A quantum Monte Carlo approach to the nonequilibrium steady state of open quantum systems

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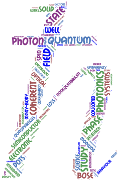
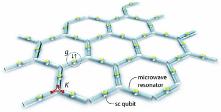
Outline

- Nonequilibrium dynamics of many-body open quantum systems
- A real-time quantum Monte Carlo approach to the steady state
- Parallel implementation, benchmarking, first results



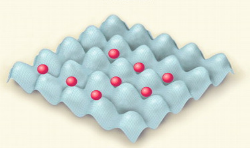
http://ltpn.epfl.ch

Coupled microcavity arrays



Koch et al., PRA (2010)

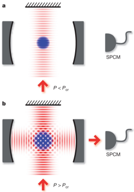
Ultracold atoms
in optical lattices



Buluta, Nori, Science 326 (2009)

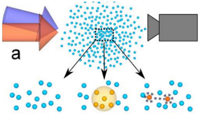
Driven open many-body dynamics

Driven-open Dicke models



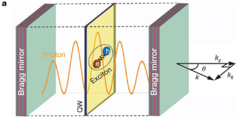
Baumann et al., Nature (2010)

Driven-dissipative Rydberg systems



Carr et al. PRL 2013

Exciton-polariton systems
in semiconductor quantum wells



Kasprzak et al., Nature (2006)

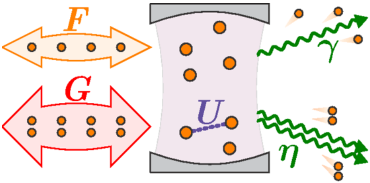
Open quantum systems

- Coupling to an external environment
- The time evolution follows the Liouville-von-Neumann master equation

$$\dot{\hat{\rho}}(t) = \mathcal{L}\hat{\rho}$$

$$\dot{\hat{\rho}} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] - \frac{\gamma}{2}\sum_j \left[\left\{\hat{K}_j^\dagger \hat{K}_j, \hat{\rho}\right\} - 2\hat{K}_j\hat{\rho}\hat{K}_j^\dagger\right]$$

- Long-time limit : nonequilibrium steady state (NESS)



Bartolo *et al.*, PRA 94, (2016)

Lindbladian real-time dynamics as a projector scheme

Hamiltonian system

- Imaginary-time dynamics of $\psi(\tau)$

$$\dot{\psi}(\tau) = -(\hat{H} - E_0)\psi(\tau)$$

- Eigenvalues E of $\hat{H}$ have $E > E_0$
- Long-time limit is ground state :

$$e^{-\tau(\hat{H}-E_0)} : \psi_{in} \xrightarrow{\tau\to\infty} \psi_0$$

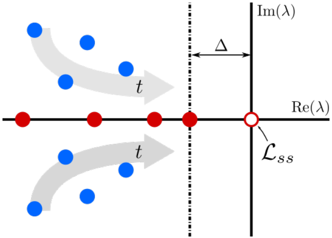
Lindbladian system

- Real-time dynamics of $\hat{\rho}(t)$

$$\dot{\hat{\rho}}(t) = \mathcal{L}\hat{\rho}$$

- Eigenvalues λ of $\mathcal{L}$ have $\mathrm{Re}(\lambda) \leq 0$
- Long-time limit is NESS :

$$e^{\mathcal{L}t} : \rho_{in} \xrightarrow{t\to\infty} \rho_{ss}$$



Overview of the FCIQMC algorithm

Projector Monte Carlo techniques

- Imaginary time dynamics $\xrightarrow{\tau \to \infty}$ exponentially decaying transients
- Stochastic implementation of the power method

$$\psi(\tau + \Delta\tau) = \hat{P}(\Delta\tau)\psi(\tau)$$

- Imaginary-time propagator

$$\hat{P}(\Delta\tau) = e^{-\Delta\tau(\hat{H} - E_0)}$$

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FCIQMC - Full Configuration Interaction Quantum Monte Carlo

- Linear projector : $\hat{P}(\Delta\tau) = \hat{I} - \Delta\tau(\hat{H} - E_0)$
- Spanning on a basis set $\{|c_i\rangle\}$

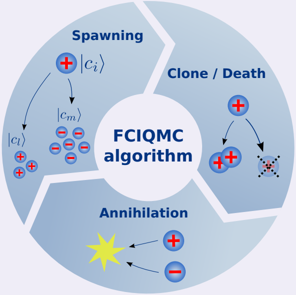
$$\psi(\tau) = \sum_i \alpha_i^\tau |c_i\rangle$$

- "Walking" : $\alpha_i \propto n_i w_i$, $w_i = \pm 1$

$$\alpha_i^{(\tau+\Delta\tau)} = [1 - \Delta\tau(H_{ii} - E_T)]\alpha_i^\tau - \Delta\tau \sum_{j\neq i} H_{ij}\alpha_j^\tau$$

Overview of the FCIQMC algorithm

Walkers do not walk.
A walker w_i can spawn another walker according to
$p_{spawn}(j|i) = -\text{sign}(\alpha_i)\frac{\Delta\tau H_{ij}}{P_{tot}}$



Decreases/increases the population on a given state
$p_{death}(i) = \Delta\tau\alpha_i(H_{ii} - E_T)$

Pairs of walkers of opposite sign are annihilated

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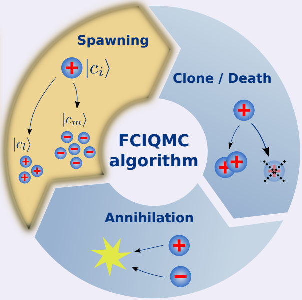

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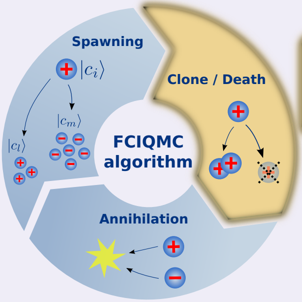

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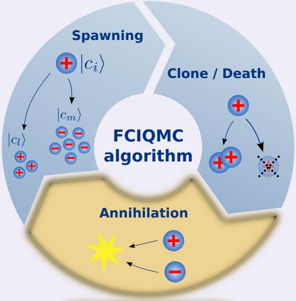

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$p_{death}(i) = \Delta\tau\alpha_i(H_{ii} - E_T)$

Pairs of walkers of opposite sign are annihilated

Why FCIQMC ?

Sign problem in QMC

- In simulation of fermions or frustrated magnets
- QMC, a large family tree $\rightarrow$ various manifestation
- An undesired state grows relative to the state of interest
- Exponential error growth

Why FCIQMC ?

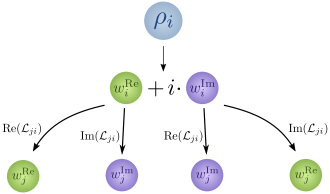
- No need to store the whole Hilbert-space
- Annihilation $\rightarrow$ stable signal to noise ratio
- Severe sign problem $\rightarrow$ increasing walker population
- Highly parallelizable algorithm

Driven-dissipative QMC - extension to open systems

- Real-time evolution leads to NESS → projector scheme MC
- Sample the complex-valued density matrix

$$\rho_i(t+\Delta t) \simeq \rho_i(t) + \sum_j (\mathcal{L}_{ij} - S\delta_{ij})\rho_j(t)\Delta t$$

- Two types of walkers : real and imaginary

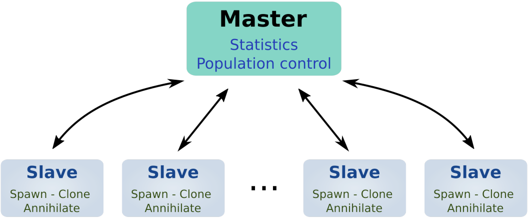


Additional refinements

- Importance sampling
- Initiator approach
- Problem-specific basis states

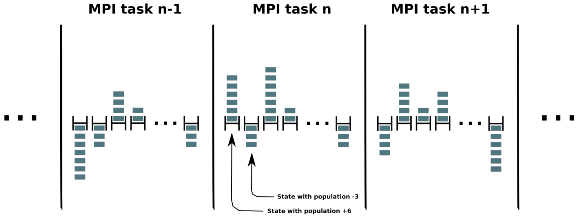
Main ideas

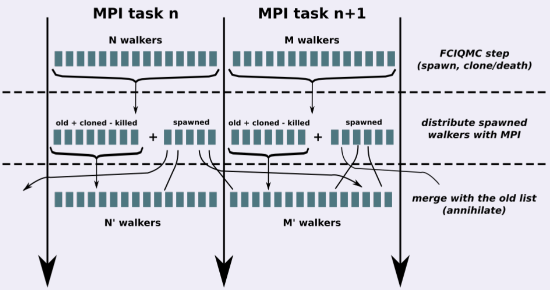
- FCIQMC is highly parallelizable
- Implemented in C++
- parallelization with MPI
- Master - Slave architecture
- Modular structure
- Efficient and scalable annihilation algorithm

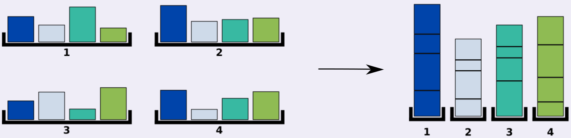


Performance

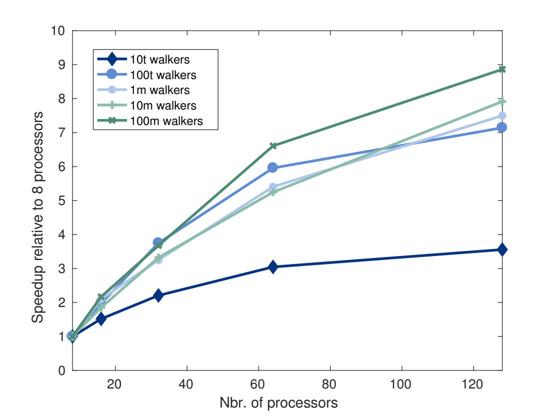
- Dual hashing procedure
  1. Hash table for storing state information
  2. Hash function for state distribution among MPI tasks
- States are coded in bitset representation → broken into 16-bit integer array




MPI task n
MPI task n+1
N walkers
M walkers
FCIQMC step
(spawn, clone/death)
old + cloned - killed
spawned
old + cloned - killed
spawned
+
+
distribute spawned
walkers with MPI
merge with the old list
(annihilate)
N' walkers
M' walkers


1
2
3
4
1
2
3
4

Increasing population → increasing parallel performance



Benchmarking

- Benchmarking and performance test on Hamiltonian systems
  1. Sign problem free - 1D antiferromagnetic Heisenberg-model
  2. Severe sign problem - 2D frustrated Heisenberg-model
- Match with analytical results even for large system sizes

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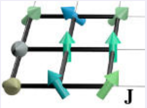
A system as a "proof of principle"

- **2D spin-1/2 lattice** governed by the **Heisenberg XYZ Hamiltonian** ($\hbar = 1$)

$$\hat{H} = \sum_{\langle i,j \rangle} \left(J_x \hat{\sigma}_i^x \hat{\sigma}_j^x + J_y \hat{\sigma}_i^y \hat{\sigma}_j^y + J_z \hat{\sigma}_i^z \hat{\sigma}_j^z \right)$$

$$\dot{\hat{\rho}} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] - \frac{\gamma}{2} \sum_j \left[\left\{ \hat{\sigma}_j^+ \hat{\sigma}_j^-, \hat{\rho} \right\} - 2 \hat{\sigma}_j^- \hat{\rho} \hat{\sigma}_j^+ \right]$$



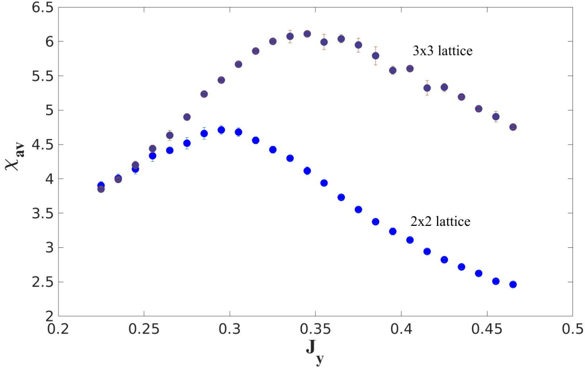
- Mean-field phase diagram known [Lee *et al.*, PRL 110, (2013)]
- Presence of dissipative phase transition [Rota *et al.*, PRB 95, (2017)]

Figure : Leblanc, Journal Phys. Cond. M. 25, (2013)

How to detect the phase transition ? [Rota *et al.* PRB 95, (2017)]

- In presence of an applied field : $\hat{H}_{ext}(h,\theta) = \sum_j h(\cos(\theta)\hat{\sigma}_j^x + \sin(\theta)\hat{\sigma}_j^y)$
- The angularly-averaged susceptibility

$$\chi_{av} = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta \frac{\partial|\vec{M}(h,\theta)|}{\partial h}\bigg|_{h=0}$$



Conclusion

Motivation

- Experimental progress
- Major challenges in simulation
- Mutual features in Lindbladian dynamics and imaginary-time Schrödinger equation
- A generalized PMC method for open systems

What's done

- Highly efficient, parallel implementation
- Benchmarking on different Hamiltonian lattice models
- A "proof of principle" on open systems
- In progress : larger system sizes, different models (e.g. driven-dissipative Bose-Hubbard, boundary dissipative problems, ...)

Thank you for your attention !

1D antiferromagnetic Heisenberg-model

- The Hamiltonian

$$\hat{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j$$

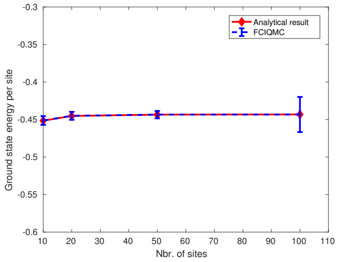
- Antiferromagnet : $J > 0$
- On bipartite lattice it is sign problem free

gauge transformation on one sublattice $\rightarrow$ all matrix elements are positive

$$\frac{J}{2}(S_i^+ S_j^- + S_i^- S_j^+) \xrightarrow{S_i^{\pm} \rightarrow (-1)^{|i|} S_i^{\pm}} -\frac{J}{2}(S_i^+ S_j^- + S_i^- S_j^+)$$

(although we don't use any transformation)

- Analytical solution known $\Rightarrow$ benchmark model



The model

- The Hamiltonian

$$\hat{H} = J_1 \sum_{\langle \mathbf{i},\hat{\mathbf{e}}\rangle} \mathbf{S}_\mathbf{i}\mathbf{S}_{\mathbf{i}+\hat{\mathbf{e}}} + J_2 \sum_{\langle \mathbf{i},\hat{\mathbf{d}}\rangle} \mathbf{S}_\mathbf{i}\mathbf{S}_{\mathbf{i}+\hat{\mathbf{d}}}$$

- where $J_1, J_2 > 0$, $\hat{\mathbf{e}}(= \hat{\mathbf{x}}, \hat{\mathbf{y}})$, and $\hat{\mathbf{d}}(= \hat{\mathbf{x}} \pm \hat{\mathbf{y}})$
- Frustrated system $\Rightarrow$ sign problem
- Complex dynamics and variety of phase transitions
  - Small frustration regime : Néel order
  - Strong diagonal interaction : collinear order
  - Intermediate coupling ratio : suggestions of various types of RVB

Order parameter estimators

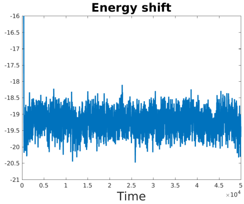
- Néel order parameter : $M^2 = \left\langle \left(\frac{1}{N} \sum_\mathbf{r} (-1)^{x+y} S^z_\mathbf{r} \right)^2 \right\rangle$
- Collinear order parameter :

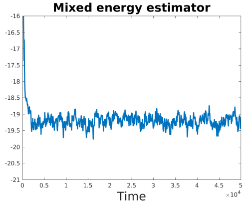
$$\chi_{col} = \left\langle \left(\frac{1}{N} \sum_\mathbf{r} \mathbf{S}_\mathbf{r}(\mathbf{S}_{\mathbf{r}+\hat{\mathbf{x}}} + \mathbf{S}_{\mathbf{r}-\hat{\mathbf{x}}} - \mathbf{S}_{\mathbf{r}+\hat{\mathbf{y}}} - \mathbf{S}_{\mathbf{r}-\hat{\mathbf{y}}}) \right)^2 \right\rangle$$

- VBS order parameter : $D^2 = \langle D_x^2 + D_y^2 \rangle$, where $D_i = \frac{1}{N} \sum_\mathbf{r} (-1)^{i_\mathbf{r}} \mathbf{S}_\mathbf{r}\mathbf{S}_{\mathbf{r}+\hat{\mathbf{i}}}$

Increasing the walker population effectively reduces the stochastical error

10.000 walkers





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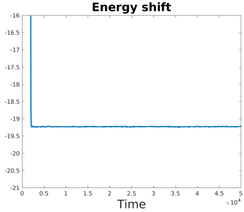
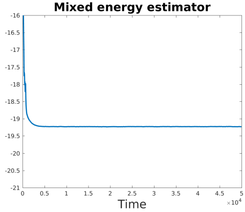
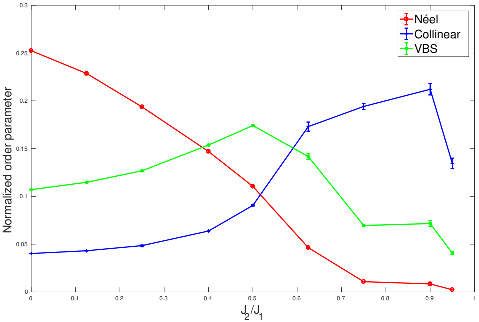




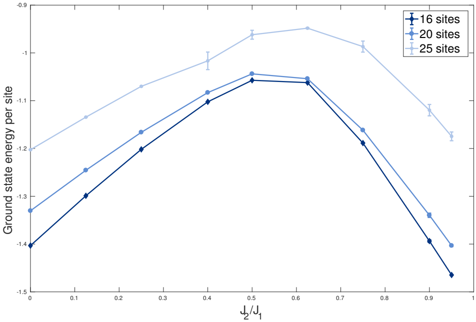
Normalized order parameter estimators

- System size : 16 sites
- Supports the occurrence of a phase transition
- VBS order parameter does not prove to be a clear indicator → the intermediate phase contains different types of spin-liquid states



Ground state energy

- Ground state energy levels from 16 up to 25 sites
- In good agreement with earlier studies
- Results with bare FCIQMC algorithm → robustness
- Clever basis, importance sampling or initiator approach would improve the efficiency



- The phase space average of a quantity A

$$\langle A \rangle = \frac{1}{Z} \sum_{c \in \Omega} A(c) p(c), \qquad Z = \sum_{c \in \Omega} p(c)$$

$\rightarrow$ but ! in QM finding $p(c)$ is not that easy

- Every D-dimensional quantum system corresponds to a $D+1$-dimensional effective classical system $\rightarrow$ various Quantum-to-classical mappings

Finite-temperature representations

- $\langle A \rangle = \frac{1}{Z} \mathrm{Tr}(A e^{-\beta \hat{H}})$
- Stochastic series expansion (SSE)
- Trotter-Suzuki decomposition

Zero-temperature projector representation

- $\langle A \rangle = \frac{1}{Z} \langle \psi_0 | A | \psi_0 \rangle$
- Projector scheme : $|\psi_0\rangle \propto \lim_{\tau \to \infty} e^{-\tau H} |\psi_{in}\rangle$
- SSE for $Z = \langle \psi_0 | \psi_0 \rangle = \langle \psi_{in} | e^{-2\tau H} | \psi_{in} \rangle$

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Sign problem

- $p(c)$ is proportional to the product of Hamiltonian elements
- Sign problem if some of the $p(c) < 0$
  - can not interpret $p(c)$ as probabilities
  - appears in simulation of fermions or frustrated magnets

"Solution"

- Sampling by using $|p(c)|$

$$Z = \sum_c p(c) = \frac{\sum_c \text{sign}\{p(c)\}|p(c)|}{\sum_c |p(c)|}$$

- BUT the mean value of the sign becomes exponentially small

$$\langle s \rangle = \frac{Z}{Z_{|p|}} = e^{-\beta N \Delta f}$$

- Exponential growth in the error

$$\frac{\Delta s}{\langle s \rangle} \sim e^{\beta N \Delta f}$$

The same limitation in PMC techniques : an undesired state grows relative to the state of interest