Simulation Methods for Open Quantum Many-Body Systems

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Scope and Challenges

Covered techniques:

- Mean-field stochastic methods
- Tensor networks (MPDO, PEPS)
- Variational methods
- vQMC
- A truncated Wigner approximation, BBGKY hierarchy equations
- Linked-cluster expansions

Other interesting regimes:

- Keldysh (real time) field theory
- PT-symmetry Q.M.
- Non-Markovian dynamics

Scope and Challenges

Open problems:

- Long-range interacting Rydberg atoms
- 2D TN
- AFM order in the 3D dissipative Ising model
- Phase transitions and universality classes of dissipative models
- Reliability of MF
- Suitable norms vs. efficient computability in variational methods

Lindblad Formulation

Quantum Master Equation

$$\frac{d}{dt}\rho = \mathcal{L}[\rho] = -i[H + H_{\text{Lamb shift}}, \rho] + \sum_{\mu} \left(L_\mu \rho L_\mu^\dagger - \frac{1}{2}\{L_\mu^\dagger L_\mu, \rho\} \right) \quad (1)$$

- $\mathcal{L}$: Liouvillian superoperator
- L_μ: Lindblad operators (dissipation channels)
- Key approximations:
  - Born-Markov: $\tau_E \ll \tau_R$ (environment correlation time $\ll$ system relaxation time)
  - Rotating wave: $\omega_s \gg \tau_R^{-1}$ (system frequency separation $\gg$ relaxation time)

Experimental Platforms:

- Quantum optics ; e.g. driven-dissipative Rydberg systems
- Circuit QED; e.g. Bose-Hubbard lattices
- Semiconductor polaritons

L_μ: **local only in the weak-coupling limit**

(Strongly correlated?)

- a slow development of correlations
- fast decay of excitations of the environment
- neglect of fast-oscillating terms
- systems need to correct

non-Markovian dynamics? Feedback:

- instantaneous feedback $\leftrightarrow$ Markovian dynamics (Lindblad form)
- delayed feedback $\leftrightarrow$ non-Markovian dynamics

Central Research Questions

- Steady-State Physics: Thermodynamic limit and the long time limit commute problem (, full time evolution)

$$\rho = \prod_i (\rho_i^{MF} + \delta\rho_i) \tag{2}$$

- Dynamical Evolution: Initial-state-dependent multiple steady states

vs. equilibrium problems

- Unsuitable: QMC, DFT, ...
- Suitable: TN, symmetries, ...

Dissipative Ising model

$$H = \frac{h}{2}\sum_i \sigma_i^x + \frac{V}{4}\sum_{\langle ij\rangle} \sigma_i^z \sigma_j^z, \quad c_i = \sqrt{\gamma}\sigma_i^- \tag{3}$$

- γ: the rate of dissipative flips
- The dissipation breaks the Z_2 Ising symmetry
- mean-field theory $\rightarrow$ bistable region?

Driven-Dissipative Bose-Hubbard

$$H = -J\sum_{\langle ij\rangle} b_i^\dagger b_j + \sum_i \left(\frac{U}{2}n_i^2 - \Delta\omega n_i + F(b_i + b_i^\dagger)\right), \quad c_i = \sqrt{\gamma} b_i \quad (4)$$

- $\Delta\omega$: the chemical potential
- F: the coherent driving because of dissipation
- The dissipation (and F) breaks the $U(1)$ symmetry
- mean-field theory $\rightarrow$ Mott lobes

Core Idea: Ensemble of Pure States

- Represent ρ as statistical ensemble: $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$
- Propagate individual trajectories $|\psi_i(t)\rangle$
- Observables via ensemble average:

$$\langle O \rangle = \sum_i p_i \langle \psi_i | O | \psi_i \rangle , \quad \text{Relative error} \sim \frac{1}{\sqrt{M}}$$

- Computational cost: $O(Md)$ (parallelizable across trajectories)

  - compared with $\mathcal{L}\rho \sim O(d^2)$

The First one of Two Key Approaches

Quantum State Diffusion (QSD)

Stochastic Schrödinger equation:

$$d\,|\psi_i(t)\rangle = -iH_{eff}\,|\psi_i(t)\rangle\,dt + \sum_j M_j\,|\psi_i(t)\rangle\,dW_j \tag{5}$$

where

$$H_{eff} = H + \sum_j \left(2\langle c_j^\dagger\rangle c_j - c_j^\dagger c_j - \langle c_j^\dagger\rangle\langle c_j\rangle\right) \tag{6}$$

- dW_j: Wiener increments

- $M_j = c_j - \langle c_j\rangle$: random fluctuations

- Maintains norm of state

The Second one of Two Key Approaches

Quantum Jump Method

1. Non-Hermitian evolution:

$$H_{\mathsf{NH}} = H - \frac{i}{2}\sum_j c_j^\dagger c_j \tag{7}$$

2. Jump trigger: When $\| \, |\psi(t)\rangle \, \| < r$ (random threshold)
3. Jump probability:

$$p_j = \frac{\langle\psi|c_j^\dagger c_j|\psi\rangle}{\sum_k \langle\psi|c_k^\dagger c_k|\psi\rangle} \tag{8}$$

- Small nonequilibrium system: new data analysis techniques $\rightarrow$ thermodynamic limit (e.g. anisotropic system)

Matrix Product Density Operators (MPDO)

- MPDO representation:

$$\rho = \sum_{\{s,s'\}=1}^{d} \prod_k M_k^{s_k,s'_k} |s\rangle \langle s'| , \quad M_k^{s_k,s'_k} \in \mathbb{C}^{D_k^2 \times D_{k+1}^2} \tag{9}$$

- Purification via MPS: $\rho = \mathrm{Tr}_a |\Psi\rangle\langle\Psi|$

$$|\Psi\rangle = \sum_{\{s,a\}} \prod_i A_i^{s_i,a_i} |s,a\rangle \tag{10}$$

- Advantages: Lower computational cost, compatible with DMRG
- Errors: Trotter decomposition, cut χ
- Disadvantages: positivity of MPDO, no bounds for MPS bond dimensions

A description of mixed states that is both efficient and locally positive semidefinite does not exist and that one can make only approximations!

Vectorized Density Matrices (Choi Isomorphism)

- Map $\rho \leftrightarrow |\rho\rangle$:

$$|\rho\rangle = \sum_{i_1=0}^{d^2-1} \cdots \sum_{i_N=0}^{d^2-1} c_{i_1 \cdots i_N} |i_1\rangle \otimes \cdots \otimes |i_N\rangle \tag{11}$$

  - $|i_l\rangle$: basis in $\mathbb{C}^{d^2}$

- TEBD algorithm for Markovian dynamics: $\mathcal{L}[\rho] = \sum_l \mathcal{L}_{l,l+1}[\rho]$
- **Positivity challenge**: purification operator $\rho = XX^\dagger$ (control error $\sim$ trace norm)

Direct MPO approaches

Some refs: Jian Cui (2015.6), Zi Cai (2013.10)

Variational method $\Rightarrow$ the null eigenvector of $\mathcal{L}$ (steady state)

- Work regimes: weakly dissipative (tuning along the sweeps)
- Disable: transient state
- steady state $\rho_s \rightarrow$ GS of the nonlocal Hamiltonian $\mathcal{L}^\dagger\mathcal{L}$

Direct MPO approaches

Evolution:

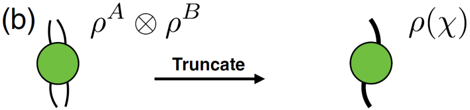
$$\mathcal{H} = \sum_{r\in\mathbb{Z}} (\mathcal{L}_r^\dagger \mathcal{L}_r)^{1/k}, \quad \mathcal{L} = \sum_{r\in\mathbb{Z}} \mathcal{L}_r \tag{12}$$

where $1/k$ is to increase the gap.

1. imaginary time evolution: $|\rho_G\rangle \approx \lim_{\tau\to\infty} \frac{e^{-\mathcal{H}\tau}|\rho_0\rangle}{||e^{-\mathcal{H}\tau}|\rho_0\rangle||}$ (pass through a highly entangled transient regime)
2. real time evolution: $|\rho_S\rangle \approx \lim_{\tau\to\infty} \frac{e^{\mathcal{L}T}|\rho_S\rangle}{||e^{-\mathcal{L}T}|\rho_S\rangle||}$ (improves the accuracy)

Corner Space Renormalization (CSR)

- For small lattices: Diagonalize $\rho^A = \sum_i p_i^A |\psi_i^A\rangle\langle\psi_i^A|$
- Merge subsystems, truncate to top-χ product states
- Convergence via increasing corner space dimension
- Applicable to finite-size driven-dissipative systems (TTN)



$$\rho(\chi) = \{|\phi_{i1}^A\rangle|\phi_{i'1}^B\rangle, |\phi_{i2}^A\rangle|\phi_{i'2}^B\rangle, \ldots, |\phi_{i\chi}^A\rangle|\phi_{i'\chi}^B\rangle\}$$

Vectorized PEPO for 2D

- Choi isomorphism in 2D: $|\dot{\rho}\rangle = \mathcal{L}\,|\rho\rangle$
- iPEPS for steady states: $|\rho_s\rangle = \lim_{t\to\infty} e^{\mathcal{L}t}|\rho(0)\rangle$
- Key challenge: H Entanglement growth vs. L_μ dissipation suppression
- Two methods: Energy of GS or Fidelity
- Success cases: Dissipative Ising model (1st-order phase transition)
- Positivity? Entanglement Monogamy: more bonds in 2D

How to deal with the positivity problem

Three methods:

1. $\rho = X^\dagger X$
2. positivity preserving algorithm (high bond dimension)
3. GS of $\mathcal{L}^\dagger \mathcal{L}$, nonlocal:
    - More approximations
    - target the variational minimization of the real part for $\langle \mathcal{L} \rangle$.

For Steady States

- Parametrize $\rho(\{\alpha_i\})$, minimize norm (e.g. trace norm):

$$\mathcal{F} = \|\mathcal{L}[\rho]\|_{\mathsf{Tr}} = \mathrm{Tr}\left(|\dot{\rho}|\right) \tag{13}$$

  - Choose variational manifold

- Trace norm:
  1. Advantages:
     1. Natural distance for density matrices;
     2. Avoid bias to mixed states (compared with Schatten p norms $[\mathrm{Tr}(|\dot{\rho}|^p)]^{1/p}\,(p > 1)$)
  2. Disadvantages: Diagonalize (solved by upper bonds)

Upper bound approximation (nn):

$$D = \sum_{ij \in \mathcal{T}} \mathrm{Tr}(|\dot{\rho}_{ij}|), \quad \rho = \prod_i \rho_i \tag{14}$$

- $\mathcal{T}$: pairs of sites connected by $\mathcal{L}$

Ref: Hendrik Weimer. "Variational Principle for Steady States of Dissipative Quantum Many-Body Systems"

Fluctuations

Dissipative Ginzburg-Landau theory based on the variational principle

- Expand upper bonds:

$$D[\phi] = \int dx \left[\sum_m v_m [\nabla \phi(x)]^m + \sum_n u_n [\phi(x)]^n \right] \tag{15}$$

  - Dynamical symmetries → Thermodynamic steady state (Keldysh formalism and FRG)

- Ginzburg-Landau-Wilson functional integral:

$$Z_{eff} = \int \mathcal{D}\phi \exp(-\beta_{eff} D[\phi]) \tag{16}$$

  - $\beta_{eff} \sim u_0$; - Perturbative RG

Full time evolution

- Lowest-order Euler approximation:

$$D = \mathrm{Tr}(|\rho(t+\tau) - \rho(t) - \tau\mathcal{L}\rho(t)|) \tag{17}$$

  - e.g. rk45 (higher correlation), ...

- Approximations: implicit midpoint method, ...

Mean-Field Dynamics

$$\frac{d}{dt}\rho_i = \mathrm{Tr}_{j\neq i}\left(\frac{d}{dt}\rho\right) = -i[H_i^{MF}, \rho_i] + \mathcal{D}_i(\rho_i) \tag{18}$$

- Variational Method (Products State) $\nLeftrightarrow$ Mean-field decoupling of the interaction in OQMS

- $\mathcal{D}_i(\rho_i)$: mean-field dissipators

- Self-consistent solution (Single-site effective problem if T-symmetry)

- Extended: Cluster MF

- N/L clusters
- Short-range physics

MF Bistability

MF Bistability regimes: absence of symmetries, ...

MF fails to capture:

- Long-range fluctuations
- First-order transitions (predicts bistability instead)
- Success in higher dimension (compared with variational principle)

Bistability: similar with limit cycles in open quantum systems

DMFT

Central Idea: Map to single impurity problem (e.g. Kondo effect)

Efficient Lindblad eq. $\rightarrow$ **Quantum transport (closed)**

- Fermi-Hubbard models

$$S_{eff} = -\int_0^\beta \int_0^\beta d\tau' \sum_\sigma f_\sigma^\dagger(\tau)\mathcal{G}_0^{-1} f_\sigma(\tau') + U\int_0^\beta f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow \qquad (19)$$

- Self-consistent solution that reproduces the dynamical Green's function $\mathcal{G}_0$

Local Green's function G_0:

$$
\begin{aligned}
G_0(i\omega_n) &= \langle c_\sigma(i\omega_n) c_\sigma^*(i\omega_n) \rangle_{S_{eff}} \\
&= \frac{1}{\mathcal{G}_0^{-1}(i\omega_n) - \Sigma(i\omega_n)} \\
&= \int d\epsilon \frac{N(\epsilon)}{i\omega_n + \mu - \Sigma(i\omega_n) - \epsilon}
\end{aligned}
$$

- ω_n: Matsubara frequencies

Projection Operator methods

Central Idea: Single site, with the non-Markovian environment

- Nakajima-Zwanzig method
- Time-convolutionless master equation
  1. Introduce corrections:
  $$\mathcal{L} = \mathcal{L}_{MF} + \Delta\mathcal{L} \tag{20}$$
  2. Removes correlations, projects onto a product state
  $$\mathcal{P}\frac{d}{dt}\rho(t) = \mathcal{L}_{MF}\mathcal{P}\rho(t) + \mathcal{P}\Delta\mathcal{L}\int_0^t dt'\mathcal{K}(t,t')\mathcal{P}\rho(t') \tag{21}$$

  - $\mathcal{K}$: The generator can be expanded $\sim \Delta\mathcal{L}$

Variational TN

Challenges: Trace norm isn't efficient in TN $\rightarrow$ Non-natural norm errors ($\sim$ dimensions, relaxation times)

Solution

- Ensemble of pure states:

$$\rho = \int p(\alpha, \tilde{\alpha}) \left|\psi(\alpha)\right\rangle \left\langle\psi(\alpha)\right| d\alpha d\tilde{\alpha} \tag{22}$$

- Variational norm:

$$D_H = \left|H_{eff} \left|\psi(\alpha)\right\rangle\right|^2, \quad H_{eff} = H - \frac{i}{2}\sum_i c_i^\dagger c_i \tag{23}$$

Variational QMC (vQMC)

Central Idea: Rewrite in terms of a sampling (classical)

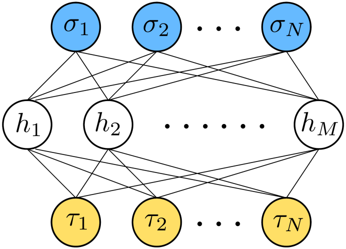
Motivation: Restricted Boltzmann machines (RBMs) in neural network simulations

Vectorized density matrix:

$$\rho(\sigma,\tau) = \frac{1}{Z}\sum_{\{h_j\}} \exp\left[\sum_{ij}\left(W_{ij}\sigma_i + W_{ij}^*\tau_i\right)h_j\right] \exp\left[\sum_i (a_i\sigma_i + a_i^*\tau_i) + \sum_j b_j h_j\right] \tag{24}$$

- $\{\sigma,\tau\}$: spin picture

- Capable: Long-range entangled quantum states, 2D directly
- RBMs wave functions $>$ MPS
- Norm:
  1. Hilbert-Schmidt norm ($D = \mathrm{Tr}(\dot{\rho}^2)/\mathrm{Tr}(\rho^2)$)
  2. the nonlocal Hermitian $\mathcal{L}^\dagger\mathcal{L}$



Semiclassical Phase-Space Dynamics

- Replace Moyal equation with classical Liouville equation
- Driven-dissipative polariton system:

$$H = \int d\boldsymbol{r} \begin{pmatrix} \psi_X^\dagger & \psi_C \end{pmatrix} \begin{pmatrix} -\frac{\nabla^2}{2m_X} + \frac{g_X}{2}|\psi_X|^2 & \frac{\Omega_R}{2} \\ \frac{\Omega_R}{2} & -\frac{\nabla^2}{2m_C} \end{pmatrix} \begin{pmatrix} \psi_X \\ \psi_C \end{pmatrix} \tag{25}$$

- $\psi_{X,C}(\boldsymbol{r}, t)$: cavity and photon field operators
- $m_{X,C}$: exciton and photon masses
- g_X: exciton-exciton interaction strength
- Ω_R: Rabi splitting.

External Drive vs. Incoherent Decay

Driven-dissipative polariton system

- System-bath (SB) Hamiltonian:

$$H_{SB} = \int d\boldsymbol{r} \left[F(\boldsymbol{r},t)\psi_C^\dagger(\boldsymbol{r},t) + h.c. \right] + \sum_{\boldsymbol{k}} \sum_{l=X,C} \left\{ \xi_{\boldsymbol{k}}^l \left[\psi_{l,\boldsymbol{k}}^\dagger(t) B_{l,\boldsymbol{k}} + h.c. \right] + \omega_{l,\boldsymbol{k}} B_{l,\boldsymbol{k}}^\dagger B_{l,\boldsymbol{k}} \right\} \tag{26}$$

  - B: the bath's bosonic annihilation and creation operators with energy ω

- Pump F: add polaritons ($\boldsymbol{k}_p$ and ω_p)

$$F(\boldsymbol{r},t) = f_p \exp\left[i(\boldsymbol{k}_p \cdot \boldsymbol{r} - \omega_p t) \right]$$

Solve from Phase-space

Central Idea: Map Fokker-Planck partial differential equation to a stochastic differential equation

Driven-dissipative polariton system (Wigner distribution)

- Stochastic differential equation:

$$i\mathrm{d}\begin{pmatrix}\psi_X\\ \psi_C\end{pmatrix} = \left[H'_{MF}\begin{pmatrix}\psi_X\\ \psi_C\end{pmatrix} + \begin{pmatrix}0\\ F\end{pmatrix}\right]\mathrm{d}t + i\begin{pmatrix}\sqrt{\kappa_X}\mathrm{d}W_X\\ \sqrt{\kappa_C}\mathrm{d}W_C\end{pmatrix} \tag{27}$$

  - Truncating limit: $g_X/(\kappa_{X,C}a^2) \ll 1$, up to 2-order derivatives
  - $\kappa_{X,C}$: the exciton and photon decay rates
  - a: lattice length

- $\mathrm{d}W_{l=X,C}$: Wiener noise terms, and

$$H'_{MF} = \begin{pmatrix} -\frac{\nabla^2}{2m_X} + g_X(|\psi_X|^2 - \frac{1}{a^2}) - i\kappa_X & \frac{\Omega_R}{2} \\ \frac{\Omega_R}{2} & -\frac{\nabla^2}{2m_C} - i\kappa_C \end{pmatrix}$$

- Developments: spin systems and quantum corrections

Particle Correlations

- Decompose correlations:

$$\rho_{\mu\nu} = \rho^c_{\mu\nu} + \rho_\mu \rho_\nu, \quad \rho^c_{\mu\nu\lambda} \simeq 0$$

- Scaling: $\rho^c_{\mathcal{S}} = O(Z^{1-|\mathcal{S}|})$ in set $\mathcal{S}$

  - Z: the coordination number of the Hamiltonian

- Generalization Functional:

$$\mathcal{F}(\alpha_\mu) = \ln\left\{\mathrm{Tr}\left[\rho \prod_\mu (1_\mu + \alpha_\mu)\right]\right\} \tag{28}$$

  - α_μ: an arbitrary operator acting on an on-site μ

$$\rho_\mu = \frac{\partial \mathcal{F}}{\partial \alpha_\mu}\Big|_{\alpha=0}, \quad \rho^c_{\mu\nu} = \frac{\partial^2 \mathcal{F}}{\partial \alpha_\mu \partial \alpha_\nu}\Big|_{\alpha=0} \tag{29}$$

Reduced Density Matrix Equations

- Dissipation equation

$$i\partial_t \rho = [H, \rho] + \sum_{\mu} \mathcal{L}_{\mu} \rho + \frac{1}{Z} \sum_{\mu\nu} \mathcal{L}_{\mu\nu} \rho \tag{30}$$

- Hierarchy equations derived by (30) via $\mathcal{F}$

$$i\partial_t \rho_{\mu} = \mathcal{L}_{\mu} + \frac{1}{Z} \sum_{k} \mathrm{Tr}_k \left(\mathcal{L}^S_{\mu k} \rho_{\mu k} \right) \tag{31}$$

with $\mathcal{L}^S_{\mu\nu} = \mathcal{L}_{\mu\nu} + \mathcal{L}_{\nu\mu}$

- Expand $\sim 1/Z$; (**Same for two lattice sites**)

- Suitable for arbitrary dimensions

Expansion in Quasilocal Clusters

- Liouvillian expansion: $\mathcal{L} = \sum_{\langle k \rangle} \alpha_k \mathcal{L}_k$

  - $k = (i, j)$: couple of i-j sites

  - α_k: local coupling strength

- Observable expansion:

$$O = \sum_{\{n_k\}} O_{\{n_k\}} \prod_k \alpha_k^{n_k} = \sum_c W_{[O]}(c) \tag{32}$$

with $n_k = 1, 2, \ldots$ for all k

- c: clusters

- $W_{[O]}(c)$: expectation in clusters

- Recurrence relation:

$$W_{[O]}(c) = O(c) - \sum_{s \subset c} W_{[O]}(s), \quad O(c) = \mathrm{Tr}\left[\hat{O}\rho_s(c)\right] \tag{33}$$

- $\rho_s(c)$: steady state in c

- Operator expectation in thermodynamic limit (T-symmetry):

$$\frac{O}{L} = \sum_{n=1}^{\infty}\left(\sum_{c_n} l(c_n) W_{[O]}(c_n)\right) \tag{34}$$

- Inner sum: topologically differences $l(c_n)$; Outer sum: cluster sizes

- Truncate cluster sizes to R

Method Performance

TABLE II. Comparison of the different simulation methods discussed in this review. We differentiate the methods by the system sizes that can be simulated, the spatial dimensions, constraints on the local Hilbert space dimension, whether or not fermionic systems can be treated, the simulation performance for inhomogeneous systems, and whether or not the correct critical exponents of phase transitions can be obtained.

	WFMC[a]	TN[b]	Variational principle	VQMC[c]	CMF[d]	TWA[e]
System size (in qubits)	20	TDL[f]	TDL	16	TDL	400
Dimensions	One, two	One, two	Any[g]	Any	Any[h]	Any
Local Hilbert space	Small	Small	Large	Large	Small	Large
Fermionic systems	Yes	Yes	Partially	No	Partially	Unknown
Inhomogeneous systems	Good	Good	Bad	Good	Good	Good
Critical exponents	Good	Good	Good[i]	Unknown	Bad	Unknown
Time-dependent $\mathcal{L}$	Yes	Yes	Yes	Yes	Yes	Yes

[a]Wave-function Monte Carlo.
[b]Tensor networks.
[c]Variational quantum Monte Carlo.
[d]Cluster mean field.
[e]Truncated Wigner approximation.
[f]Systems in the thermodynamic limit.
[g]Works better in higher dimensions.
[h]Works better in higher dimensions.
[i]For states with thermal statistics.

References I

[1] Hendrik Weimer, Augustine Kshetrimayum, and Román Orús. Simulation methods for open quantum many-body systems. Rev. Mod. Phys., 93:015008, Mar 2021.