Field-theoretical description of many-body random walks on graphs

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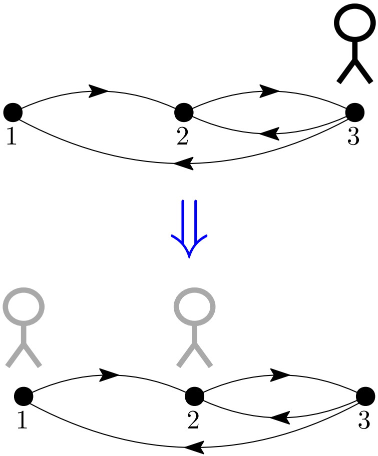
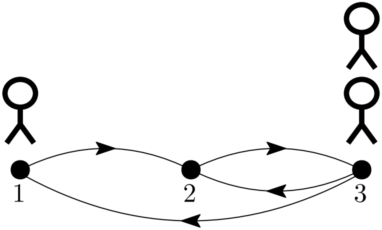
One-particle random walk on a graph



Linear evolution of the probability distribution (linear algebra)

Multi-particle random walk on a graph



Independent evolution $\oplus$ **interparticle interactions**

$$\Downarrow$$

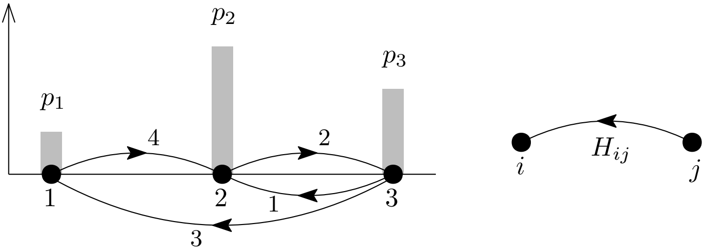
Non-linear behaviour (particle influenced by configuration of the others)

Outline

- One-particle walk
- Many walkers (Reaction networks)
- Master equation and Rate equation
- Quantum (Fock-space) techniques
- The Hamiltonian and evolution of operators

Main reference: [Baez2012] (see last slide with bibliography)

One-particle random walk on a graph



- Graph (oriented, weighted) with vertex set $V = \{1, 2, 3\}$
- Probability distribution $\vec{p} = (p_1, p_2, p_3)$
- Weights $\to$ Transition rate matrix $\mathsf{H} = \begin{pmatrix} -4 & 0 & 3 \\ 4 & -2 & 1 \\ 0 & 2 & -4 \end{pmatrix}$

  H is *infinitesimal stochastic*: $H_{ij} \geq 0 \ (i \neq j)$ and $\sum_{i \in V} H_{ij} = 0 \ (\forall j)$ ($\Rightarrow$ conservation of probability)

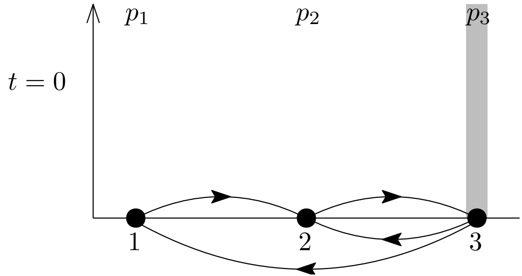
One-particle random walk on a graph

- Evolution equation (continuous time):

$$\frac{d}{dt}\vec{p} = \mathsf{H}\vec{p}, \quad \text{that is} \quad \frac{d}{dt}p_i = \sum_{\substack{j \\ j\neq i}} (H_{ij}p_j - H_{ji}p_i) \tag{1}$$

(c.f. Schrödinger equation $i\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle$)

- Solution: $\vec{p}(t) = e^{t\mathsf{H}}\vec{p}(0)$



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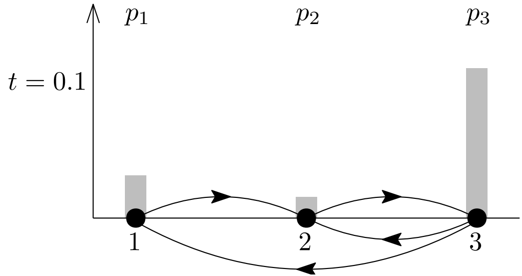

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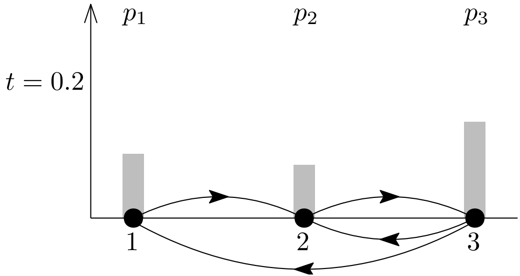

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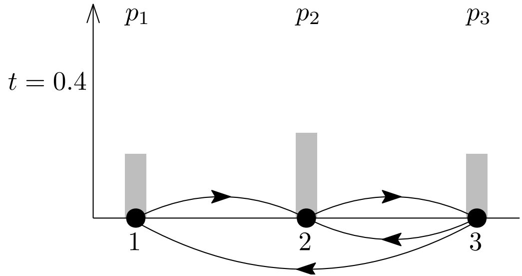

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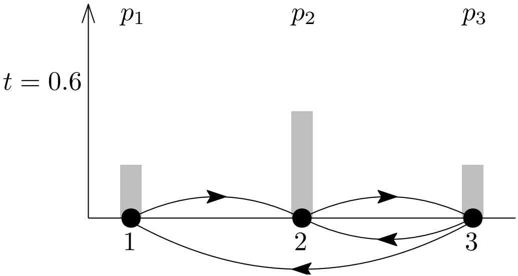

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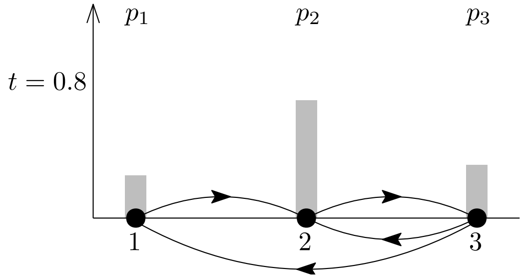

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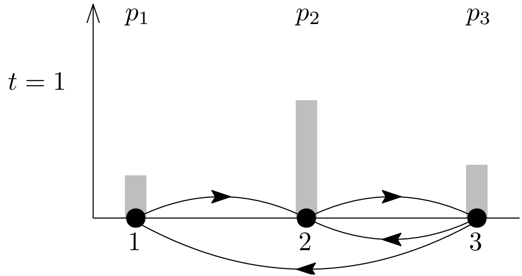
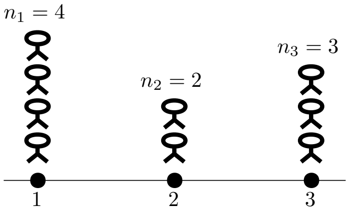


Many walkers

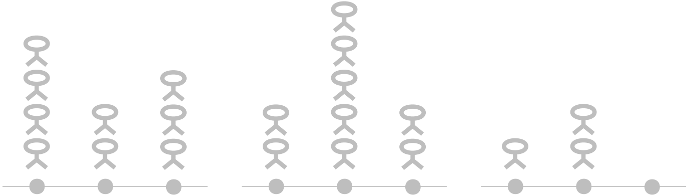
- From **particle description** ("where are individual particles located") to **field description** ("how many particles occupy individual places")

- **Indistinguishable** particles
  $\rightarrow$ definite **(micro)state** characterized by **occupation numbers**

  $\vec{n} = (n_1, \ldots, n_k) \in \mathbb{N}_0^k$



- Statistical **(macro)state**: $(\psi_{\vec{n}})_{\vec{n} \in \mathbb{N}_0^k}$ (list of microstate probabilities)

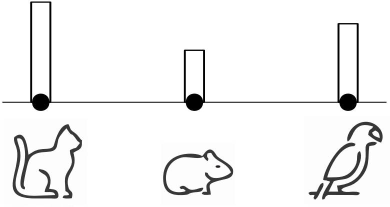


Many walkers - examples

- Population dynamics:

  vertices $\leftrightarrow$ animal species

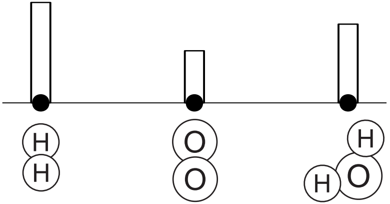
  evolution $\leftrightarrow$ birth, death, predation



- Chemical reaction networks:

  vertices $\leftrightarrow$ substances

  evolution $\leftrightarrow$ chemical reactions

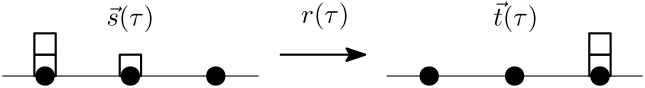


Complexes and transitions

- Complex: occupation vector ($\in \mathbb{N}_0^k$) with (typically) small entries

- Elementary transition τ: change of one complex into another

  $\vec{s}(\tau)$ ... source complex
  $\vec{t}(\tau)$ ... target complex
  $r(\tau)$ ... rate constant



Example: chemical reaction $2H_2 + O_2 \rightarrow 2H_2O$

Master equation

Evolution of statistical state:

$$\frac{d}{dt}\psi_{\vec{n}'} = \sum_{\vec{n}} H_{\vec{n}'\vec{n}}\psi_{\vec{n}} \tag{2}$$

where **many-body transition rate matrix**

$$H_{\vec{n}'\vec{n}} = \sum_{\tau} \underbrace{r(\tau)\vec{n}^{\underline{\vec{s}(\tau)}}}\big(\underbrace{\delta_{\vec{n}',\vec{n}+\vec{t}(\tau)-\vec{s}(\tau)}} - \underbrace{\delta_{\vec{n}',\vec{n}}}\big) \tag{3}$$

trans. rate for occup. $\vec{n}$	$\vec{n}$ becoming $\vec{n}'$ via τ	$\vec{n}'$ transitioning away

Notation:

- Vector exponent $\vec{n}^{\underline{\vec{s}}} \equiv n_1^{\underline{s_1}} \cdots n_k^{\underline{s_k}}$
- Falling power $n^{\underline{s}} \equiv n(n-1)\cdots(n-s+1)$
- Kronecker delta $\delta_{\vec{n}',\vec{n}} = 1$ if $\vec{n}' = \vec{n}$ (otherwise $\delta_{\vec{n}',\vec{n}} = 0$)

Remark: Matrix H is infinitesimal stochastic, $\sum_{\vec{n}'} H_{\vec{n}'\vec{n}} = 0$ $(\forall\vec{n})$

Rate equation

Evolution of average occupations $\vec{x} = (x_1, \ldots, x_k)$ ($x_i = \sum_{\vec{n}} n_i \, \psi_{\vec{n}}$):

$$\frac{d}{dt}\vec{x} = \sum_{\tau} r(\tau)\big(\vec{t}(\tau) - \vec{s}(\tau)\big)\vec{x}^{\,\vec{s}(\tau)} \tag{4}$$

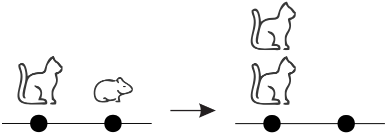
Non-linear system of equations (*dynamical system*)

Good approximation (reduction) of the master equation for large occupation numbers [Baez2013]

Example: Lotka-Volterra predator-prey model

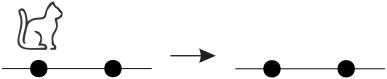
Elementary transitions: $\tau \in \{p, b, d\}$

- **p**redation:
  $\vec{s}(p) = (1,1) \xrightarrow{r_p} (2,0) = \vec{t}(p)$



- **b**irth:
  $\vec{s}(b) = (0,1) \xrightarrow{r_b} (0,2) = \vec{t}(b)$

- **d**eath:
  $\vec{s}(d) = (1,0) \xrightarrow{r_d} (0,0) = \vec{t}(d)$



Rate equations: (x_1 ... predator population, x_2 ... prey population)

$$\frac{dx_1}{dt} = r_p x_1 x_2 - r_d x_1 \quad , \quad \frac{dx_2}{dt} = -r_p x_1 x_2 + r_b x_2 \tag{5}$$

Statistical state - power series representation

→ For each vertex $i = 1, \ldots, k$ introduce auxiliary variable z_i

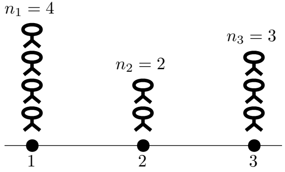
→ Represent statistical state $(\psi_{\vec{n}})_{\vec{n} \in \mathbb{N}_0^k}$ by power series (probability generating function)

$$\Psi(z_1, \ldots, z_k) = \sum_{\vec{n}} \psi_{\vec{n}} \, z_1^{n_1} \cdots z_k^{n_k} \quad , \quad \Psi(\vec{1}) \equiv \Psi(1, \ldots, 1) = 1 \tag{6}$$

Stochastic **Fock space**: all real (formal) power series in $z_1, \ldots, z_k$

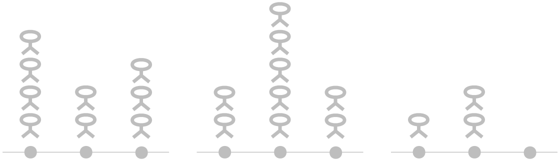
1) Definite microstate

$\Psi = z_1^4 z_2^2 z_3^3$



2) Statistical mixture of microstates

$\Psi = \psi_{4,2,3} z_1^4 z_2^2 z_3^3 + \psi_{2,5,2} z_1^2 z_2^5 z_3^2 + \psi_{1,2,0} z_1 z_2^2$



Examples

- Product state: two independent particles A and B with location distributions $\vec{p}^A$ and $\vec{p}^B$

$$\Psi(\vec{z}) = (\vec{p}^A \cdot \vec{z})(\vec{p}^B \cdot \vec{z}) = \sum_{i,j} \frac{1}{2} \underbrace{(p_i^A p_j^B + p_i^B p_j^A)}\, z_i z_j \qquad (7)$$

symmetry $\rightarrow$ indistinguishability

- Coherent state (single vertex, resp. many vertices):

$$\Psi(z) = e^{x(z-1)} = \sum_{n=0}^{\infty} \underbrace{e^{-x} \frac{x^n}{n!}}\, z^n \quad , \quad \Psi(\vec{z}) = e^{\vec{x} \cdot (\vec{z} - \vec{1})} \qquad (8)$$

Poisson distribution with mean x

Creation and annihilation operators

Inspired by quantum field theory (second quantization [Kleinert2016, Ch. 2]),
$\rightarrow$ introduce for each vertex **creation operator** $a_i^\dagger$:

$$a_i^\dagger \Psi = z_i \Psi \quad , \quad a_i^\dagger \vec{z}^{\vec{n}} = z_1^{n_1} \cdots z_i^{n_i+1} \cdots z_k^{n_k} \tag{9}$$

and **annihilation operator** a_i:

$$a_i \Psi = \frac{\partial}{\partial z_i} \Psi \quad , \quad a_i \vec{z}^{\vec{n}} = n_i \, z_1^{n_1} \cdots z_i^{n_i-1} \cdots z_k^{n_k} \tag{10}$$

- $a_i^\dagger$ adds (for every microstate) one particle onto vertex i
- a_i removes one particle from vertex i (n_i particles to choose from)
- Commutation relations: $[A, B] \equiv AB - BA$

$$[a_i, a_j^\dagger] = \delta_{ij} \quad , \quad [a_i, a_j] = 0 \quad , \quad [a_i^\dagger, a_j^\dagger] = 0 \tag{11}$$

See [Doi1976] [Grassberger1980] [Baez2012] [Baez2013]

Hamiltonian operator

Turn the many-body transition rate matrix

$$H_{\vec{n}'\vec{n}} = \sum_{\tau} r(\tau) \vec{n}^{\underline{\vec{s}(\tau)}} (\delta_{\vec{n}',\vec{n}+\vec{t}(\tau)-\vec{s}(\tau)} - \delta_{\vec{n}',\vec{n}}) \tag{12}$$

into the **Hamiltonian operator**

$$\hat{H} = \sum_{\tau} r(\tau) \left(\vec{a}^{\dagger\,\vec{t}(\tau)} - \vec{a}^{\dagger\,\vec{s}(\tau)} \right) \vec{a}^{\vec{s}(\tau)} \tag{13}$$

$\rightarrow$ Then master equation turns into evolution equation for generating series $\Psi(\vec{z}, t)$ [Baez2013]:

$$\boxed{\frac{d}{dt}\psi_{\vec{n}'} = \sum_{\vec{n}} H_{\vec{n}'\vec{n}} \psi_{\vec{n}} \quad \rightarrow \quad \frac{\partial}{\partial t}\Psi = \hat{H}\,\Psi} \tag{14}$$

Follows from: $(a^s z^n = n^{\underline{s}} z^{n-s})$

$$\sum_{\vec{n}'} H_{\vec{n}'\vec{n}} \vec{z}^{\vec{n}'} = \sum_{\tau} r(\tau) \vec{n}^{\underline{\vec{s}(\tau)}} (\vec{z}^{\vec{n}+\vec{t}(\tau)-\vec{s}(\tau)} - \vec{z}^{\vec{n}}) = \hat{H} \vec{z}^{\vec{n}} \tag{15}$$

Examples of Hamiltonian operators

- Non-interacting walkers:
  $\vec{s}(i,j) = (0,\ldots,\overset{j}{1},\ldots,0) \xrightarrow{r_{ij}} (0,\ldots,\overset{i}{1},\ldots,0) = \vec{t}(i,j)$

$$\hat{H} = \sum_{i,j=1}^{k} r_{ij}(a_i^\dagger - a_j^\dagger)a_j \qquad (16)$$

- Lotka-Volterra model:
  $a_1^\dagger, a_1$ ... predator operators; $a_2^\dagger, a_2$ ... prey operators

$$\hat{H} = r_p({a_1^\dagger}^2 - a_1^\dagger a_2^\dagger)a_1 a_2 + r_b({a_2^\dagger}^2 - a_2^\dagger)a_2 + r_d(1 - a_1^\dagger)a_1 \qquad (17)$$

- Branching process (on one vertex):
  $\vec{s}(m) = (1) \xrightarrow{r_m} (m) = \vec{t}(m)$

$$\hat{H} = r_0(1 - a^\dagger)a + \sum_{m=2}^{\infty} r_m({a^\dagger}^m - a^\dagger)a \qquad (18)$$

Evolution operator

- The Hamiltonian $\hat{H}$ defines **time evolution operator** $U(t)$ via:

$$\frac{dU}{dt} = \hat{H} U \quad , \quad U(0) = 1 \tag{19}$$

Assuming, for simplicity, that rate constants $r(\tau)$ (and therefore $\hat{H}$) are time-independent: $U(t) = e^{t\hat{H}}$

- State evolution can be cast, using $\Psi(\vec{z}) = \Psi(\vec{a}^\dagger)\, 1$, and $\hat{H}\, 1 = 0$, as

$$\Psi(\vec{z}, t) = U(t)\Psi(\vec{z}, 0) = \Psi(\underbrace{e^{t\hat{H}} \vec{a}^\dagger e^{-t\hat{H}}}_{\vec{A}^\dagger(t)}, 0)\, 1 \tag{20}$$

Here $\vec{A}^\dagger(t)$ satisfies $(\forall i)$

$$\boxed{\frac{dA_i^\dagger}{dt} = [\hat{H}, A_i^\dagger] = U(t)\, [\hat{H}, a_i^\dagger]\, U^{-1}(t) \quad , \quad A_i^\dagger(0) = a_i^\dagger} \tag{21}$$

Example: Branching process

Hamiltonian

$$\hat{H} = r_0(1 - a^\dagger)a + \sum_{m=2}^{\infty} r_m({a^\dagger}^m - a^\dagger)a \tag{22}$$

yields equation for $A^\dagger(t)$ (recall: $[a, a^\dagger] = 1$)

$$\frac{dA^\dagger}{dt} = r_0(1 - A^\dagger) + \sum_{m=2}^{\infty} r_m({A^\dagger}^m - A^\dagger) \quad , \quad A^\dagger(0) = a^\dagger \tag{23}$$

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→ Assuming $r_m = 0$ for $m \geq 2$ (particles only vanish at rate r_0)

$$A^\dagger(t) = 1 - e^{-r_0 t} + e^{-r_0 t} a^\dagger \tag{24}$$

→ Evolved state reads

$$\Psi(z, t) = \Psi(1 - e^{-r_0 t} + e^{-r_0 t} z, 0) = \sum_n \psi_n(0)(1 - e^{-r_0 t} + e^{-r_0 t} z)^n \tag{25}$$

Time evolution transformed z to $1 - e^{-r_0 t} + e^{-r_0 t} z$.

Example: Non-interacting walkers

Hamiltonian

$$\hat{H} = \sum_{i,j=1}^{k} r_{ij}(a_i^\dagger - a_j^\dagger)a_j \tag{26}$$

yields

$$\frac{dA_j^\dagger}{dt} = \sum_i r_{ij}(A_i^\dagger - A_j^\dagger) = \sum_i A_i^\dagger H_{ij} \quad , \quad A^\dagger(0) = a^\dagger, \tag{27}$$

where we denoted $H_{ij} = r_{ij}$ (for $i \neq j$) and $H_{jj} = -\sum_i r_{ij}$ elements of a 'rate matrix' H.

$\rightarrow$ We find

$$A_j^\dagger(t) = \sum_i a_i^\dagger (e^{t\mathsf{H}})_{ij} \quad \rightarrow \quad \Psi(\vec{z}, t) = \Psi(e^{t\mathsf{H}^\intercal}\vec{z}, 0) \tag{28}$$

For one particle: $((0, \ldots, \underset{i}{1}, \ldots, 0) \rightarrow i)$

$$\Psi(\vec{z}, t) = \sum_j \psi_j(0) \sum_i z_i (e^{t\mathsf{H}})_{ij} = \sum_i \overbrace{\sum_j (e^{t\mathsf{H}})_{ij}\psi_j(0)}^{\psi_i(t)} z_i \tag{29}$$

Example: Lotka-Volterra model

Hamiltonian

$$\hat{H} = r_p({a_1^\dagger}^2 - a_1^\dagger a_2^\dagger)a_1 a_2 + r_b({a_2^\dagger}^2 - a_2^\dagger)a_2 + r_d(1 - a_1^\dagger)a_1 \tag{30}$$

yields

$$\frac{dA_1^\dagger}{dt} = r_p({A_1^\dagger}^2 - A_1^\dagger A_2^\dagger)A_2 + r_d(1 - A_1^\dagger) \tag{31}$$

$$\frac{dA_2^\dagger}{dt} = r_p({A_1^\dagger}^2 - A_1^\dagger A_2^\dagger)A_1 + r_b({A_2^\dagger}^2 - A_2^\dagger) \tag{32}$$

where $\vec{A}(t) = e^{t\hat{H}}\vec{a}\,e^{-t\hat{H}}$

Example: Lotka-Volterra model

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$$\frac{dA_2^\dagger}{dt} = r_p({A_1^\dagger}^2 - A_1^\dagger A_2^\dagger)A_1 + r_b({A_2^\dagger}^2 - A_2^\dagger) \tag{32}$$

where $\vec{A}(t) = e^{t\hat{H}}\vec{a}\,e^{-t\hat{H}}$

$$\rightarrow \frac{dA_1}{dt} = r_p(-2A_1^\dagger + A_2^\dagger)A_1 A_2 + r_d A_1 \tag{33}$$

$$\frac{dA_2}{dt} = r_p A_1^\dagger A_1 A_2 + r_b(-2A_2^\dagger + 1)A_2 \tag{34}$$

System of coupled, non-linear, operator-valued differential equations.

Evolution of average occupations

- Define **occupation number operators**:

$$N_i = a_i^\dagger a_i \quad , \quad N = N_1 + \cdots + N_k \tag{35}$$

such that $N_i \vec{z}^{\,\vec{n}} = z_i \frac{\partial}{\partial z_i}(z_1^{n_1} \cdots z_k^{n_k}) = n_i \vec{z}^{\,\vec{n}}$

- Expected (or average) value: $\langle \ldots \rangle \equiv (\ldots)|_{\vec{z}=\vec{1}}$

$$\langle \Psi \rangle = 1 \quad \text{(normalization of probability)} \tag{36}$$

$$\langle N_i \Psi \rangle = \sum_{\vec{n}} \psi_{\vec{n}}\, n_i \quad \text{(average occupation number)} \tag{37}$$

- Evolution of $x_i = \langle N_i \Psi \rangle$:

$$\frac{d}{dt}\langle N_i \Psi \rangle = \langle N_i \hat{H} \Psi \rangle = \sum_{\tau} r(\tau)\big(t_i(\tau) - s_i(\tau)\big)\langle \vec{N}^{\vec{s}(\tau)} \Psi \rangle \tag{38}$$

If $\langle \vec{N}^{\vec{s}(\tau)} \Psi \rangle = \langle \vec{N} \Psi \rangle^{\vec{s}(\tau)}$ we get $\frac{d}{dt}\vec{x} = \sum_\tau r(\tau)\big(\vec{t}(\tau) - \vec{s}(\tau)\big)\vec{x}^{\,\vec{s}(\tau)}$

(for coherent states holds [Baez2013])

Analogies with quantum theory

One-particle random walk	$\leftrightarrow$	One-particle quantum mechanics
probability distribution $\vec{p}$		quantum state (wave function) $\|\psi\rangle$
transition rate matrix H		one-particle Hamiltonian H

Many-body random walk $\leftrightarrow$ Many-body quantum mechanics

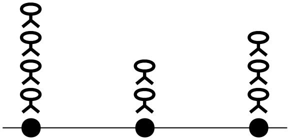
Occupation number description	$\leftrightarrow$	Field theory (second quantization)
Hamiltonian $\hat{H}$		Hamiltonian $\hat{H}$
non-interacting walkers		free quantum field theory (QFT)
master equation for $\Psi(\vec{z})$		QFT in Schrödinger picture
evolution of operators $\vec{A}^{\dagger}, \vec{A}$		QFT in Heisenberg picture
rate equation for $\vec{x}$		classical field equations

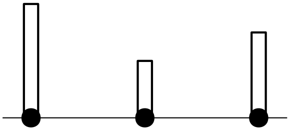
Despite similarities in formalism, the typical questions to address can be rather different.

Outlook

- We only considered one field (variables $\vec{z}$ and operators $\vec{a}^\dagger, \vec{a}$).
  $\rightarrow$ Easily generalized to **several fields**: $\vec{z}, \vec{w}, \ldots$ and $\vec{a}^\dagger, \vec{a}, \vec{b}^\dagger, \vec{b}, \ldots$
- Mean-field approximation: expansion of $\hat{H}$ up to **quadratic order** in creation and annihilation operators around 'classical' mean values.
- Path-integral approach [Peliti1985]
- In physics the background (spacetime) often simple, uniform (flat). Complex networks have rich, often non-rigid, structure.
  $\rightarrow$ Evolution of networks (i.e., of rates $r(\tau)$) — plasticity

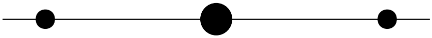
Summary





$$a_i^\dagger, a_i$$

$$z_i$$



References

Thank you for your attention.

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