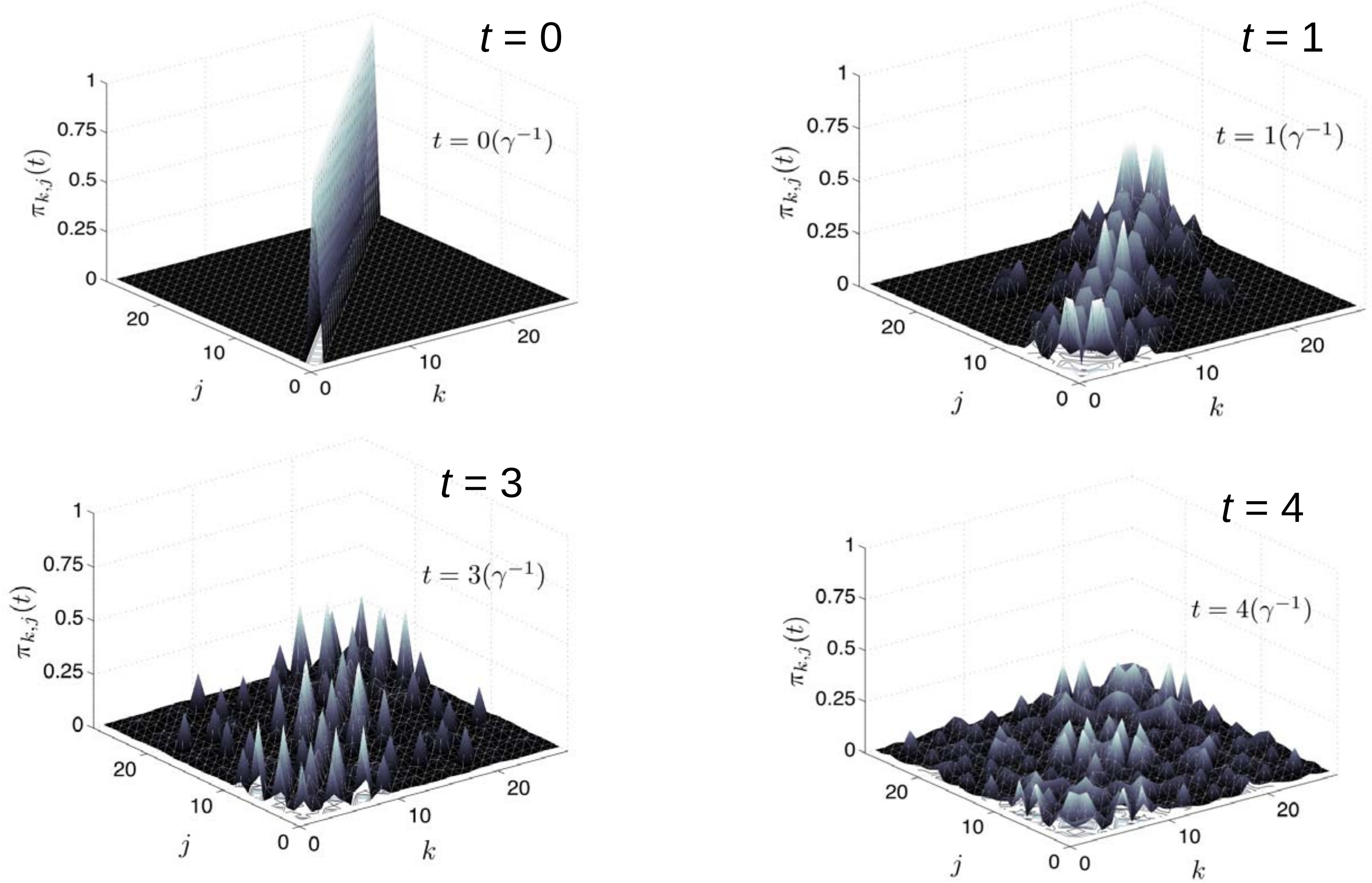
E. Agliari, A.B., O. Mülken, J. Phys. A **41**, 445301 (2008)



Exact probability $\pi_{kj}(t)$ for the CTRW starting from j = 1 (apex) to reach sites k = 1, 2, 5 and 14.

$\pi_{kj}(t)$ for the finite dual Sierpinski gasket with g = 3

E. Agliari, A.B., O. Mülken, J. Phys. A **41**,445301 (2008)

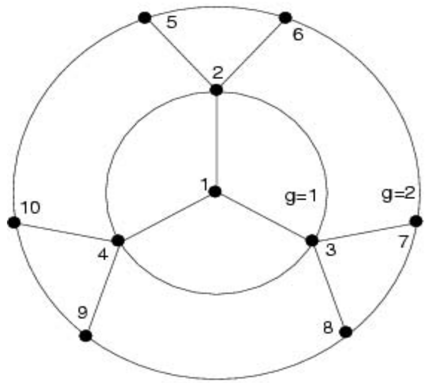


The walker stays a long time close to its original node; the π_{kj} are large only for clusters of sites directly connected by bonds.

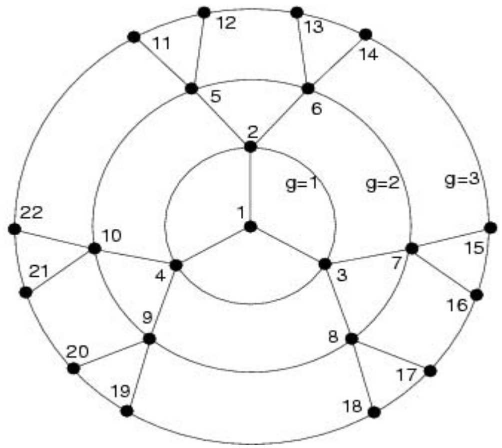
Dendrimers – Hyperbranched networks

O. Mülken and A.B., J. Chem. Phys. **124**, 124905 (2006)

Dendrimers



g = 2



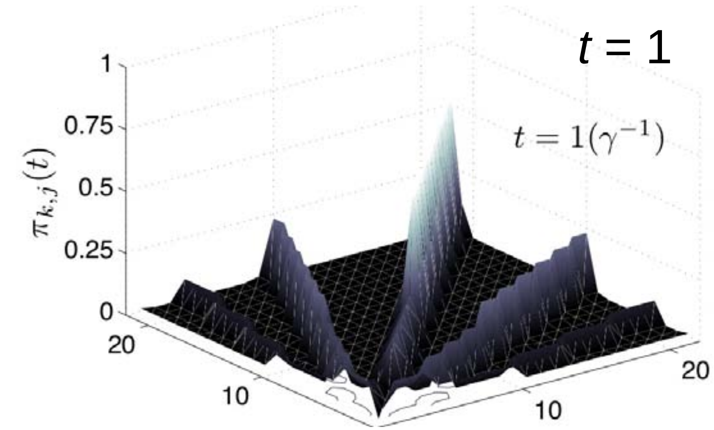
g = 3

- Chemical realisation: hyperbranched macromolecules with a very regular structure
- Their number of nodes grows exponentially with their generation
- They show highly degenerated eigenvalues
- They display a strong dependence of CTQW on the initial conditions

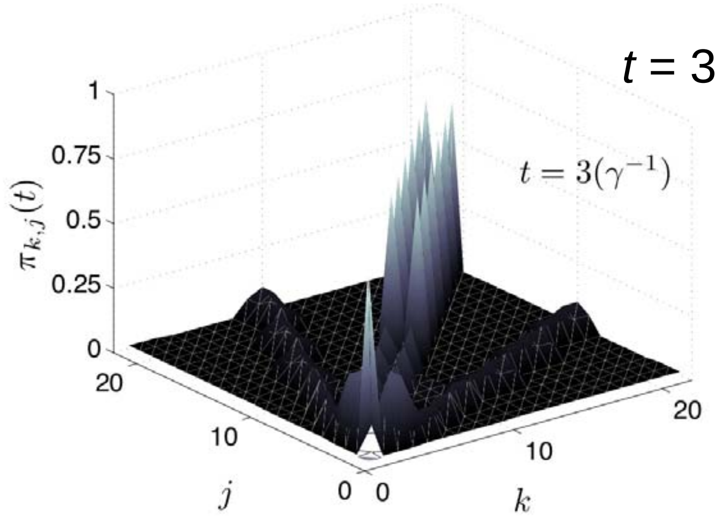
$\pi_{kj}(t)$ for the dendrimer with f = 3 and g = 3

E. Agliari, A.B., O. Mülken, J. Phys. A **41**, 445301 (2008)

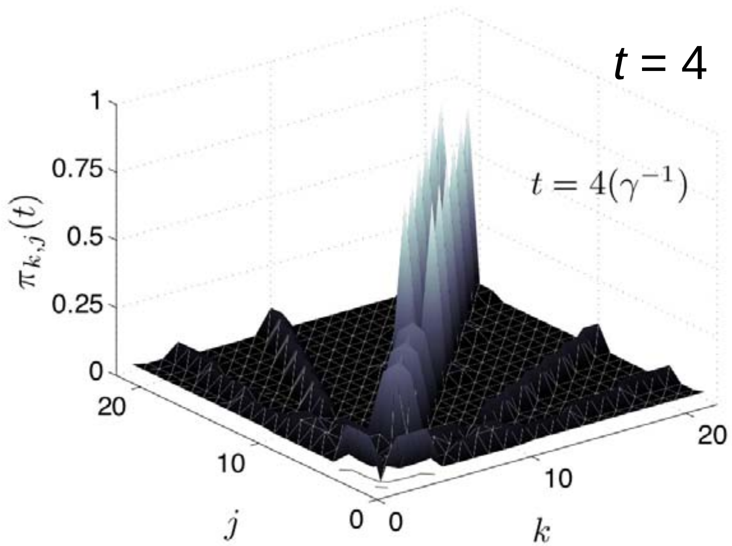
t = 1



t = 3



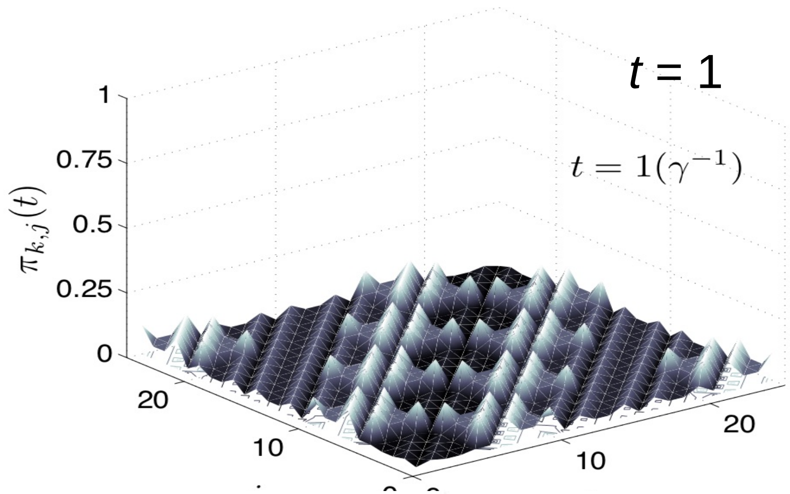
t = 4

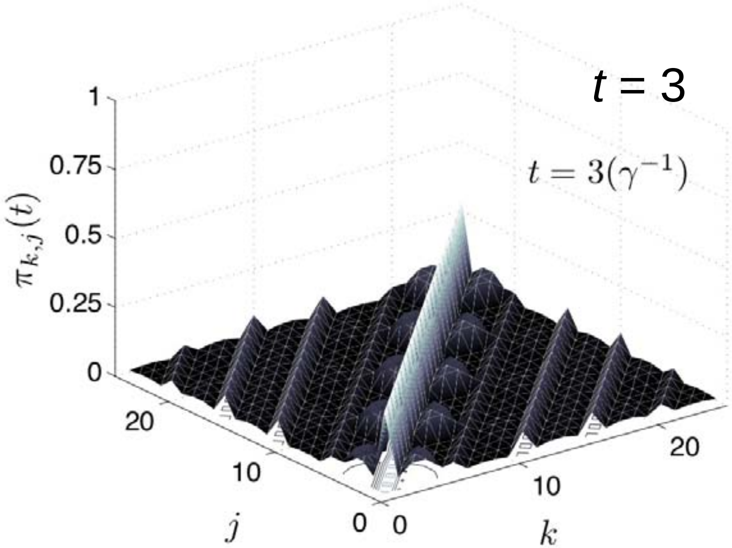


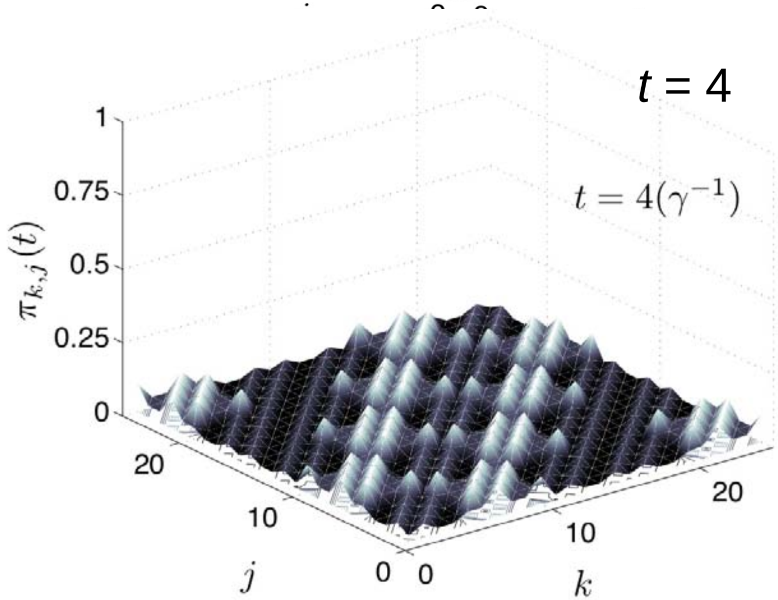
Findings: A large fraction of π_{kj} is localized on particular pairs of nearest-neighbor sites; again the walker stays a long time close to its original node.

$\pi_{kj}(t)$ for a square torus of linear size $L = 5$

E. Agliari, A.B., O. Mülken, J. Phys. A **41**, 445301 (2008)





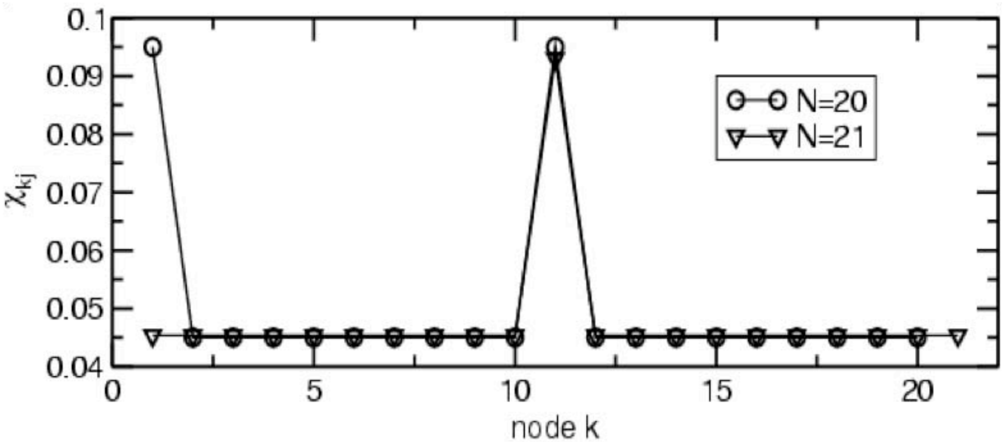


Finding: The distribution spreads quickly and regularly over the whole structure

1D regular networks – Situation at long times

O. Mülken and A.B., Phys. Rev. E **71**, 036128 (2005)

- The long time average χ_{kj} reflects the parity of the lattice



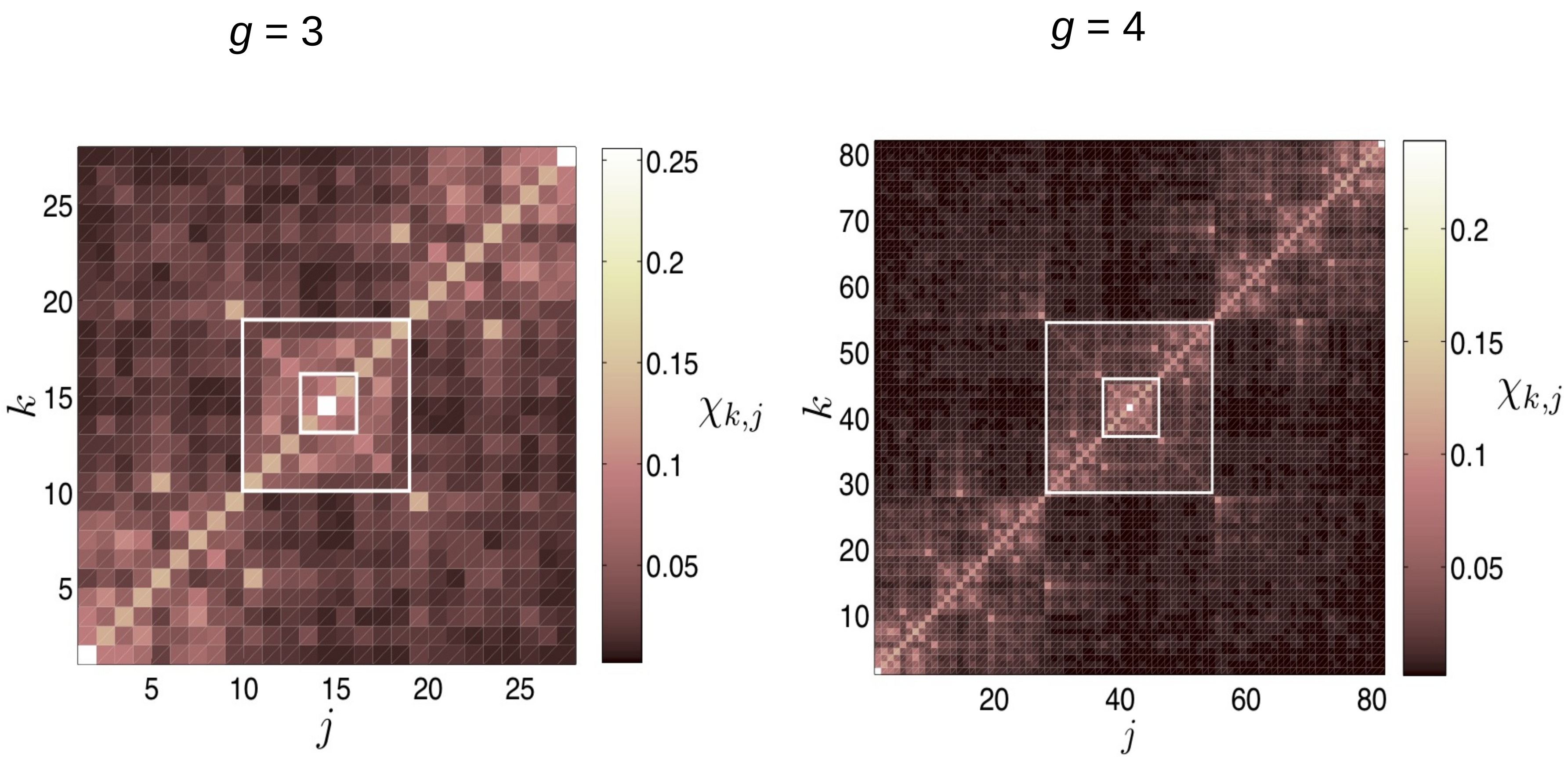
- Odd *N:* One peak at *j*, equal distribution over all other nodes
- Even *N*: Two peaks at *j* and $j \pm N/2$, reflecting constructive interference at $j \pm N/2$

$$\chi^0_{kj} \begin{cases} (2N-1)/N^2 & \text{for } k=j \\ (N-1)/N^2 & \text{else} \end{cases} ; \quad \chi^0_{kj} = \begin{cases} (2N-2)/N^2 & \text{for } k=j, j+N/2 \\ (N-2)/N^2 & \text{else} \end{cases}$$

- Reminder: for CTRW one has equipartition, $p_{kj} = 1/N$

χ_{kj} for finite dual Sierpinski gaskets

E. Agliari, A.B., O. Mülken, J. Phys. A **41**, 445301 (2008)

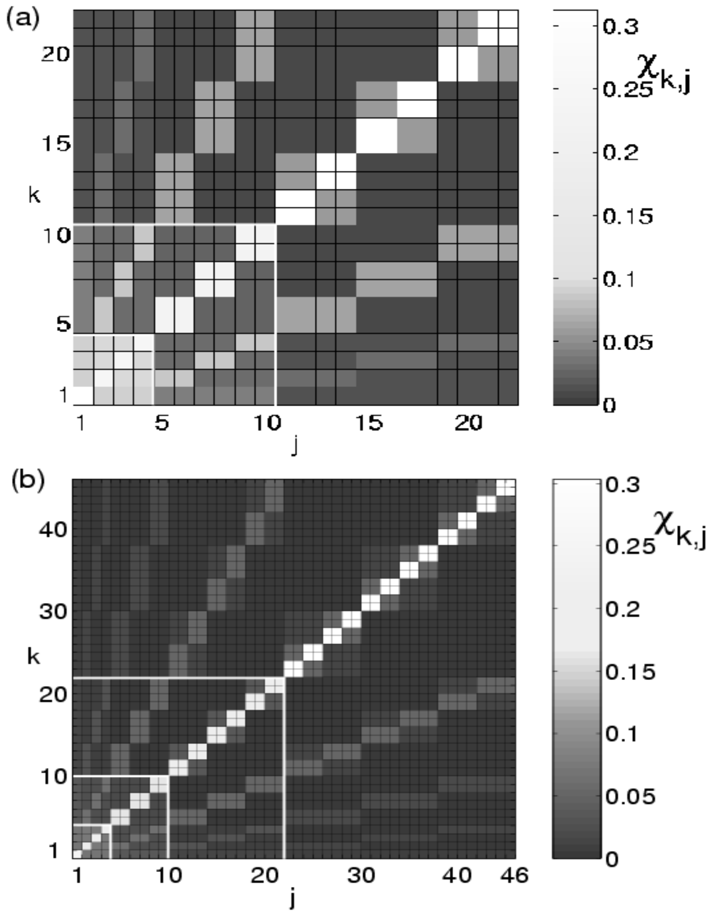


Note that the global maxima lay on the main diagonal. The patterns are self-similar, as exemplified by the indicated substructures.

χ_{kj} for dendrimers (hyperbranched networks)

O. Mülken, V. Bierbaum, A.B., J. Chem. Phys. **124**, 124905 (2006)

- Depending on the initial condition, the $\pi_{kj}(t)$ cluster
- For excitations starting at the center: we find concentric transport
- For excitations starting at a peripheral site: the excitation stays close to the initial node



Most evident in the long time average

$$\chi_{kj} = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\ \pi_{kj}(t)$$

$$= \sum_{n,m} \delta_{E_n,E_m} \langle k|\Psi_n\rangle\langle\Psi_n|j\rangle\langle j|\Psi_m\rangle\langle\Psi_m|k\rangle$$

•We find a self-similar structure for the χ_{kj}

•The clusters of equal probabilities depend on the initial condition

•Mapping to a line possible if $j = 1$

•The CTRW leads to equipartition

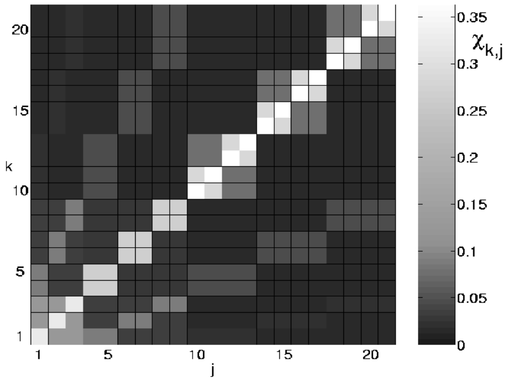
χ_{kj} for Husimi cacti

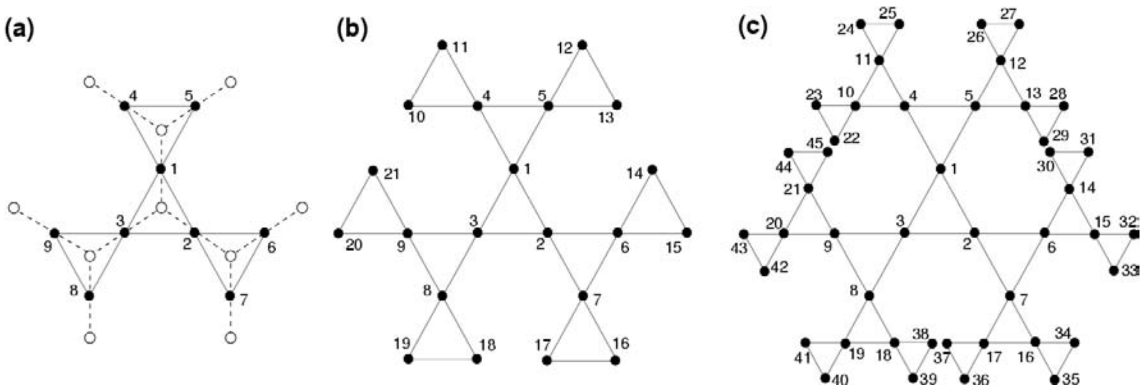
O. Mülken, A.B., V. Bierbaum, Physica A **371**, 10 (2006)

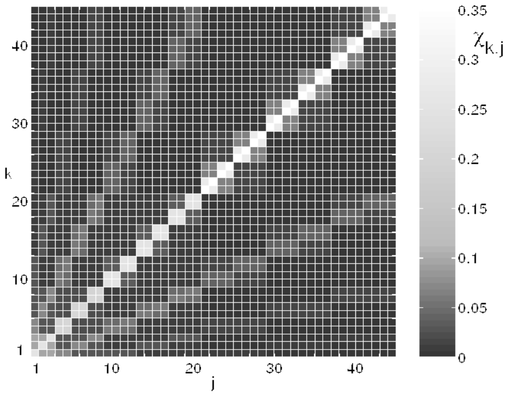
Husimi cacti:

Construction: Replace the bonds of dendrimers by nodes and connect neighboring nodes.

Thus: The Husimi cacti are dual to the dendrimers and have loops.







- The results are similar to those of the dendrimers.
- There is almost no influence of the loops on the CTQW.

The CTQW transport efficiency

O. Mülken and A.B., Phys. Rev. E**73**, 066117 (2006)

The return probabilities $\pi_{jj}(t)$ allow to quantify the transport performance

- $1-\pi_{jj}(t)$: probability to be at any of the nodes $k \neq j$
- Average over all j: global statement

$$\bar{\pi}(t) \equiv \frac{1}{N}\sum_j \pi_{jj}(t) = \frac{1}{N}\sum_j \left|\sum_n e^{-iE_n t}\langle \Psi_n | j \rangle\langle j | \Psi_n \rangle\right|^2$$

Quick decay of $\bar{\pi}(t)$: fast propagation through the network

Slow decay of $\bar{\pi}(t)$: slow propagation through the network

Classical case (CTRW):

$$\bar{p}(t) = \frac{1}{N}\sum_n e^{-E_n t}\langle \Psi_n | \overbrace{\sum_j | j \rangle\langle j |}^{=1} \Psi_n \rangle = \frac{1}{N}\sum_n e^{-E_n t}$$

Quantum case (CTQW):

To evaluate $\bar{\pi}(t)$ one needs the eigenstates $|\Psi_n\rangle$!

The CTQW transport efficiency (continued)

O. Mülken and A.B., Phys. Rev. E **73**, 066117 (2006)

Simplification of the quantum mechanical evaluation

Remark: There exists a lower bound (based on the Cauchy-Schwarz inequality):

$$\bar{\pi}(t) = \frac{1}{N}\sum_j \left|\alpha_{jj}(t)\right|^2 \geq \left|\frac{1}{N}\sum_j \alpha_{jj}(t)\right|^2 = \left|\bar{\alpha}(t)\right|^2$$

- $\bar{\alpha}(t)$ depends only on the eigenvalues E_n

$$\left|\bar{\alpha}(t)\right|^2 = \left|\frac{1}{N}\sum_n e^{-iE_n t}\left\langle \Psi_n \left| \underbrace{\sum_j |j\rangle\langle j|}_{=1} \right| \Psi_n \right\rangle\right|^2 = \left|\frac{1}{N}\sum_n e^{-iE_n t}\right|^2$$

- $\left|\bar{\alpha}(t)\right|^2$ oscillates:

  Use envelope $\mathrm{env}\left(\left|\bar{\alpha}(t)\right|^2\right)$ to compare to $\bar{p}(t)$

Transport efficiency over rings and dendrimers

O. Mülken and A.B., Phys. Rev. E **73**, 066117 (2006)

Examples:

(a) Discrete ring

$$\bar{p}(t) = (1/N)\sum_n e^{-E_n t}$$ is dominated by the smallest E_n

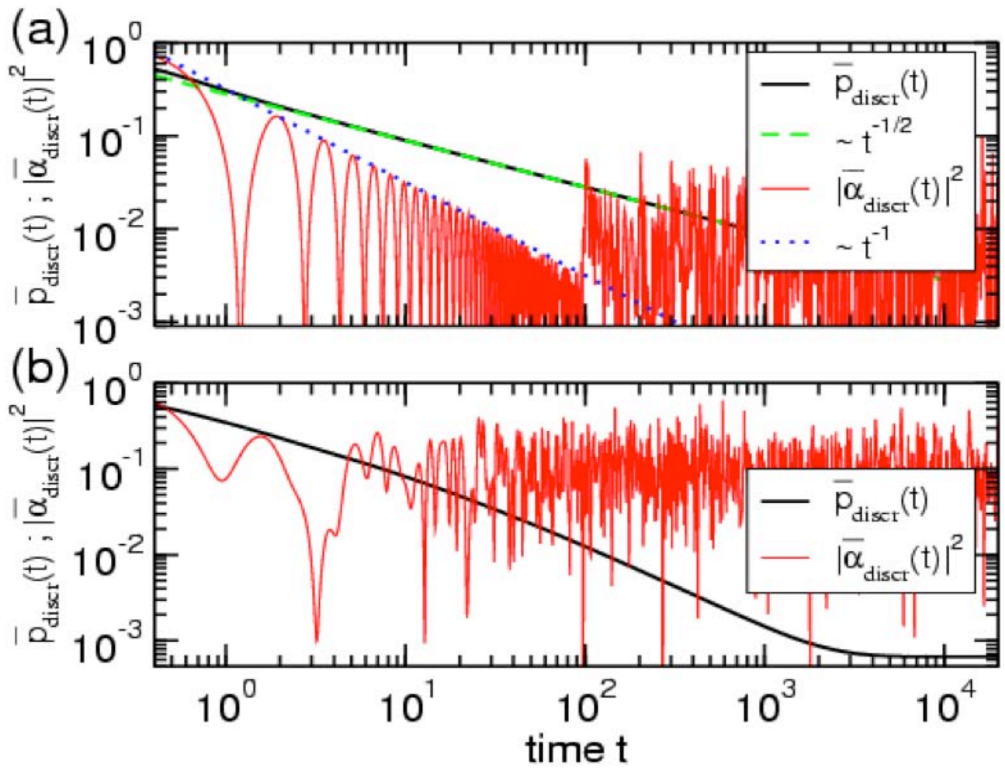
$$E_n = 2 - 2\cos(2\pi n/N);$$ for n small: $E_n \approx 4\pi^2 n^2/N^2$.

$$\bar{p}(t) \sim t^{-1/2}$$

Quantum mechanically

$$\mathrm{env}\left[\bar{\pi}(t)\right] \sim t^{-1}$$

(b) Dendrimer with g = 10



General remarks on the efficiency of the transport

O. Mülken and A.B., Phys. Rev. E 73, 066117 (2006)

Continuous DOS $\rho(E): \bar{p}(t) = \int dE\, \rho(E) e^{-Et}$ and $\bar{\pi}(t) \geq \left| \int dE\, \rho(E) e^{iEt} \right|^2$

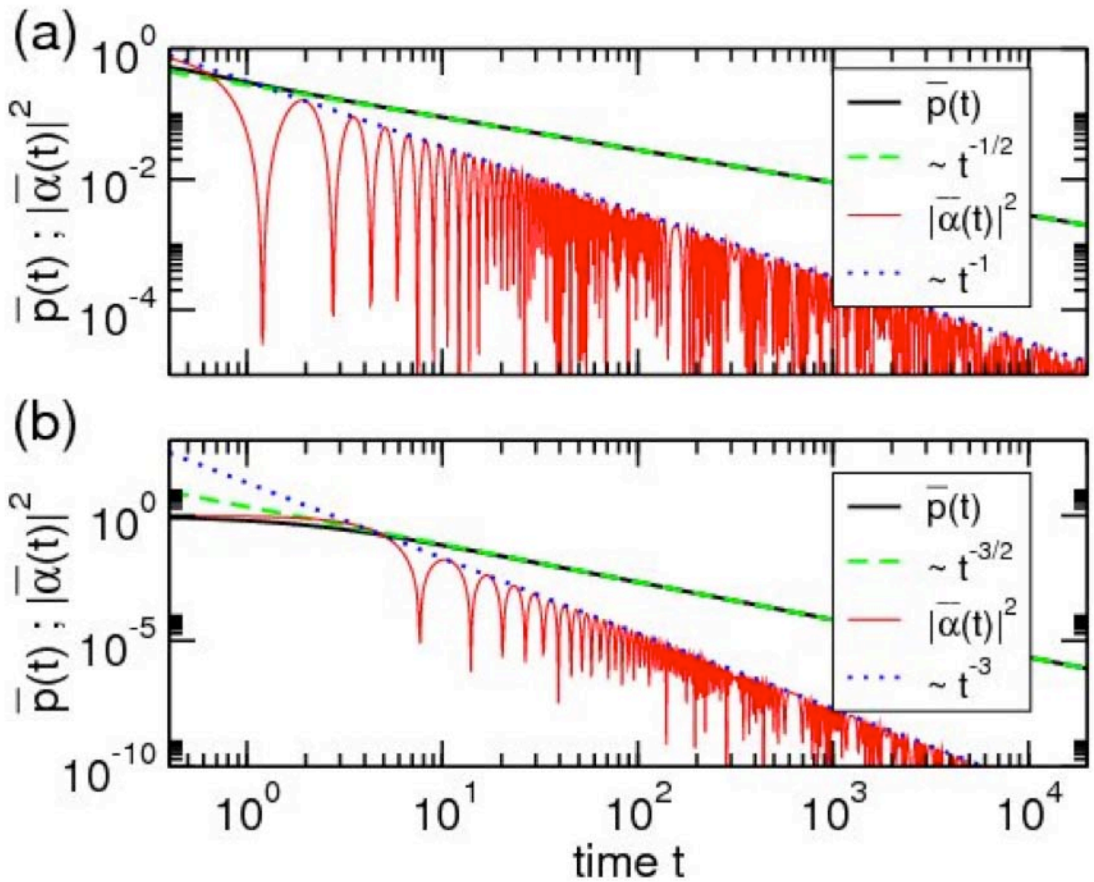
$\rho(E) \sim E^{\nu}$

Classical:

$\bar{p}(t) \sim t^{-(1+\nu)}$

Quantum:

$\mathrm{env}\left(\left| \bar{\alpha}(t) \right|^2 \right) \sim t^{-2(1+\nu)}$



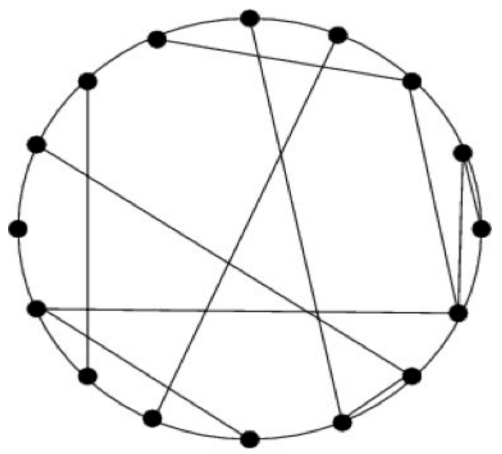
(a) 1D regular network, (b) random graph with the DOS given by Wigner's semicircle law.

CTQW over Small-World Networks (SWN)

O. Mülken, V. Pernice, A.B., Phys. Rev. E **76**, 051125 (2007)

- SWN are models for systems with short and long range interactions.

- Applications in various fields.
- Statistical statements – ensemble average.



SWN: ring with additional bonds

We find for CTQWs over SWN:

- A fast transport through the SWN.
- No equipartition but a strong dependence on the initial node.
- No Anderson localization.

$\langle \bar{p}(t) \rangle_R$ and $\langle \bar{\pi}(t) \rangle_R$ for CTQW over SWN

O. Mülken, V. Pernice, A.B., Phys. Rev. E **76**, 051125 (2007)

Increasing the number of additional bond leads for CTRW and CTQW to a faster decay for the return probabilities

- Long time average, also over the realizations R:

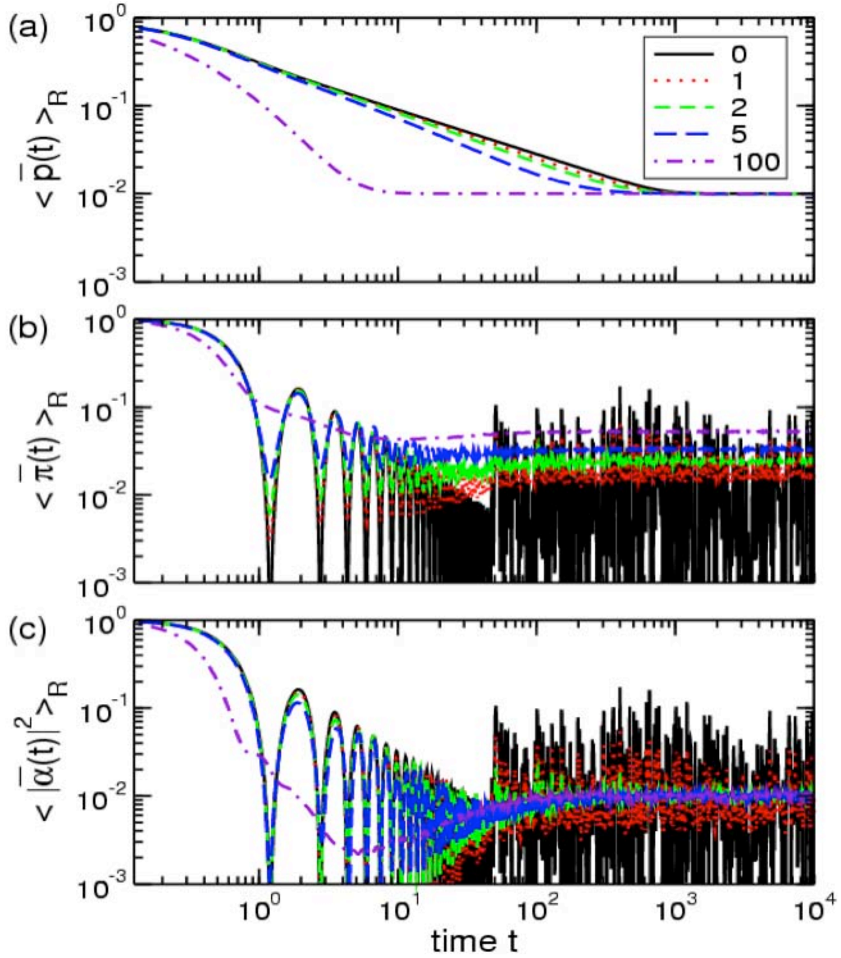
$$\langle \bar{\chi} \rangle_R = \left\langle \lim_{T\to\infty} \frac{1}{T} \int_0^T dt \bar{\pi}(t) \right\rangle_R$$

- The E_n of SWN are almost always non-degenerate.

$$\langle \bar{\chi} \rangle_R = \frac{1}{RN} \sum_{r,j,n} \left| \langle j | \Psi_{n,r} \rangle \right|^4$$

- $\langle \bar{\chi} \rangle_R$ depends on the eigenstates.
- We find localized eigenstates at the band edges.
- For the ring, equipartition: $1 / N^2$

Here, $N = 100$.



Trapping in the CTQW picture

O. Mülken, A.B., T. Amthor, C. Giese, M. Reetz-Lamour, M. Weidemüller,
Phys. Rev. Lett. **99**, 090601 (2007)

The moving entities (ions, electrons, excitons) may get trapped

Model: Out of the *N* nodes *M* are traps (absorbing sinks)

We denote the set of traps by $\mathcal{M}$

Let T_0 (classical) and H_0 (quantal) denote the situation without traps.

We introduce the traps by including a trapping matrix (operator) $\mathbf{\Gamma}$

$$\Gamma_{mm} = \begin{cases} \Gamma > 0 & \text{for} \quad m \in \mathcal{M} \\ 0 & \text{else} \end{cases}$$

Then

- CTRW: $\mathrm{T} = \mathrm{T}_0 - \Gamma,$
- CTQW: $\mathrm{H} = \mathrm{H}_0 - i\Gamma,$

Implications of trapping in the CTQW scheme

O. Mülken, A.B., T. Amthor, C. Giese, M. Reetz-Lamour, M. Weidemüller,
Phys. Rev. Lett. **99**, 090601 (2007)

Properties of **H**

- **H** is non-hermitian **H** ≠ **H**†
- **H** has *N* complex eigenvalues, $E_j = \varepsilon_j - i\gamma_j$
- **H** has *N* left and *N* right eigenstates, $\left|\Psi_j\right\rangle$ and $\left\langle\tilde{\Psi}_j\right|$; generally:

$$\left\langle\tilde{\Psi}_j \middle| \Psi_{j'}\right\rangle = \delta_{jj'} \text{ and } \sum_j \left|\Psi_j\right\rangle\left\langle\tilde{\Psi}_j\right| = 1$$

The γ_j determine the temporal decay of $\pi_{kj}(t) = \left|\alpha_{kj}(t)\right|^2$

$$\alpha_{kj}(t) = \sum_m \exp(-\gamma_m t)\exp(-i\varepsilon_m t)\left\langle k \middle| \Psi_m\right\rangle\left\langle\tilde{\Psi}_m \middle| j\right\rangle$$

General situation for trapping

O. Mülken, A.B., T. Amthor, C. Giese, M. Reetz-Lamour, M. Weidemüller,
Phys. Rev. Lett. **99**, 090601 (2007)

In an ideal experiment one would excite one node $j \notin \mathcal{M}$ and read out the probability $\pi_{kj}(t)$ to be at node $k \notin \mathcal{M}$ at time *t*. Realistically, each node which is not a trap can be excited with equal probability.

In this case the mean survival probabilities are:

$$\Pi_M(t) = \frac{1}{N-M} \sum_{j \notin \mathcal{M}} \sum_{k \notin \mathcal{M}} \pi_{kj}(t) \quad \text{and} \quad P_M(t) \equiv \frac{1}{N-M} \sum_{j \notin \mathcal{M}} \sum_{k \notin \mathcal{M}} p_{kj}(t)$$

$$\Pi_M(t) \equiv \frac{1}{N-M} \sum_j e^{-2\gamma_j t} \left[1 - 2 \sum_{m \in \mathcal{M}} \langle \tilde{\Psi}_j | m \rangle \langle m | \Psi_j \rangle \right]$$

$$+ \frac{1}{N-M} \sum_{j,j'} e^{-i(E_j - E^*_{j'})t} \left[\sum_{m \in \mathcal{M}} \langle \tilde{\Psi}_{j'} | m \rangle \langle m | \Psi_j \rangle \right]^2$$

CTQW trapping behaviour

O. Mülken, A.B., T. Amthor, C. Giese, M. Reetz-Lamour, M. Weidemüller,
Phys. Rev. Lett. **99**, 090601 (2007)

For small M / N and t large $\Pi_M(t)$ simplifies considerably:

- At long times the oscillating term drops out and for small M / N we can assume

  $2\sum_{m\in\mathcal{M}}\langle\tilde{\Psi}_j|m\rangle\langle m|\Psi_j\rangle << 1.$ Then:

$$\Pi_M(t) \approx \frac{1}{N-M}\sum_j \exp\left(-2\gamma_j t\right)$$

- Asymptotically, $\Pi_M(t)$ is dominated by the γ_j values closest to zero:

$$\Pi_M(t) \approx \exp(-2\gamma_{\min} t)$$

- Such long times are not of much experimental relevance
- The γ_j often scale in a large j range, $\gamma_j \sim aj^{\mu}$. For densely distributed γ_j and at intermediate times:

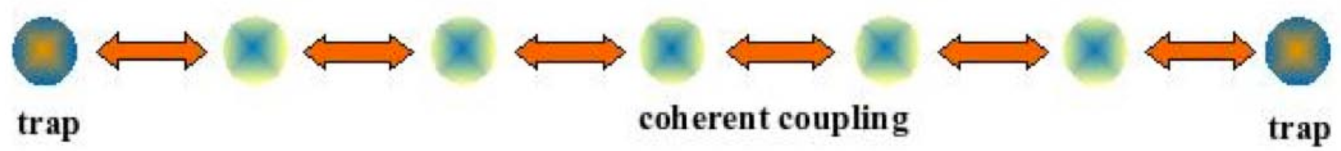
$$\Pi_M(t) \approx \int d\chi e^{-2at\chi^{\mu}} = \int dy \frac{e^{-y^{\mu}}}{(2at)^{-1/\mu}} \sim t^{-1/\mu}$$

Experimental design using Rydberg gases

O. Mülken, A.B., T. Amthor, C. Giese, M. Reetz-Lamour, M. Weidemüller,
Phys. Rev. Lett. **99**, 090601 (2007)

Example:

Chain of length *N* with two traps (*M* = 2) located at its ends (*m* = 1 and *m* = *N*); description within a nearest-neighbor tight-binding model



(Courtesy of M. Weidemüller's group)

- CTQW Hamiltonian:

$$\mathbf{H} = +\sum_{n=2}^{N-1}\Big(2|n\rangle\langle n| - |n-1\rangle\langle n| - |n+1\rangle\langle n|\Big)$$
$$+\Big(|1\rangle\langle 1| - |2\rangle\langle 1|\Big) + \Big(|N\rangle\langle N| - |N-1\rangle\langle N|\Big)$$
$$-i\Gamma|1\rangle\langle 1| - i\Gamma|N\rangle\langle N|$$

Trapping in CTRW

O. Mülken, A.B., T. Amthor, C. Giese, M. Reetz-Lamour, M. Weidemüller,
Phys. Rev. Lett. **99**, 090601 (2007)

- CTRW transfer matrix:

$$\mathrm{T} = -\sum_{n=2}^{N-1}\Big(2\left|n\right\rangle\left\langle n\right| - \left|n-1\right\rangle\left\langle n\right| - \left|n+1\right\rangle\left\langle n\right|\Big)$$

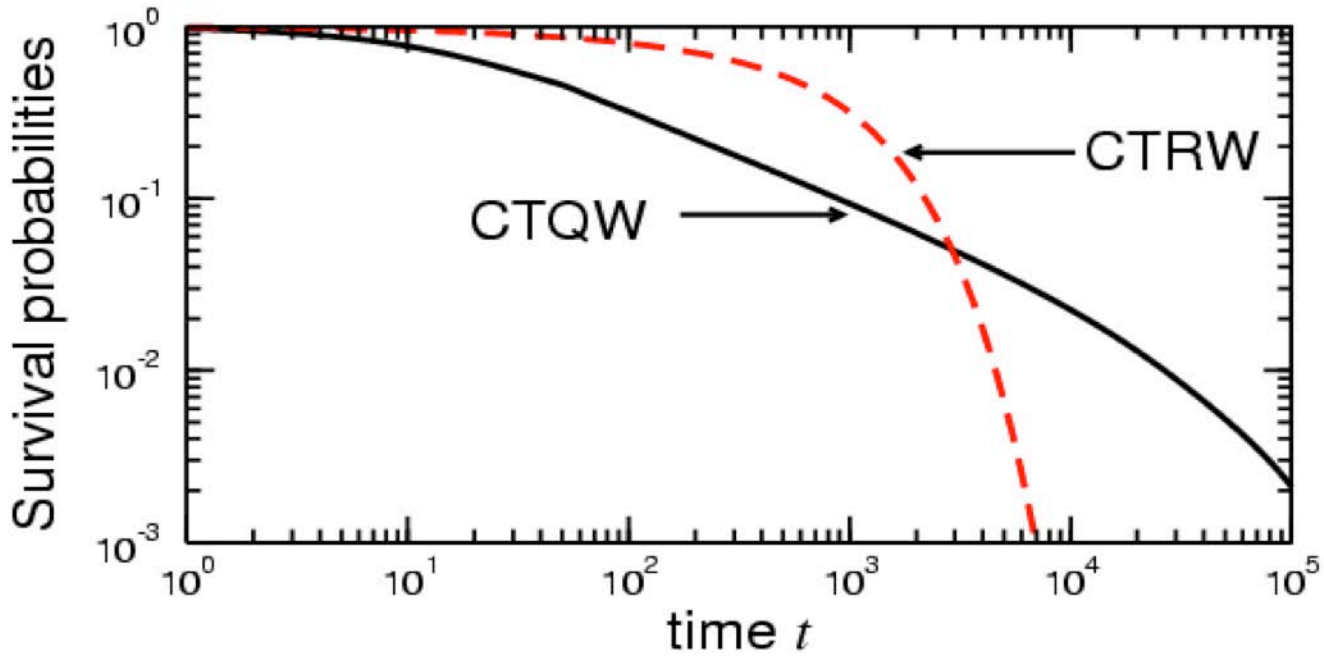
$$-\Big(\left|1\right\rangle\left\langle 1\right| - \left|2\right\rangle\left\langle 1\right|\Big) - \Big(\left|N\right\rangle\left\langle N\right| - \left|N-1\right\rangle\left\langle N\right|\Big)$$

$$-\Gamma\left|1\right\rangle\left\langle 1\right| - \Gamma\left|N\right\rangle\left\langle N\right|$$

Temporal decay of $\Pi_M(t)$ and of $P_M(t)$:

O. Mülken, A.B., T. Amthor, C. Giese, M. Reetz-Lamour, M. Weidemüller,

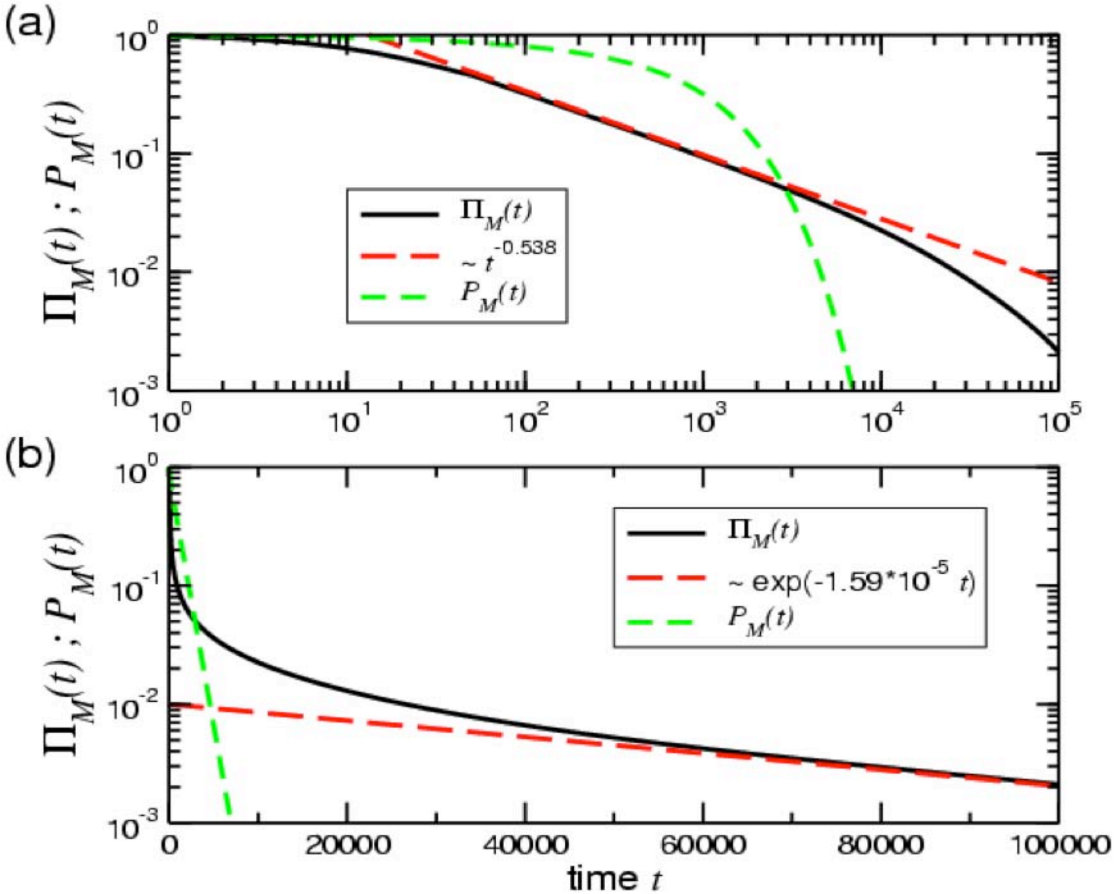
Phys. Rev. Lett. **99**, 090601 (2007)



Analysis of trapping in CTRW and in CTQW

O. Mülken, A.B., T. Amthor, C. Giese, M. Reetz-Lamour, M. Weidemüller,
Phys. Rev. Lett. **99**, 090601 (2007)

The temporal decay of $\Pi_M(t)$ and $P_M(t)$:



$\Pi_M(t)$ and $P_M(t)$ for $N = 100$ and $\Gamma = 1$.

Now, $P_M(t)$ and $\Pi_M(t)$ differ strongly:

i) $P_M(t)$ decays practically in an exponential manner

ii) $\Pi_M(t)$ shows two regimes:

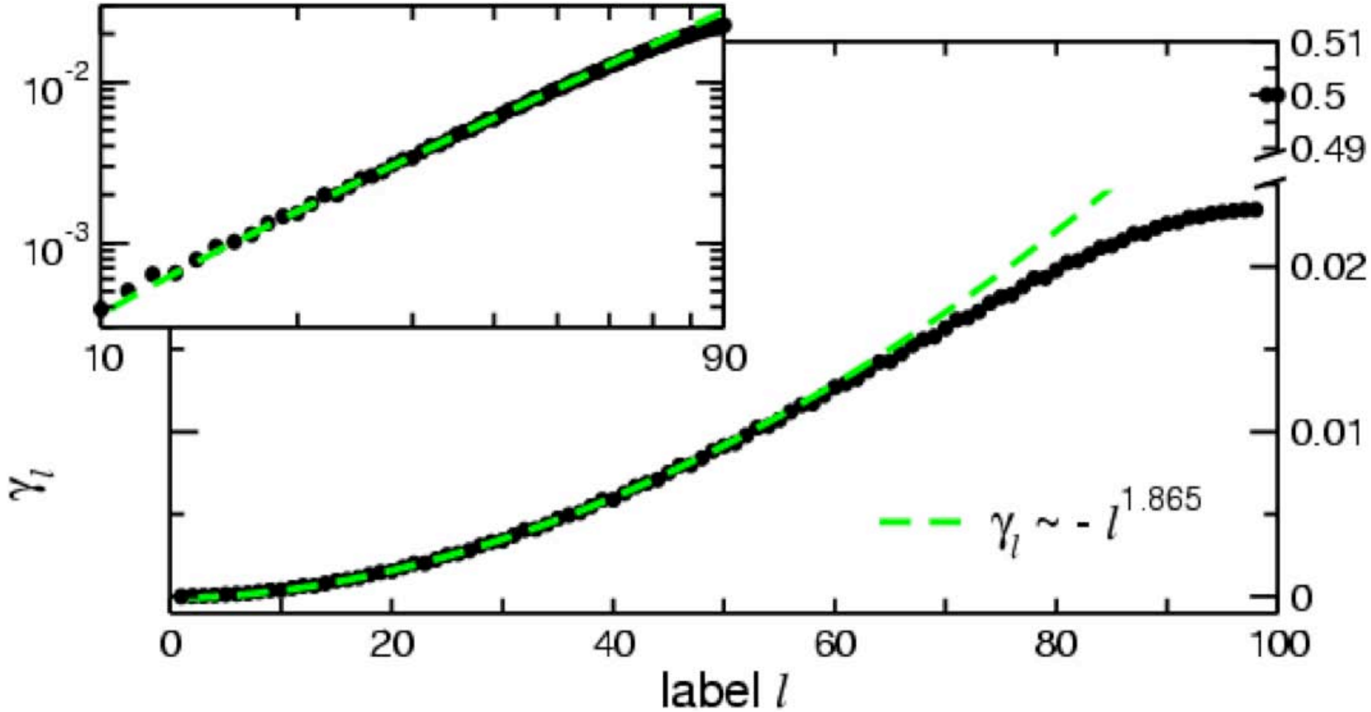
- A power-law decay at intermediate t

$$\Pi_M(t) \sim t^{-0.538} \quad (0.538 = 1/\mu)$$

- An exponential decay at very long t

Imaginary part of the spectrum under trapping

O. Mülken, A.B., T. Amthor, C. Giese, M. Reetz-Lamour, M. Weidemüller,
Phys. Rev. Lett. **99**, 090601 (2007)



γ_l (dots) in ascending order for $N = 100$ and $\Gamma = 1$.

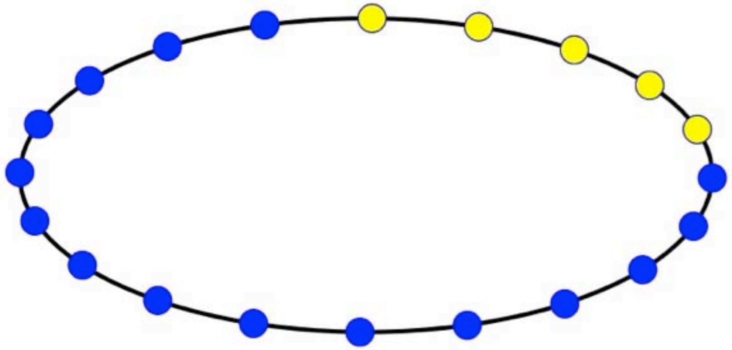
For the imaginary part of the spectrum, $E_j = \varepsilon_j - i\gamma_j$, we find

$\gamma_j \sim a j^{\mu}$ for $10 \leq j \leq 60$, with $\mu = 1.865$

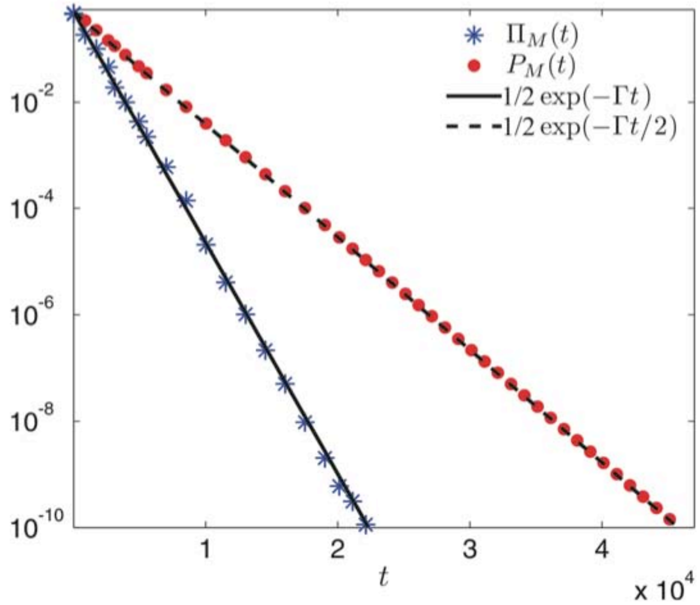
CTQW and trapping on a ring

E. Agliari, O. Mülken and A.B., Internat. J. Bifurc. Chaos **20**, 271 (2010)

Different distributions of traps act differently in CTRW and CTQW



Consecutive arrangement of traps



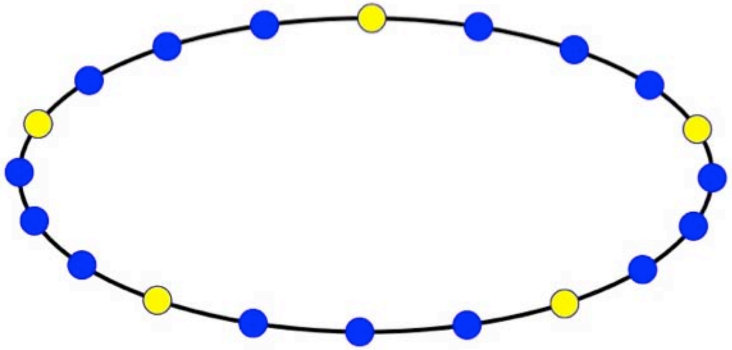
Survival probabilities for a consecutive arrangement of traps

N= 48, M = 24

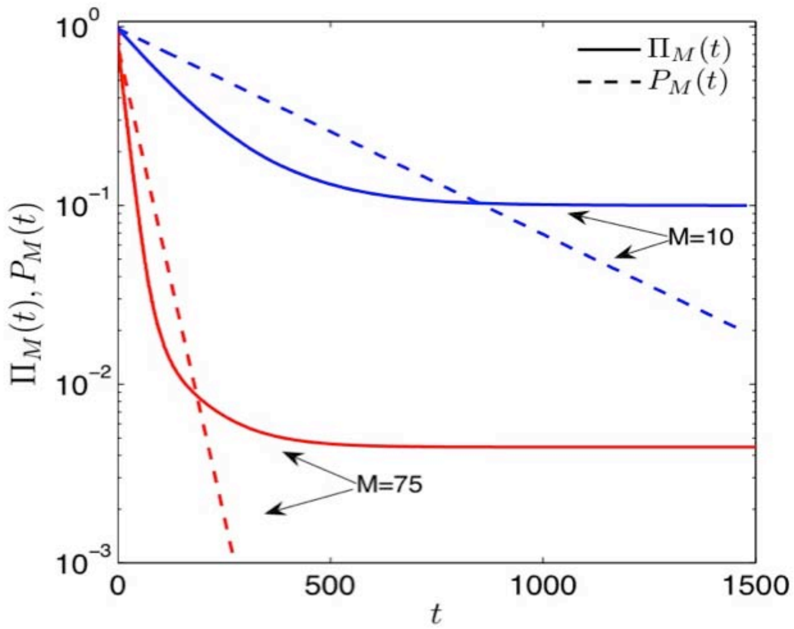
CTRW: $P_M(t)$; CTQW: $\Pi_M(t)$

Difference between CTQW and CTRW trapping on a ring

E. Agliari, O. Mülken and A.B., Internat. J. Bifurc. Chaos **20**, 271 (2010)



Periodic arrangement of traps



Survival probabilities for a periodic arrangement of traps, N=300.
CTRW: $P_M(t)$; CTQW: $\Pi_M(t)$

The CTQW decay curves tend to a plateau value because some of the modes have nodes at all traps' positions and hence do not „see" the traps.

CTQW with long-range interactions

O. Mülken, V. Pernice, A.B., Phys. Rev. E **77**, 021117 (2008)

Experimental realization of system with traps based on an assembly of Rydberg atoms with dipole-dipole interactions going as R^{-3} ($R = |k-j|$: Distance between two nodes).

- Classically: CTRWs with $R^{-\gamma}\left(\gamma > 3\right)$ belong to the same universality class as CTRW with NN-interactions:
- For $\gamma > 3$ the mean square displacement (MSD) goes as t
- For $\gamma < 3$ the MSD diverges
- Quantum mechanically: The MSD goes as t^2 for all $\gamma \geq 2$

- The MSD is related to the average probability to be at initial node:

$$\left\langle R_\gamma^2(t) \right\rangle_{qm} = \frac{1}{N} \sum_{k=1}^{N} \left|k-j\right|^2 \pi_{kj}^{(\gamma)}(t) \sim \left[\bar{\pi}_\gamma(t)\right]^2$$

where $$\bar{\pi}_\gamma(t) \equiv \frac{1}{N} \sum_{j=1}^{N} \pi_{jj}^{(\gamma)}(t) \geq \left| \frac{1}{N} \sum_{j=1}^{N} \alpha_{jj}^{(\gamma)}(t) \right|^2 \equiv \left|\bar{\alpha}_\gamma(t)\right|^2$$

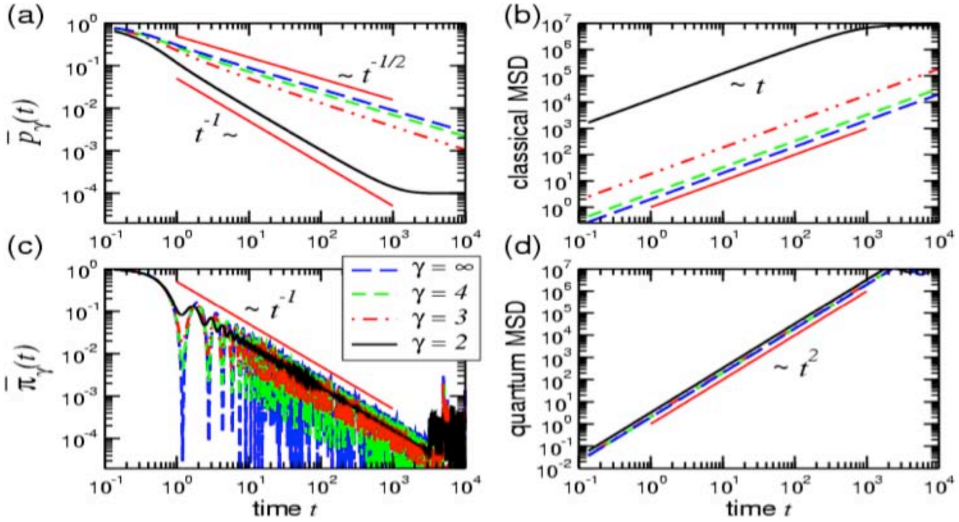
Study of $\bar{p}$ and $\bar{\pi}$ for CTQW and long-range interactions

O. Mülken, V. Pernice, A.B., Phys. Rev. E **77**, 021117 (2008)

Example: A ring without traps:

$$\bar{\pi}_\gamma(t) = \left|\bar{\alpha}_\gamma(t)\right|^2 = \left|\frac{1}{2\pi}\int_0^{2\pi} d\theta \exp\left[iE_\gamma(\theta)t\right]\right|^2$$

$$E_\gamma(\theta) = \sum_{R=1}^{\infty} R^{-\gamma}\left[2-2\cos(\theta R)\right]$$



Left: $\bar{p}_\gamma(t)$ and $\bar{\pi}_\gamma(t)$
Right: classical and quantum MSD for a ring (N=1000) without traps.

Stationary phase approximation:
For $\gamma = 2$ one has one stat. point, $\theta_0 = \pi$

$$\left|\bar{\alpha}_\gamma(t)\right|^2 \approx \frac{1}{2\pi t\left|E''_\gamma(\theta_0)\right|} \sim t^{-1}$$

For $\gamma > 2$ one has two points, $\theta_0 = 0$ and π

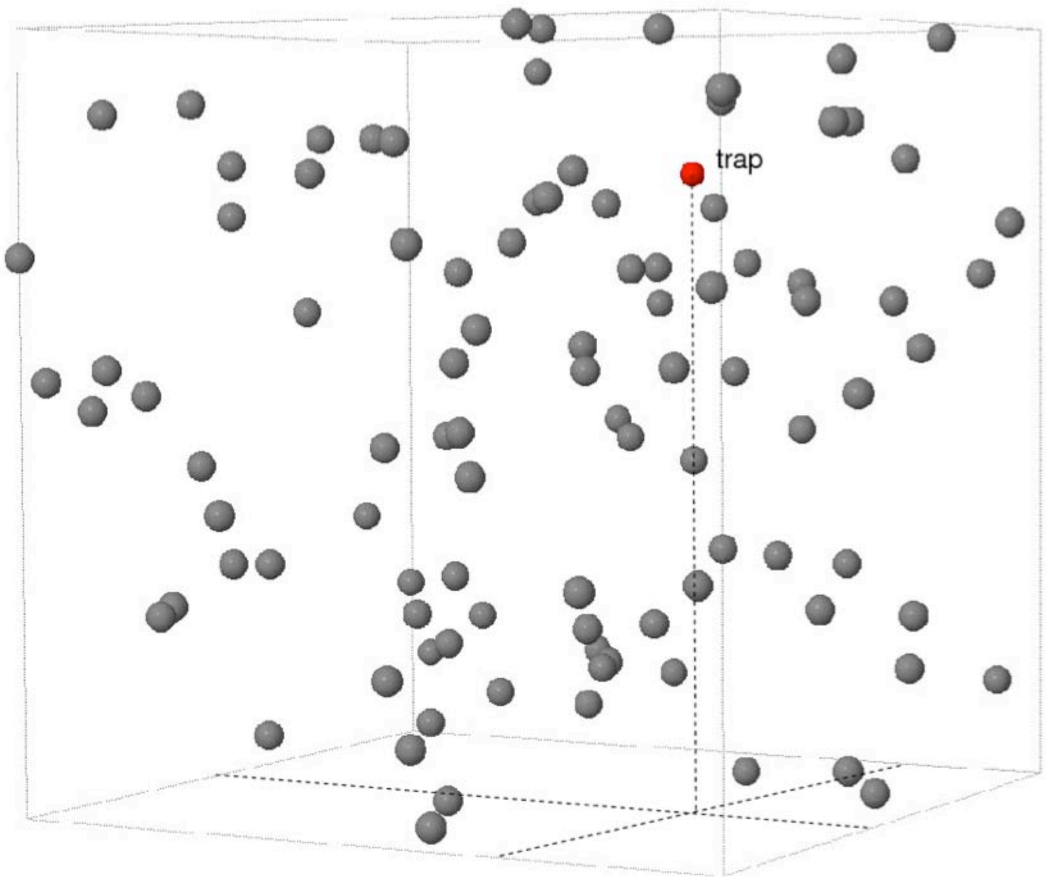
$$\left|\bar{\alpha}_\gamma(t)\right|^2 \approx \frac{1}{2\pi t}\left(\frac{1}{\left|E''_\gamma(0)\right|} + \frac{1}{\left|E''_\gamma(\pi)\right|} + \frac{2\cos\left\{t\left[E_\gamma(0)-E_\gamma(\pi)\right]+\pi/2\right\}}{\sqrt{\left|E''_\gamma(0)E''_\gamma(\pi)\right|}}\right) \sim t^{-1}$$

For $\gamma \geq 2$: $\bar{\pi}_\gamma(t) \sim t^{-1}$

Trapping under long range interactions

O. Mülken and A.B., Physica E 42, 576 (2010)

Disordered system with one trap



Random configuration of N = 100 nodes in a cube

- N nodes placed at random in a 3d box (coordinates $\left\{x^{(i)}\right\}$)
- Distance between j and k:

$$\Delta_{jk} = \left[\sum_{i=1}^{3}\left(x_j^{(i)} - x_k^{(i)}\right)^2\right]^{1/2}$$

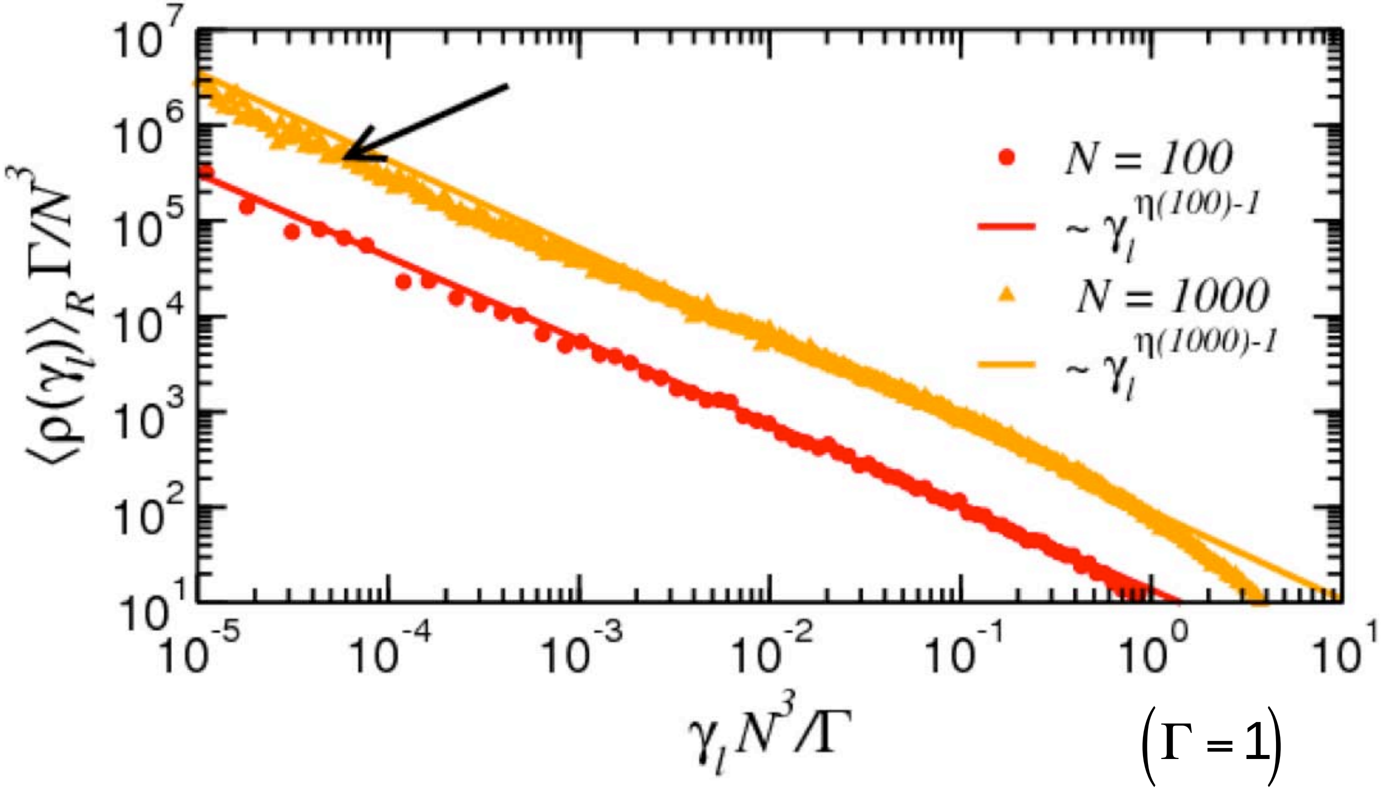
- Interactions decay as Δ_{jk}^{-3}:

$$\langle k|H_0|j\rangle = \begin{cases} -\Delta_{jk}^{-3} & \text{for} \quad k \neq j \\ \sum_{k\neq j}\Delta_{jk}^{-3} & \text{for} \quad k = j \end{cases}$$

Trapping under long range interactions

O. Mülken and A.B., Physica E **42,** 576 (2010)

Disordered systems with one trap



$\left(\Gamma = 1\right)$

$\left\langle \rho(\gamma) \right\rangle_R \approx \mathcal{L}^{-1}\left\{ \left\langle \Pi(t) \right\rangle_R \right\}$ with $\left\langle \Pi(t) \right\rangle_R \sim t^{\eta(N)}$

Best fit: $\left\langle \rho(\gamma_j) \right\rangle_R \sim \gamma_j^{\eta(N)-1}$

Slight bending of $\Pi(t)$ as reflected in the $\rho(\gamma)$, see arrow.

Trapping under long range interactions

O. Mülken and A.B., Physica E **42,** 576 (2010)

Disordered systems; one trap

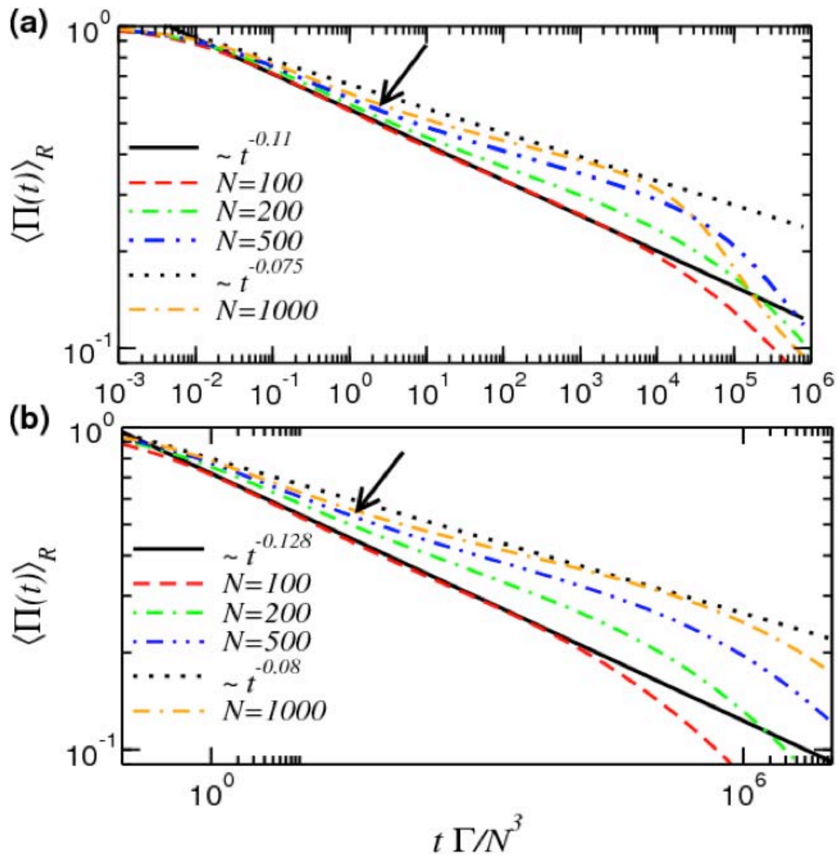
- Ensemble averages

$$\left\langle \Pi(t) \right\rangle_R \equiv \frac{1}{R} \sum_{r=1}^{R} \left[\Pi(t) \right]_r$$

- The correspondence between $\left\langle \Pi(t) \right\rangle_R$ and $\left\langle \gamma_j \right\rangle_R$ is not straightforward

- For all t, exp $(-2\gamma_j t)$ is convex and Jensen's inequality yields:

$$\left\langle \Pi(t) \right\rangle_R \geq \frac{1}{N} \sum_{l=1}^{N} \exp\left(-2t \left\langle \gamma_j \right\rangle R\right)$$



$\left\langle \Pi(t) \right\rangle_R$ for different N:

(a) for $T = 10^{-6}$ and **(b)** for $T = 1$

$\Rightarrow$ Scaling, $\left\langle \Pi(t) \right\rangle_R \sim t^{\eta(N)}$

Take-home messages

Transport over a given network can take place coherently, incoherently or show an intermediate behavior: the CTQWs are purely quantum-mechanical, the CTRWs are purely classical:

CTRW

- classical transport
- Master equation for $p_{kj}(t)$
- probability $\sum_k p_{kj}(t) = 1$
- incoherent
- diffusive motion
- irreversible
- equipartition at long t

CTQW

- quantum transport
- Schrödinger equation for $\alpha_{kj}(t)$
- probability $\sum_k \left|\alpha_{kj}(t)\right|^2 = 1$
- coherent
- wave interference
- reversible
- unitary time evolution

There's plenty of room in the middle…

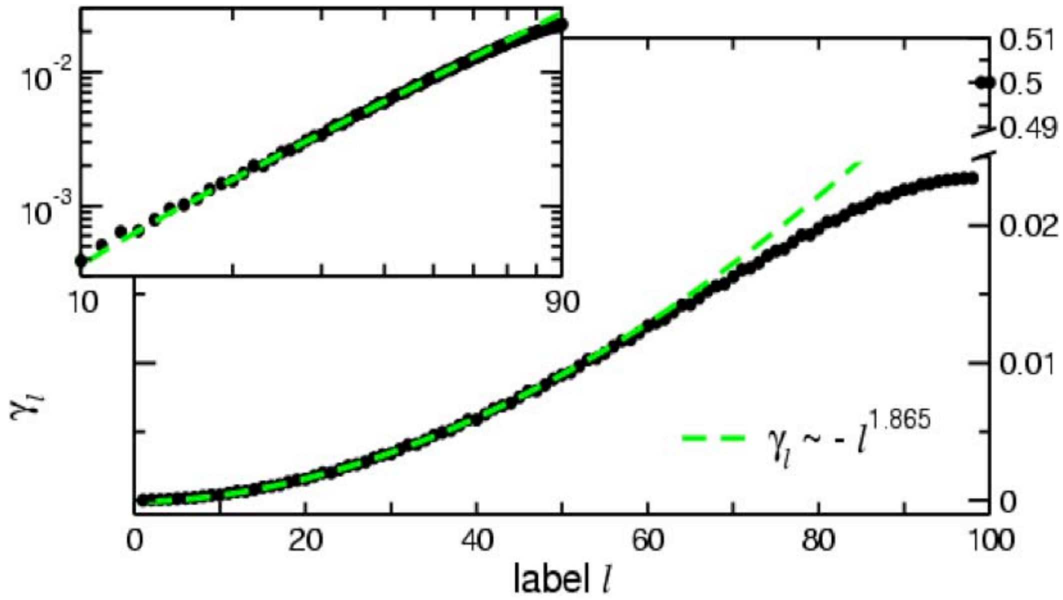
Analysis of the imaginary part of the spectrum

O. Mülken, A.B., T. Amthor, C. Giese, M. Reetz-Lamour, M. Weidemüller,
Phys. Rev. Lett. **99**, 090601 (2007)

The imaginary part of the spectrum, $E_j = \varepsilon_j - i\gamma_j$:
$\gamma_j \sim a j^{\mu} (\mu = 1.865)$
for $10 \le j \le 60$

Time scale in units of
$\left[\hbar / \langle j \pm 1 | H_0 | j \rangle \right]$

For Rydberg gases
$\langle j \pm 1 | H_0 | j \rangle / \hbar \ \geq 1\mathrm{MHz} : \mathrm{ns} - \mu\mathrm{s}$

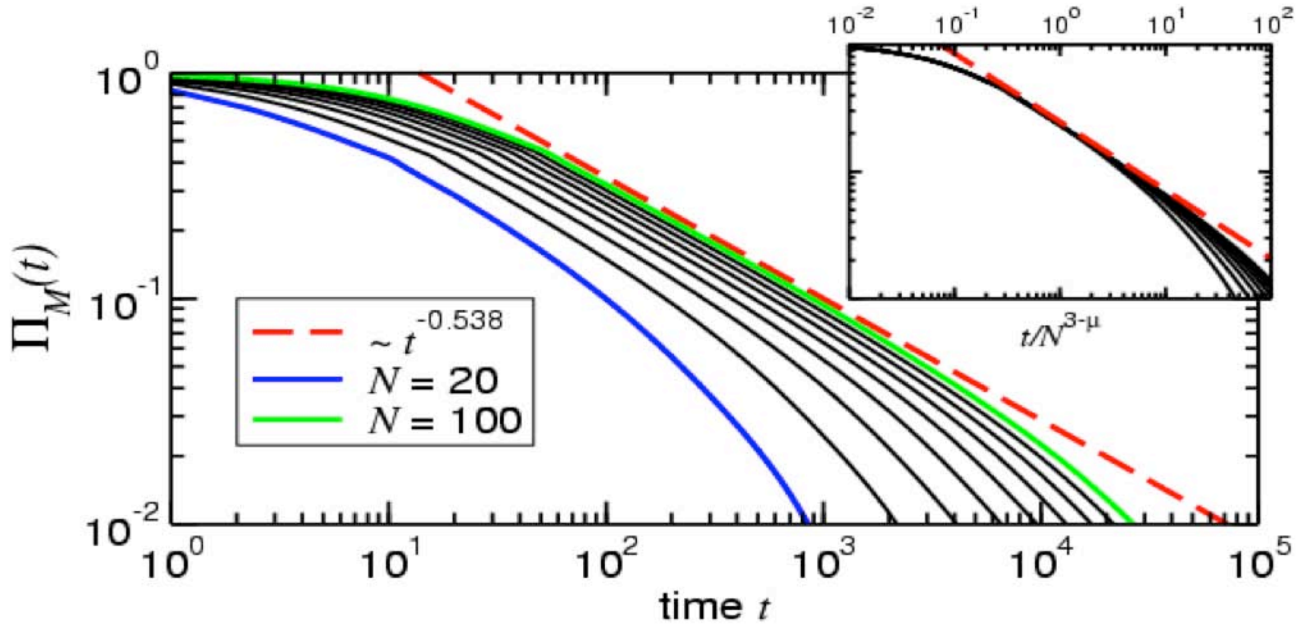


γ_l (dots) in ascending order for N=100 and $\Gamma = 1$

- $\gamma_j \in [0.0012, 0.012]$ translates to experimentally accessible times of about $10 - 100\mu\mathrm{s}$
- The smallest decay rate $\gamma_{\min} = 7.94 \times 10^{-6}$ corresponds to experimentally unrealistically long times

Dependence of $\Pi_M(t)$ on N

O. Mülken, A.B., T. Amthor, C. Giese, M. Reetz-Lamour, M. Weidemüller,
Phys. Rev. Lett. **99**, 090601 (2007)



N – dependence of $\Pi_M(t)$ for $\Gamma = 1$.

For larger N and intermediate t, $\Pi_M(t)$ scales with N:

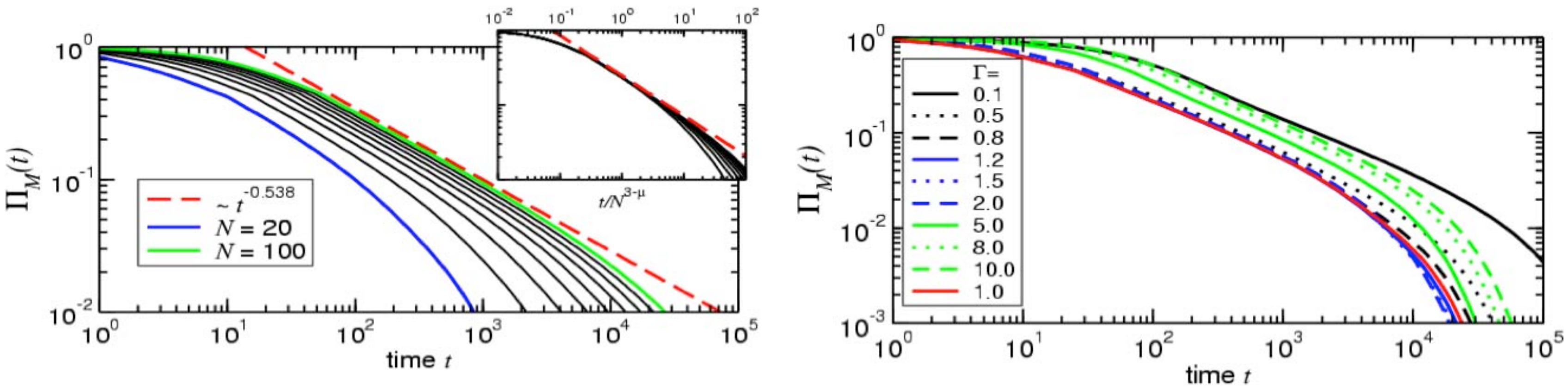
$$\Pi_M(t) \sim \sum_j \exp\left(-2N^{-3} j^{\mu} t\right) = \sum_j \exp\left[-2\left(j / N\right)^{\mu} N^{-(3-\mu)} t\right]$$

Dependence of $\Pi_M(t)$ on N and on Γ

O. Mülken, A.B., T. Amthor, C. Giese, M. Reetz-Lamour, M. Weidemüller,

Phys. Rev. Lett. **99**, 090601 (2007)

Parameter dependence of $\Pi_M(t)$:



Left: N-dependence of $\Pi_M(t)$ for Γ =1. Right: Γ-dependence of $\Pi_M(t)$ for N = 50.

- The N-dependence of $\Pi_M(t)$: For larger N and intermediate t $\Pi_M(t)$ scales with N ($a \sim N^{-3}$ for a linear system)
- The Γ-dependence of $\Pi_M(t)$: Values of Γ close to 1 lead to the quickest decay, being of the same order as $H_{j,j\pm1} = -1$.

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