Continuous-time Quantum Walks

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Based on joint works with Paul Krapivsky, Jean-Marc Luck, Sylvain Prolhac and Dries Sels.

Outline

Introduction: A brief review of quantum walks

1. **Survival of quantum particles in presence of traps**

   Zeno effect and 'quantum' Lifshitz, Donsker-Varadhan tails.

2. **Open System with a source/sink:**

   the Lindblad approach.

Concluding remarks.

Introduction

Discrete-time quantum walks

We define a unitary dynamics given by an operator U on the lattice Hilbert space $\ell^2(\mathbb{Z})$ in discrete time such as the (wave function) ψ satisfies

$$|\psi(t+1)\rangle = U|\psi(t)\rangle$$

For $\psi_n(t+1)$ to be a linear combination of $\psi_{n-1}(t), \psi_n(t)$ and $\psi_{n+1}(t)$, the operator U is taken to be of the form

$$\mathbf{U} = \alpha \mathbf{1} + \beta \mathbf{s} + \gamma \mathbf{s}^\dagger$$

where $\mathbf{s}$ and $\mathbf{s}^\dagger$ are the right and left-shift operators on $\mathbb{Z}$.
Unitarity, $UU^\dagger = U^\dagger U = 1$, leads to
$\alpha\alpha^* + \beta\beta^* + \gamma\gamma^* = 1,\ \alpha^*\gamma + \beta^*\alpha = 0 \text{ and } \beta\gamma^* = 0$
Solutions with $\alpha, \beta, \gamma \in \mathbb{C}$ are trivial.
These coefficients must be taken in a non-commutative matrix algebra in order to obtain a non-trivial solution to the problem (cf Dirac's equation):

A discrete-time random walk requires an internal degree of freedom *(a coin, a spin)* in addition to the space position.

The Hadamard walk

The position Hilbert space is $\mathcal{H}_p \simeq \ell^2(\mathbb{Z})$

The internal degree of freedom, denoted by C, belongs to the Hilbert space $\mathcal{H}_C = \mathrm{Span}\,(|+1\rangle, |-1\rangle) \simeq \mathbb{C}^2$.

The Unitary operator U acting on $\mathcal{H}_C \otimes \mathcal{H}_p$ is defined as

$$U = \hat{S}(\hat{H} \otimes 1_p)$$

where

$$\hat{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

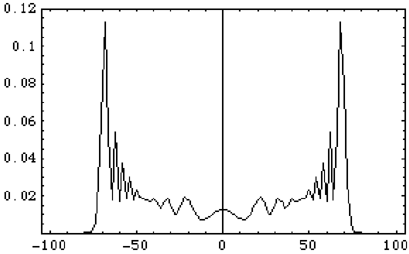
is the Hadamard matrix and $\hat{S}$ is the conditional shift operator given by

$$\hat{S} = \sum_{\sigma=\pm 1, n \in \mathbb{Z}} |\sigma, n+\sigma\rangle\langle\sigma, n|$$

The evolution depends on the initial condition $\psi(0)$.

The even Hadamard walk Probability distribution

The probability distribution of the position observable X_t after 100 time-steps, with symmetric initial condition $|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}\left(|+1\rangle_C + i|-1\rangle_C\right) \otimes |0\rangle_P$, is given by



A weak-convergence result holds for $t \to \infty$ (Grimmett et al. 2004):

$$\frac{X_t}{t} \Rightarrow v$$

where the random variable $v \in [-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}]$ is distributed with density

$$f(v) = \frac{1}{\pi(1-v^2)\sqrt{1-2v^2}}$$

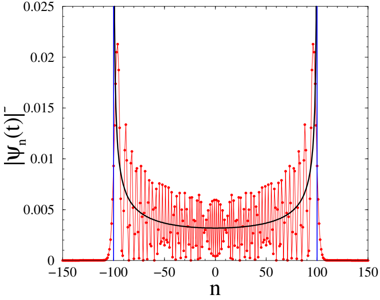
Continuous-time Quantum Walks

In continuous time, a quantum walk on a line is simply described by a Schrödinger equation (on the lattice):

$$i\frac{d\psi_n(t)}{dt} = \psi_{n+1}(t) + \psi_{n-1}(t) \quad \text{with } \psi_n(0) = \delta_{na}$$

Assuming the particle is launched from $a = 0$, we have

$$\psi_n(t) = \int \frac{dq}{2\pi} \mathrm{e}^{\mathrm{i}nq - 2\mathrm{i}t\cos q} = \mathrm{i}^{-n} J_n(2t) \text{ (Bessel)}$$



Ballistic Spreading

The typical scale of the continuous time Q. W. grows linearly with time

$$\langle n^2 \rangle = 2t^2, \ \ \langle n^4 \rangle = 6t^4 + 2t^2$$

The maximal spreading velocity, $V = 2$, separates an allowed region from a (exponentially) forbidden region:

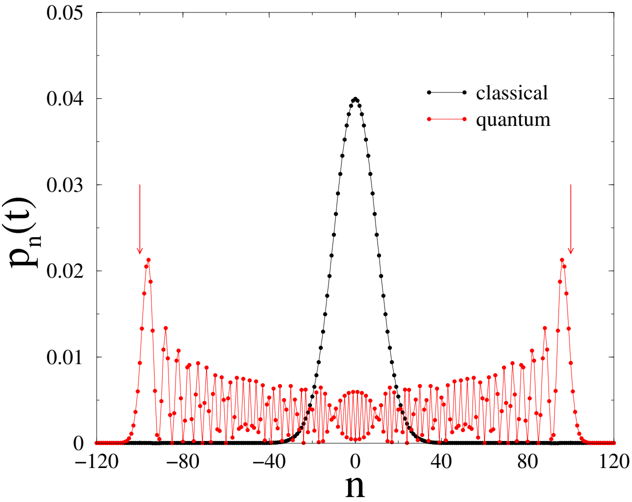
- *Allowed region* $(|n| < 2t)$

$$|\psi_n(t)|^2 \to \frac{1}{\pi\sqrt{4t^2 - n^2}}$$

- *Ballistic peaks* $(n \approx\approx \pm 2t)$

$$\text{For } \ |n| = 2t + z\, t^{1/3}, \ \ \psi_n(t) \approx \mathrm{i}^{-n} t^{-1/3} \mathrm{Ai}(z)$$

Profiles Classical versus Quantum



Note that ballistic spreading is merely a consequence of Heisenberg Uncertainty Principle.

Quantum Walks and Quantum Computing

Quantum Walks can be viewed as quantum-mechanical generalizations of classical random walks, first introduced in

Y. Aharonov, L. Davidovich and N. Zagury, 1993, *Quantum random Walks*, Phys. Rev. A **48** 1687-1690.

• Toy-models of elementary quantum dynamics with entanglement, many-body effects etc... S. E. Venegas-Andraca, 2012, Quant. Inf. Proc. **11** 1015-1106

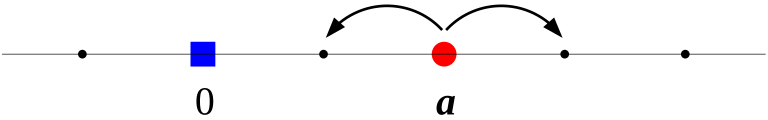
• Quantum Algorithms can be reformulated in terms of Quantum Walks: A.M. Childs and J. Goldstone, 2004, *Spatial Search by quantum walks*, PRA **70** 022314.

• Universal models of quantum computation: A.M. Childs, 2009, *Universal Computation by quantum walk*, PRL **102**, 180501.

A good framework to study the interplay between statistical and quantum effects.

Survival of a Quantum Walk

Survival of a 1d Walk in presence of a single trap



The classical case (Reminder): Put a classical trap of strength γ at site 0 and launch a (classical) random-walk from a :

$$\frac{dP_n}{dt} = P_{n+1} + P_{n-1} - 2P_n - \gamma\delta_{n,0}P_0(t)$$

When $t \to \infty$, the survival probability $S(t) = \sum_{n\in\mathbb{Z}} P_n(t)$ decays to 0 and we have

$$S(t) \simeq \frac{b}{\sqrt{\pi t}} \quad \text{with} \quad b = a + \frac{2}{\gamma}$$

What can one say for a quantum walk?

Effective non-unitary evolution

The trap is modeled as optical potential (Wigner) of strength γ:

$$\mathrm{i}\,\frac{\mathrm{d}\psi_n(t)}{\mathrm{d}t} = \psi_{n+1}(t) + \psi_{n-1}(t) - \mathrm{i}\gamma\,\delta_{n0}\,\psi_n(t)$$

with $\psi_n(0) = \delta_{na}$. The survival probability is then given by

$$S(t) = \sum_n |\psi_n(t)|^2 = 1 - 2\gamma \int_0^t |\psi_0(\tau)|^2 \,\mathrm{d}\tau$$

In the limit $t \to \infty$, the quantum particle has an asymptotic probability of *not* being trapped given by

$$S_\infty = 1 - 2\gamma \int_0^\infty |\psi_0(\tau)|^2 \,\mathrm{d}\tau \;\; > 0$$

The dynamics can be solved exactly using Green functions techniques.

Expression of the Survival Probability

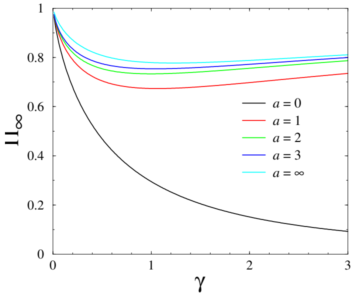
Taking Fourier transform in space and Laplace in time, we obtain

$$\widehat{\psi(q,s)} = \frac{\mathrm{i}(\mathrm{e}^{-\mathrm{i}qa} - \gamma\,\widehat{\psi}_0(s))}{\mathrm{i}s - 2\cos q} \text{ and } \widehat{\psi}_0(s) = \frac{1}{\gamma + \sqrt{s^2+4}}\left(\frac{\sqrt{s^2+4}-s}{2\mathrm{i}}\right)^a$$

This leads to an exact formula for the survival probability as a function of the initial position a:

$$S_\infty = 1 - \frac{4\gamma}{\pi}\left[\int_0^{\pi/2} \frac{\sin\theta\,\mathrm{d}\theta}{(\gamma+2\sin\theta)^2} + \int_0^\infty \frac{\sinh\theta\,\mathrm{d}\theta}{\gamma^2+4\sinh^2\theta}\,\mathrm{e}^{-2a\theta}\right]$$

The Zeno Effect



- Monotonic behavior for $a = 0$: $S_\infty \simeq \frac{1}{2\gamma^2}$ for large γ.

- Non-monotonic for $a \neq 0$: *paradoxical transparency* for $\gamma \to \infty$.

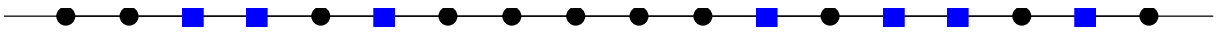
This is an instance of the Quantum Zeno Effect: repeated measurements of a quantum system tend to freeze its dynamics (Degasperis, Fonda, Ghirardi 1974; Misra, Sudarshan 1977; Turing 1954).

$$S_\infty \approx 1 - \frac{16a^2}{(4a^2 - 1)\pi\gamma}$$

See recent works of E. Barkai et al and A. Dhar et al.

Quantum Walk with a finite random concentration of traps

Traps are randomly and independently located on $\mathbb{Z}$ with a concentration c. How does the survival probability $S(t)$ of the quantum walker decay with time?



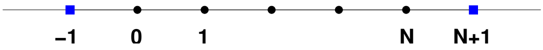
$$\mathrm{i}\,\frac{\mathrm{d}\psi_n(t)}{\mathrm{d}t} = \psi_{n+1}(t) + \psi_{n-1}(t) - \mathrm{i}\gamma\,\varepsilon_n\,\psi_n(t)$$

$$\varepsilon_n = \begin{cases} 1 & \text{trap with Prob.} \quad c \\ 0 & \text{no trap with Prob.} \quad 1 - c. \end{cases}$$

Parris, Edwards & Parris (1989); KLM (2014)

Classical Particle: Lifshitz and Donsker-Varadhan estimate

For a classical walker, the asymptotic behaviour of the survival is found thanks to a Lifshitz tail argument, by estimating the decay rate in a trap-free region of size N



On a finite sample of size N, the survival rate decreases as $S_N(t) \sim \mathrm{e}^{-\lambda t}$ with $\lambda \simeq \frac{\pi^2}{N^2}$.

Weighing this decay rate with the probability $(1-c)^N$ of finding a free region of size N and optimizing over N for large t (saddle point), we recover the celebrated stretched exponential formula

$$S_{\mathrm{clas}}(t) \sim \exp\left(-\frac{3}{2}\left(2\pi^2|\log(1-c)|^2 t\right)^{1/3}\right)$$

In dimension d, the $1/3$ exponent becomes $d/(d+2)$.

The quantum Lifshitz Donsker-Varadhan formula

For a quantum-walker, the spectrum of the effective Hamiltonian is complex. It can be shown that the lowest decay mode in a region of size N is the eigenvalue with smallest imaginary part

$$\lambda = -2\mathrm{Im}(E_1) \simeq \frac{8\pi^2 f}{N^3 \gamma}$$

The stretched exponential law for the survival probability of a quantum walker is then obtained as

$$S_{\mathrm{QW}}(t) \sim \exp\left(-\frac{4}{3}\left(\frac{24\pi^2 f}{\gamma}|\log(1-c)|^3 t\right)^{1/4}\right)$$

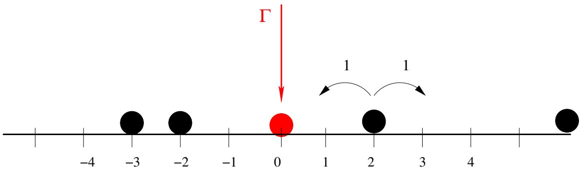
The classical $1/3$ exponent has become $1/4$ for the quantum problem. In arbitrary dimensions, the exponent is $d/(d+3)$ in the quantum case.

Inserting particles

Symmetric exclusion with a source

Consider (classical) random walkers with exclusion on $\mathbb{Z}$. A particle is inserted at site 0, with rate Γ if the site is empty.

What is the statistics of $N(t)$ the total number of particles in the lattice at time t (starting from an empty state)?



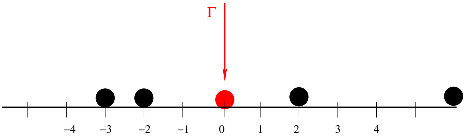
$$\langle N \rangle \simeq \begin{cases} 4\sqrt{\frac{t}{\pi}} & d = 1 \\ \frac{2\pi t}{\ln t} & d = 2 \\ \frac{\Gamma}{1+\Gamma W_d} t & d > 2 \end{cases} \qquad \langle N^2 \rangle_c \simeq \begin{cases} 4(3 - 2\sqrt{2})\sqrt{\frac{t}{\pi}} & d = 1 \\ V_2 \frac{t}{\ln t} & d = 2 \\ \frac{\Gamma}{1+\Gamma W_d} t & d > 2 \end{cases}$$

where $W_d = \frac{d}{2} \int_0^{2\pi} \dots \int_0^{2\pi} \prod_{i=1}^{d} \frac{dq_i}{2\pi} \frac{1}{\sum_{i=1}^{d}(1-\cos q_i)}$ is the Watson integral.

Note that the leading order terms do not depend on Γ for $d = 1, 2$.

Quantum version with Free Fermions

What happens if we replace SEP particles by free fermions?



Unitary Evolution: $U(t) = \mathrm{e}^{iHt}$ with $H = \sum_n c_n^\dagger c_{n+1} + c_n c_{n+1}^\dagger$
The effective dynamics for the insertion of particles at site 0 and at rate Γ is given by

$$\partial_t \rho = -\mathrm{i}[H, \rho] + \Gamma \left(2L\rho L^\dagger - \{L^\dagger L, \rho\} \right)$$

where ρ is the density matrix and the insertion operator is given by

$$\boxed{L = c_0^\dagger}$$

In continuous set-up, see M. Butz and H. Spohn, *Dynamical Phase transition for a quantum particle source* (2010).

Closed equations for correlators

The average particle number in the system grows linearly with time

$$N(t) \simeq C_d(\Gamma)t$$

We wish to determine how the growth factor depends on the injection rate Γ and on the dimension d.

Using the Lindblad equation, one derives closed evolution equations for the 2-point correlators $\sigma_{i,j}(t) = \langle c_i^\dagger c_j \rangle_t$

$$\dot{\sigma}_{i,j} = \mathrm{i}\left(\sigma_{i+1,j} + \sigma_{i-1,j} - \sigma_{i,j+1} - \sigma_{i,j-1}\right) - \Gamma\left(\delta_{i,0}\sigma_{i,j} + \delta_{j,0}\sigma_{i,j} - 2\delta_{i,0}\delta_{j,0}\right)$$

The average total number of particles is

$$N(t) = \sum_{n=-\infty}^{\infty} \sigma_{n,n}(t)$$

One can compute this average by studying the *dual* problem of removing particles at the origin, with Lindblad (Kraus) operator $L = \sqrt{\Gamma}\, c_0$.

Average number of particles

In the dual problem, we start with a system full of holes and we remove holes at the origin. The equations for the two-body correlators are given by

$$\frac{d\sigma_{i,j}}{dt} = \mathrm{i}\left(\sigma_{i+1,j} + \sigma_{i-1,j} - \sigma_{i,j+1} - \sigma_{i,j-1}\right) - \Gamma\left(\delta_{i,0}\sigma_{i,j} + \delta_{j,0}\sigma_{i,j}\right)$$

Exact solutions of these equations can be constructed by factorization of wave-functions for the non-unitary optical potential

$$\sigma_{i,j}(t) = \psi_i(t)\psi_j^*(t)$$

where the wave-functions obey the non-unitary Schrödinger equation

$$\mathrm{i}\,\frac{\mathrm{d}\psi_n(t)}{\mathrm{d}t} = \psi_{n+1}(t) + \psi_{n-1}(t) - \mathrm{i}\Gamma\,\delta_{n0}\,\psi_n(t)$$

This one-body dynamics is strictly identical to the one we studied for the survival problem, and it can readily be solved by going to Fourier-Laplace transform.

Values of the growth rates

Exact expression for $C_d(\Gamma)$ can be derived by using lattice Green functions.

- In d =1:

$$C_1(\Gamma) = 2\Gamma - \frac{2\Gamma^2}{\pi}\left[\gamma^{-2} + \left(\gamma^{-1} - \gamma^{-3}\right)\tan^{-1}\gamma\right]$$

with $\gamma = \sqrt{(\Gamma/2)^2 - 1}$

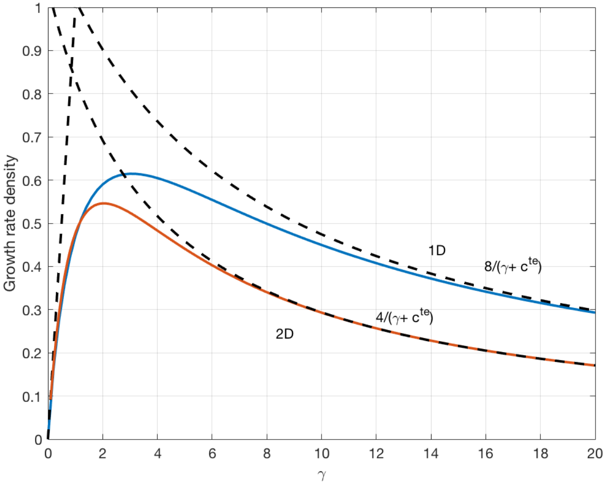
- In d =2: $C_2(\Gamma) = 2\Gamma - \frac{16}{\pi}\Gamma^2[I_1(\Gamma) + I_2(\Gamma)]$ with

$$I_1 = \int_0^1 dx \, \frac{K(x) + K(x')}{[\Gamma K(x)]^2 + [\Gamma \, K(x') + 2\pi]^2} \text{ and } I_2 = \int_0^1 \frac{dx}{\Gamma^2 x^2 + [2\pi/K(x)]^2}$$

where $K(x) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - x^2 \sin^2\theta}}$ is the complete elliptic integral.

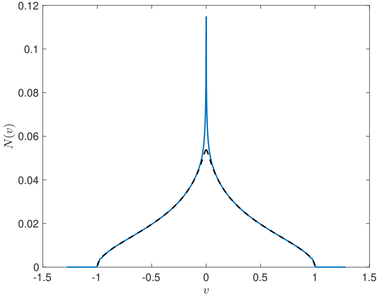
The calculation of higher moments of N, of its full statistics, of the density profiles at a given time, are interesting open problems, that may be probed experimentally on cold atoms.

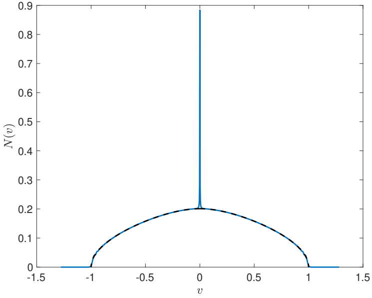
Growth rate: Zeno effect



For large Γ, the growth rate decreases with Γ as $C_d(\Gamma) \simeq \frac{2d}{\Gamma}$

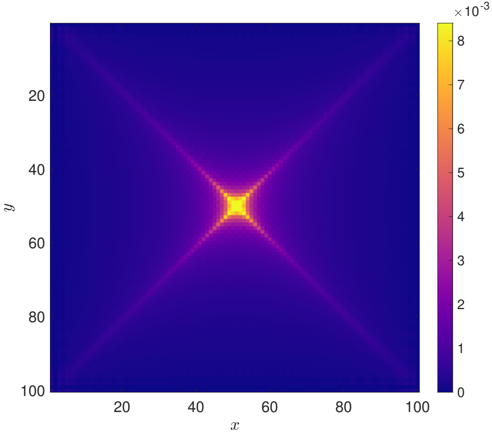
Density profiles





Density profile of injected particles for $\Gamma = 0.05$ and $\Gamma = 2.5$. Blue line shows the numerical exact result obtained at a time $t = 200$ in rescaled coordinates.

Density profile in 2d



Density profile on a 100×100 square lattice at time $t = 25$ for $\Gamma = 0.1$.

Open questions

We have calculated the average growth of the number of particles as a function of time.

• Can we determine the variance?

• Can we calculate the full counting statistics (Large deviations)?
(For the semi-infinite set-up see Sasamoto et al. 1901.07228.)

• What happens for bosons?

• Can we find density profiles (done for free fermions in 1d)?

• Is there a hydrodynamic description?

Conclusion

Quantum walks are the quantum analogs of classical walks. They provide an intuition on Quantum Mechanics different from that from microscopic physics.

Quantum walks can be defined and studied for their own sake or in relation with quantum information theory.

Many probabilistic or statistical mechanics problems can be restated for quantum walkers: recurrence times, survival probabilities, asymptotic distributions etc...

Classical Stochastic Interacting Particle Systems (like the ASEP) are extensively studied to understand non-equilibrium physics, hydrodynamic limits, large deviations, dynamical phase transitions.

It is often thought that the word ‘exclusion’ in ASEP reflects a kind of 'Pauli Exclusion Principle'. This is not quite true. However, comparing SEP with free fermions is instructive. Besides, some of the mathematical structures involved are similar and integrability plays a key-role.

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