The walk- and path-sum methods for quantum many-body physics

P.-L. Giscard, S. Thwaite, M. Kiffner, D. Jaksch

Department of Physics, University of Oxford, United-Kingdom

Centre for Quantum Technologies, National University of Singapore, Singapore

Introduction

Problem considered:

Many-body system S with N constituents each with d internal levels: typical model for cold atoms in optical lattices. The coherent evolution is described by $U = \exp[-iHt]$ ($\hbar = 1$) with H the Hamiltonian. Computational cost of a direct evaluation of U scales as d^{3N}.

Walk-sum:

Walk-sums approximate analytically any chosen pieces of U without any prior knowledge about the system under study. Computational cost at fixed order scales polynomially with N.

- Walk-sum express any quantum-evolution as a sum of walks on a graph
- Reduces many-body physics to few-body physics exactly
- Yields Feynman path-integrals for systems with continuous degrees of freedom
- Is part of a wider approach to matrix-functions valid independently of physics

Walk-sum: physical derivation

Consider S to comprise two subsystems: small S with d_S levels and the rest S'

$\longrightarrow$ **Idea:** if S' is frozen in configuration μ, evolving S is **easy**

$\longrightarrow$ **Goal:** describe the evolution of S is terms of situations where **only** S evolves

- Consider the projectors on a complete orthogonal set of configurations of S':

$$\hat{\varepsilon}_\mu = \underbrace{|\mu\rangle\langle\mu|}_{\text{Projects } S' \text{ in configuration } \mu} \otimes \overbrace{\mathcal{I}_S}^{\text{Identity on } S} \quad \text{with} \quad \sum_\mu \hat{\varepsilon}_\mu = \mathcal{I}_S$$

- "Freeze" S' in a configuration μ by projecting S' onto μ every δt

$$\text{Expand } U(t) = \lim_{\delta t \to 0} \prod_{n=0}^{t/\delta t} \Big(\sum_\mu \hat{\varepsilon}_\mu\Big)\delta U \quad \ldots.$$

S' jumps from μ to ν

$$\ldots. \text{ yields terms like } \quad \hat{\varepsilon}_\nu\, U(t)\, \hat{\varepsilon}_\mu = \lim_{\delta t\to 0} \underbrace{\hat{\varepsilon}_\nu\, \delta U\, \hat{\varepsilon}_\nu\, \delta U \cdots \hat{\varepsilon}_\nu\, \delta U}\; \overbrace{\hat{\varepsilon}_\nu\, \delta U\, \hat{\varepsilon}_\mu} + \cdots$$

Zeno measurement of $\hat{\varepsilon}_\nu \Rightarrow S'$ frozen in ν

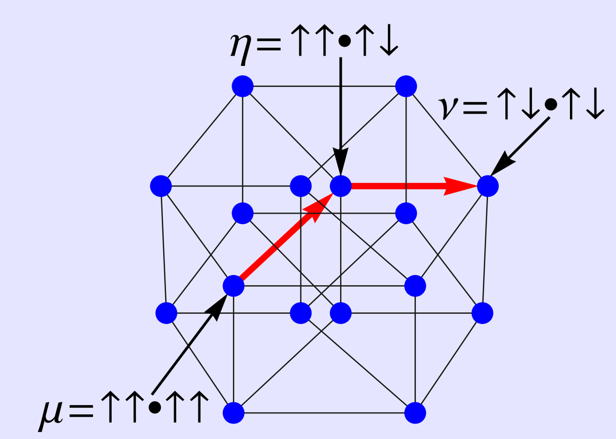
S evolves according to a small effective U_ν

Configuration space of S'...

... is a graph $\mathcal{G}$!

- *Vertices = configurations*
- *Edges = allowed transitions*

Ex: 5 spin-1/2 system, S central spin



A walk of S', $\mu \to \eta \to \nu$

- General expansion has jump $\mu \to \nu$ at any time, jumps to intermediary configurations η etc. We find

Walk-sum formula

$$\hat{\varepsilon}_\nu\, U(t)\, \hat{\varepsilon}_\mu = |\nu\rangle\langle\mu| \otimes \sum_{W(\mathcal{G})_{\nu\mu}} i^{-n} \underbrace{\int_0^t \int_0^{t_n} \cdots \int_0^{t_2}} U_\nu\, H_{\nu\leftarrow\eta_{n-1}} \cdots U_{\eta_2}\, H_{\eta_2\leftarrow\mu}\, U_\mu\, dt_1 \cdots dt_n \qquad (\star)$$

- Sum on strings of jumps of S' $\longrightarrow$ Sum on histories — **Walk-sum on $\mathcal{G}$**
- Continuous sums on jump times
- S' jumps, S affected by $H_{\beta\leftarrow\alpha}$ — $d_S \times d_S$ matrix
- Evolution operator of S when S' is frozen in μ from 0 to t_1 — $d_S \times d_S$ matrix

What walk-sum yields

We have obtained the *conditional* evolution operators $U_{\nu\leftarrow\mu}$ defined by the walk-sum in ($\star$)

- $U_{\nu\leftarrow\mu}$ is a $d_S \times d_S$ piece of U

$$U(t) = \sum_{\nu,\mu} \underbrace{|\nu\rangle\langle\mu|}_{S' \text{ from } \mu \text{ to } \nu} \otimes \underbrace{U_{\nu\leftarrow\mu}(t)}_{\text{Exact evolution of } S}$$

- Represents the evolution of S, knowing S' starts in μ and finishes in ν
- Integrals are convolutions: Laplace domain $\to$ only $+$ and $\times$ of $d_S \times d_S$ matrices required
- Effective matrices U_ν and $H_{\nu\leftarrow\mu}$ easy to compute !

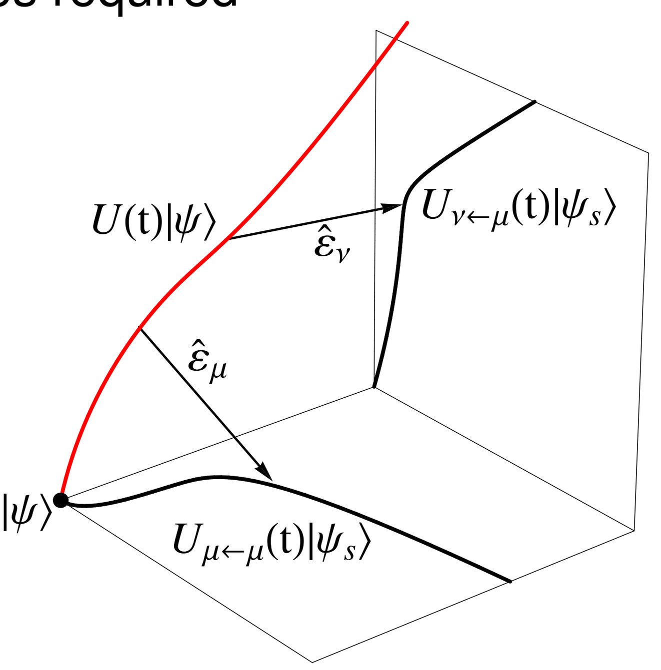
$$U_\nu = e^{-iH_\nu t} \quad \text{with} \quad \hat{\varepsilon}_\nu H \hat{\varepsilon}_\nu = \hat{\varepsilon}_\nu \otimes H_\nu$$
$$\hat{\varepsilon}_\nu H \hat{\varepsilon}_\mu = |\nu\rangle\langle\mu| \otimes H_{\nu\leftarrow\mu}$$

$\longrightarrow$ H_ν: small effective Hamiltonian acting on S when S' frozen in ν

$\longrightarrow$ H_ν and $H_{\nu\leftarrow\mu}$ are pieces of the full Hamiltonian H

- $U_{\nu\leftarrow\mu}$ is expressed as a sum of walks = sum of histories of S'

$\longrightarrow$ Number of walks of length K on $\mathcal{G}$ scales as poly(N)



Implementation, advantages and limitations

Unique procedure to follow: arXiv:1204.5087

1. Divide the system into the two parts S and S'
2. Compute the effective H_μ and $H_{\nu\leftarrow\mu}$ required
3. If possible, draw the graph $\mathcal{G}$
4. Decide which $U_{\nu\leftarrow\mu}$ are of interest
5. Compute these via the walk-sum

Advantages

- Free to choose S
- Can tackle 2D and 3D systems
- Observed to work best with strong long-range interactions
- Smooth monotonous convergence

Limitations

- No rigorous criterion exists to decide when to implement walk-sum
- Walk-sum is a perturbation theory with the jumps of S' perturbing S

Rydberg excited Mott insulators

Model:

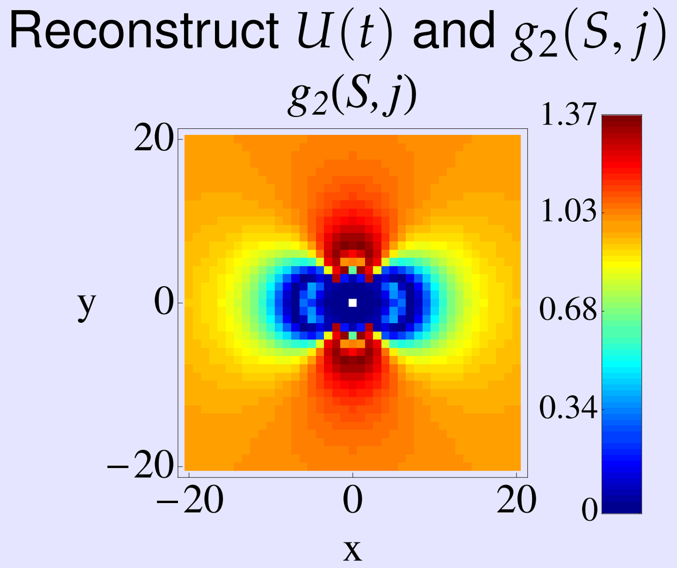
- Lattice of spin-1/2 + strong long-range interaction

$$H = \sum_i \Big\{ \Delta |\uparrow_i\rangle\langle\uparrow_i| - \frac{1}{2}\Omega\, \sigma_x^i + \frac{1}{2}\sum_{j\neq i} \frac{A}{|i-j|^3} |\uparrow_i\uparrow_j\rangle\langle\uparrow_i\uparrow_j| \Big\}$$

- Graph $\mathcal{G}$ = N-hypercube
- Initial state $|\downarrow_1 \cdots \downarrow_N\rangle \equiv |0\rangle$

Density-density correlation function $g_2(S,j)$?

- S central atom,
- Compute all $U_{K\leftarrow 0}$ with $K \leq 6$ excitations
- Reconstruct $U(t)$ and $g_2(S,j)$



- A: dipole-dipole int.
- $\Delta = \Omega$, π-pulse
- 1 atom / pixel $\Rightarrow N \simeq 1700$ atoms

More examples: arXiv:1204.5087, arXiv:1108.1177

The walk- and path-sum methods for quantum many-body physics

P.-L. Giscard, S. Thwaite, M. Kiffner, D. Jaksch
Department of Physics, University of Oxford, United-Kingdom
Centre for Quantum Technologies, National University of Singapore, Singapore

Centre for Quantum Technologies

From walk-sum to path-sum

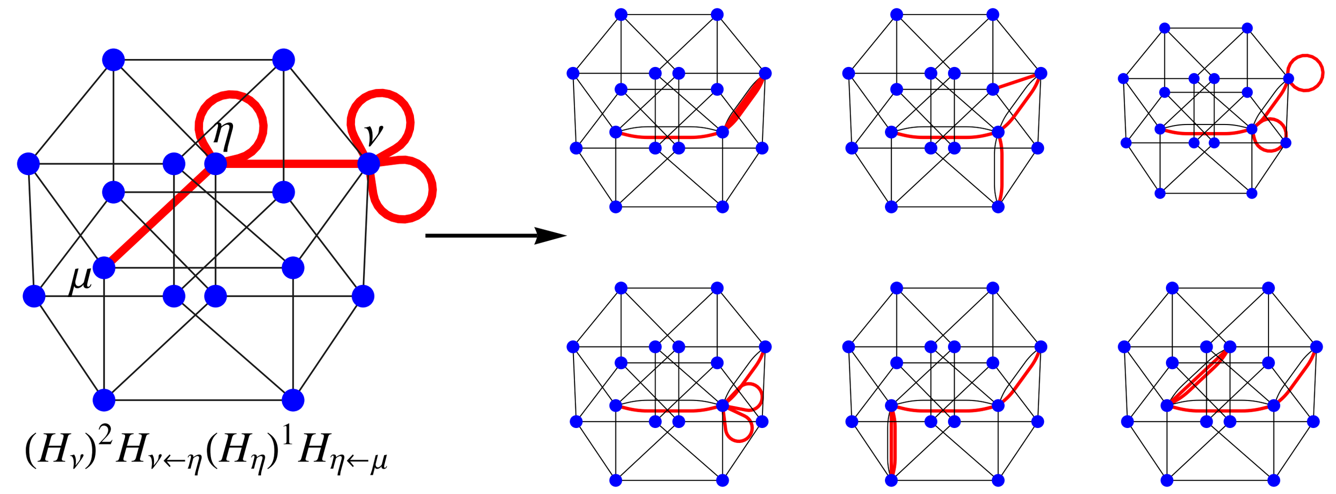
Like walk-sum, path-sum computes any piece $U_{\nu\leftarrow\mu}$ of U.
To understand path-sum, we take a new look on the derivation of walk-sum.

Graph $\mathcal{G}_L$

- *Vertex*: configuration of S'
- *Edge* $\mu\to\nu$: associate weight $H_{\nu\leftarrow\mu}$
- *Walk weight*: product of edge weights

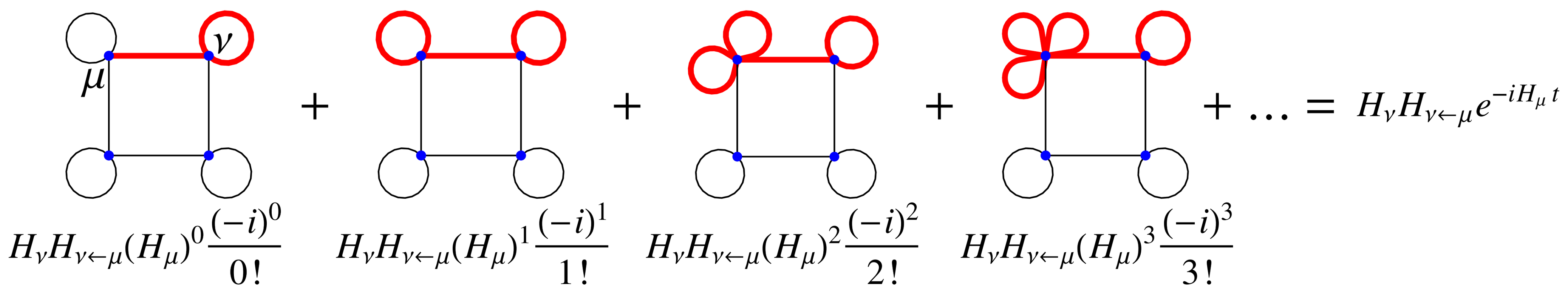
Remember H_μ and $H_{\nu\leftarrow\mu}$ = pieces of H

$\longrightarrow$ Terms of power-series of H = walks on $\mathcal{G}_L$



Walks = terms of power-series of H

- The sum of walks differing only by loops can be calculated !



The loops of $\mathcal{G}_L$ are eliminated through exact resummations, thus yielding the ***walk-sum*** *(★) on $\mathcal{G}$*

- $U_\nu = \exp[-iH_\nu t]$: an effective vertex weight representing the sum of all loops
- **Path-sum sums all cycles** this way
  - $\longrightarrow$ Reduces the walk-sum to sum over acyclic walks: the simple paths
  - $\longrightarrow$ Effective vertex weight $\tilde{U}_\nu$ representing the sum of all cycles

Path-sum

- Path-sum gives the $U_{\nu\leftarrow\mu}$ operators by summing over the **simple paths** of $\mathcal{G}$
  - $\longrightarrow$ A simple path is forbidden to visit any vertex more than once
- Path-sum is non-perturbative
- Path-sum yields a generalized Dyson equation
  - $\longrightarrow$ Path-sum also gives an explicit formula for the self-energy !

Conclusion:

Features	**Walk-sum**	**Path-sum**
Physical derivation	✔	×
Perturbative	✔	×
Valid in 2D and 3D	✔	✔
Valid for any choice of S	✔	✔
Valid for any Hamiltonian	✔	✔
Valid for any matrix function	×	✔
Criterion to decide practicality	×	×
Smooth monotonous convergence	✔	?
Systems with continuous degrees of freedom	Path-Integrals	✔

Walk-sum:
Works best for systems with strong long-range interactions. A discrete equivalent to Feynman path-integrals.

Path-sum:
Generalized Dyson equation valid for any S, explicitly gives the self-energy. Works for all matrices, all functions.

The path-sum formula

- Gives $U_{\nu\leftarrow\mu}$ in the Laplace domain

S' jumps

$$U_{\nu\leftarrow\mu}(t) = \mathfrak{L}^{-1}\Big\{\sum_{P_{\mathcal{G};\nu\mu}} i^{-n}\,\tilde{U}_{\mathcal{G}\backslash\{\mu,\dots,\eta_n\}}[\nu]\; H_{\nu\leftarrow\eta_n}\cdots\tilde{U}_{\mathcal{G}\backslash\{\mu\}}[\eta_2]\; H_{\eta_2\leftarrow\mu}\;\tilde{U}_{\mathcal{G}}[\mu]\Big\}(t)$$

Sum over the simple paths

Effective evolution operator of S while S' undergoes arbitrary cyclic evolution off μ
Represents the sum of all cycles off μ on $\mathcal{G}$

$$\tilde{U}_{\mathcal{G}}[\mu] = \Big[s\mathcal{I} - H_\mu - \sum_{C_{\mathcal{G};\mu}} i^{-m}\, H_{\mu\leftarrow\lambda_m}\tilde{U}_{\mathcal{G}\backslash\{\mu,\dots,\lambda_{m-1}\}}[\lambda_m]\cdots\tilde{U}_{\mathcal{G}\backslash\{\mu\}}[\lambda_2]\, H_{\lambda_2\leftarrow\mu}\Big]^{-1} \iff G = \left[G_0^{-1} - \Sigma\right]^{-1}$$

Sum over the simple cycles

Progressively smaller configuration space

Generalized Dyson equation

- Valid for any S, discrete degrees of freedom
- G dressed propagator: $\tilde{U}_\mu$ evolves S exactly
- G_0 bare propagator: $[s\mathcal{I} - H_\mu]^{-1}$ evolves S with S' static
- Σ self energy: sum over the simple cycles
  - $\longrightarrow$ Finite explicit formula for Σ

Derivation: arXiv:1202.5523

How do we use path-sum?

Demonstrative example: two atoms

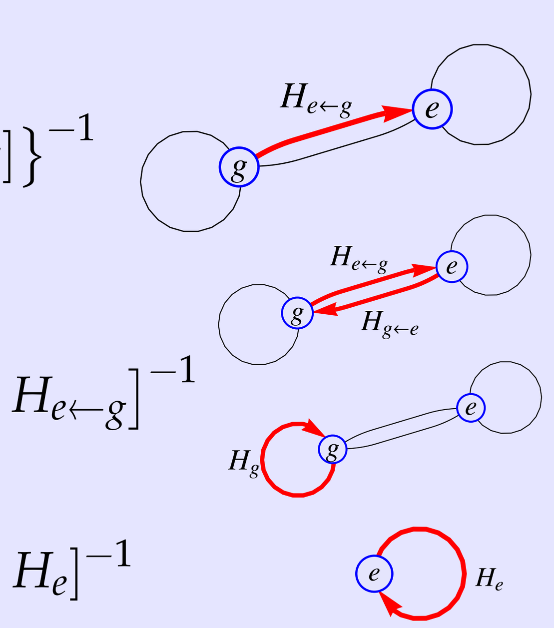
- Each atom has 2 levels: $g \equiv$ and $e \equiv$
- $S =$ atom 1
  - $\longrightarrow$ S' atom 2 $\Rightarrow$ $\mathcal{G}$ has 2 vertices
- What is $U_{e\leftarrow g}$? *one simple path ...*

$$U_{e\leftarrow g} = \mathcal{L}^{-1}\{\tilde{U}_{\mathcal{G}\backslash\{g\}}[e]\, H_{e\leftarrow g}\, \tilde{U}_{\mathcal{G}}[g]\}^{-1}$$

... and a sum on the simple cycles

$$\tilde{U}_{\mathcal{G}}[g] = [s\mathcal{I} - H_g - H_{g\leftarrow e}\,\tilde{U}_{\mathcal{G}\backslash\{g\}}[e]\, H_{e\leftarrow g}]^{-1}$$

$$\tilde{U}_{\mathcal{G}\backslash\{g\}}[e] = [s\mathcal{I} - H_e]^{-1}$$



General matrix functions: arXiv:1112.1588

This work is supported by a Scatcherd European scholarship and EPSRC funding

Mail: p.giscard1@physics.ox.ac.uk