NUMERICAL METHODS AND VARIATIONAL APPROACHES FOR OPEN QUANTUM SYSTEMS

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⇒ • The open Quantum Many-Body problem:
general scenario

Strong interactions lie at the heart of many prominent aspects of quantum mechanics

→ high-T_c superconductivity
→ quantum phase transitions
→ quantum magnetism
→ many-body localization
→ quantum transport
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} notably known to be HARDLY ATTACHABLE many-body problems

→ Theoretical toy models:
- quantum spin chains & networks
- Hubbard-like models (fermionic/bosonic)

→ Experimental platforms:
- ultracold atoms
- trapped ions
- superconducting circuits
:

} controllable Quantum simulators
→ detailed microscopic knowledge
→ high external tunability

→ high coherence over large time scales
→ good access for measurements

- **example: ultracold bosons trapped in optical lattices**

$$\hat{H}_{BH} = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_j \hat{n}_j^2$$

hopping — on-site repulsion

Bose-Hubbard

($\hat{b}_j^{(\dagger)}$ bosonic creation/annihilation operators; $\hat{n}_j = \hat{b}_j^\dagger \hat{b}_j$ number op.)

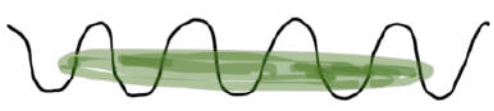
- if $U \gg J$ the interaction term dominates

$$|\psi_{g.s.}\rangle \sim \prod_{j=1}^{L} (\hat{b}_j^\dagger)^p |0\rangle$$

Mott Insulator (Fock state)

- if $U \ll J$ the kinetic term dominates:

$$|\psi_{g.s.}\rangle \sim \left[\sum_{j=1}^{L} \hat{b}_j^\dagger \right]^N |0\rangle$$



Superfluid (Coherent state)

M. Fisher, P. Weichman, G. Grinstein, D. Fisher, PRB 40, 546 (1989)
D. Jaksch, C. Bruder, J. Cirac, C. Gardiner, P. Zoller, PRL 81, 3108 (1998)
M. Greiner, O. Mandel, T. Esslinger, T. Hansch, I. Bloch, Nature 415, 39 (2002)

Q. Why should we care about the coupling to an external environment?

strong interactions + coupling with a bath ⇒ competition between coherent dynamics & incoherent processes

several quantum optical platforms cannot be reliably described neglecting the system/bath coupling

- ultracold atoms → excited Rydberg atoms (see, e.g. A. Browaeys, T. Lahaye,

Nature Phys. 16, 132 (2020)

↓ driven systems in optical superlattices

S. Diehl, A. Micheli, A. Kantian, B. Kraus, H. Büchler, P. Zoller, Nature Phys. 4, 878 (2008)

- nonlinear photon dynamics → arrays of optomechanical cavities

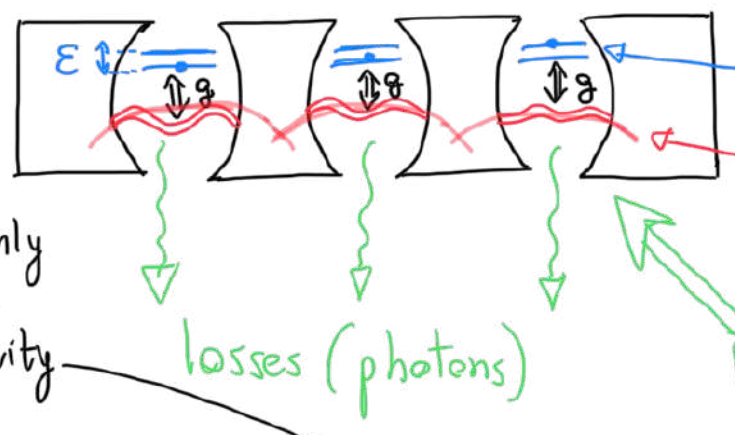
M. Ludwig, F. Marquardt, PRL 111, 073603 (2013)

↓ Coupled QED/superconducting cavities

A. Houck, H. Türeci, J. Koch, Nature Phys. 8, 292 (2012)

e.g. arrays of nonlinearly coupled cavities

a simplified picture



we consider only (one) photonic mode per cavity

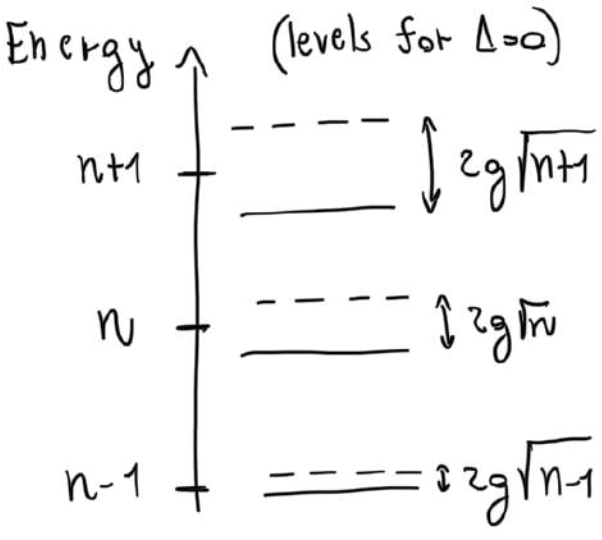
Inside each cavity ≈ Jaynes-Cummings model:

$\hat{a}(\dagger)$ photon operators

$\hat{\sigma}^{\alpha}$ Pauli matrices

$$\hat{H}_{JC} = \omega \hat{a}^{\dagger}\hat{a} + \varepsilon \hat{\sigma}^{+}\hat{\sigma}^{-} + g(\hat{\sigma}^{+}\hat{a} + \hat{\sigma}^{-}\hat{a}^{\dagger})$$

@ small g (light-matter interaction)



$$E_n^{\pm} = n\omega + \frac{\Delta}{2} \pm \sqrt{ng^2 + \frac{\Delta^2}{4}}$$

$$\Delta = \varepsilon - \omega$$

$U_{eff} \sim J_n^2 E(n) > 0$ effective onsite nonlinearity

→ For (many) coupled cavities:

$$\hat{H}_{JCH} = \sum_{i=1}^{L} \hat{H}_{JC,i} - t \sum_{\langle i,j \rangle} \hat{a}_i^{\dagger} \hat{a}_j$$

Jaynes-Cummings-Hubbard

$\approx \hat{H}_{BH}$ for dressed photons

(atomic/photonic excitations: POLARITONS)

Q. How can we take into account natural cavity LOSSES (or/and cavity pumping)?

A brief (not too formal) mathematical intro

J. Preskill, "Lecture Notes on Quantum Information and Computation" http://theory.caltech.edu/people/preskill/ (1998)

C. Gardiner, P. Zoller, "Quantum Noise" (Springer-Verlag, 2000)

H. Breuer, F. Petruccione, "The Theory of Open Quantum Systems" (Oxford Univ. Press, 2002)

(A) Closed quantum systems

Q given quantum state is described by a normalized vector $|\psi(t)\rangle$ in a Hilbert space $\mathcal{H}$

The evolution of $|\psi\rangle$ is dictated by the (ħ=1)

Schrödinger equation: $i\frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$

$\hat{H}$ ↑ Hamiltonian Operator

Observables correspond to Hermitian operators $\hat{A}$.

The statistics of measurement outcomes is determined by

$$\langle A \rangle = \langle \psi(t)|\hat{A}|\psi(t)\rangle$$

When many quantum objects interact together, we are dealing with many-body Hamiltonians

(B) Open quantum systems

A given quantum state of an open system is described by a density matrix $\rho(t)$ in a Hilbert space $\mathcal{H}$. (ρ is hermitian, positive, and $\mathrm{Tr}[\rho]=1$)

The evolution of $\rho(t)$ is dictated by a suitable master equation.

It can be shown that the most general form of master equation which preserves all the properties of ρ at any time (i.e. completely positive trace-preserving dynamical semigroup) is the so-called Lindblad master equation:

$$\text{(*)}\quad \frac{d\rho(t)}{dt} = \underbrace{-i[\hat{H},\rho]}_{\text{unitary evolution}} + \sum_j \gamma_j \left[\hat{L}_j \rho \hat{L}_j^\dagger - \frac{1}{2}\{\hat{L}_j^\dagger \hat{L}_j, \rho\}\right]$$

γ_j: dissipation rate $\gamma_j > 0$

$\hat{L}_j$: jump operators (Lindblad op.)

V. Gorini, A. Kossakowski, E. Sudarshan, J. Math. phys. 17, 821 (1976)
G. Lindblad, Commun. Math Phys. 48, 119 (1976)

e.g. for photonic losses in a cavity array, the suitable jump operator is $\hat{L}_j = \hat{a}_j$

(*) This master eq. holds under certain approximations:

- Born approx. (weak system-bath coupling)
- Markov approx. (neglect memory effects in system/bath coupling)
- Secular approx. (neglect fast oscillations)

- A realistic theoretical model for coupled QED cavities:

$$\frac{d\rho}{dt} \equiv \mathcal{L}[\rho] = -i[\hat{H}_{JCH},\rho] + \sum_{\alpha,j} \gamma_j^{(\alpha)} \left(\hat{L}_j^{(\alpha)} \rho \hat{L}_j^{(\alpha)\dagger} - \frac{1}{2}\{\hat{L}_j^{(\alpha)\dagger}\hat{L}_j^{(\alpha)}, \rho\}\right)$$

also called Liouvillian

$$\hat{H}_{JCH} = \sum_j \underbrace{\omega_j \hat{a}_j^\dagger \hat{a}_j}_{\text{photon energy}} + \underbrace{\varepsilon_j \hat{\sigma}_j^+ \hat{\sigma}_j^-}_{\text{atom splitting}} + \underbrace{g_j \left(\hat{\sigma}_j^+ \hat{a}_j + \hat{\sigma}_j^- \hat{a}_j^\dagger\right)}_{\text{light-matter coupling in each cavity}}$$

(in the rotating frame)

$$+ \sum_j \underbrace{\Omega_j \left(\hat{a}_j^\dagger + \hat{a}_j\right)}_{\text{laser (coherent) driving}} - \sum_{\langle i,j \rangle} \underbrace{t_{ij} \hat{a}_i^\dagger \hat{a}_j}_{\text{photon hopping between neighboring cavities}}$$

$\hat{L}_j^{(e)} = \hat{a}_j$ incoherent photon losses (e) on each cavity, of strength $\gamma_j^{(e)}$

$\hat{L}_j^{(p)} = \hat{a}_j^\dagger$ incoherent photon pumping (p) on each cavity, of strength $\gamma_j^{(p)}$

→ can be approximated by a dissipative Bose-Hubbard model for polaritons:

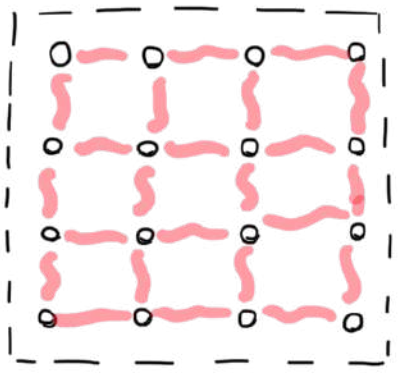
$$\hat{H} \sim -t \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + U \sum_j \hat{n}_j^2 + \Omega \sum_j \left(\hat{b}_j^\dagger + \hat{b}_j\right)$$

$$\hat{L}_j^{(e)} = \hat{b}_j \quad ; \quad \hat{L}_j^{(p)} = \hat{b}_j^\dagger$$

[see, e.g., A. Tomadin, R. Fazio, J. Opt. Soc. Am. B 27, a130 (2010)
A. Houck, H. Türeci, J. Koch, Nat. Phys. 8, 292 (2012)]

The challenge: exponentially growing Hilbert space!

$$\frac{d\rho}{dt} = -i[\hat{H},\rho] + \sum_{j=1}^{N} \gamma_j \left(\hat{L}_j \rho \hat{L}_j^\dagger - \frac{1}{2}\{\hat{L}_j^\dagger \hat{L}_j, \rho\} \right)$$



N sites

$$\hat{H} \sim -t \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + U \sum_j \hat{n}_j^2 \quad ; \quad \hat{L}_j = \hat{b}_j$$

single-site states:

$$\{|0\rangle, |1\rangle, |2\rangle, \ldots, |n_{MAX}\rangle\}$$

⇓

Brute-force integration techniques of the master equation severely limited to a small number of sites:

$$\dim \mathcal{H}_N = (n_{MAX}+1)^N$$

⇒ the Liouvillian $\mathcal{L}$ ($\dot{\rho} = \mathcal{L}[\rho]$) is a matrix acting on the space of linear operators in $\mathcal{H}$

→ $\mathcal{L}$ is a matrix of size $(n_{MAX}+1)^{2N} \times (n_{MAX}+1)^{2N}$

→ not even hermitian!

- even for spin-½ systems the problem becomes rapidly intractable

# spins	$\dim \mathcal{H}$	$\dim \mathcal{L}$
1	$2^1 = 2$	$2^2 \times 2^2 = 4 \times 4$
2	$2^2 = 4$	$4^2 \times 4^2 = 16 \times 16$
3	$2^3 = 8$	$8^2 \times 8^2 = 64 \times 64$
4	$2^4 = 16$	$16^2 \times 16^2 = 256 \times 256$
5	$2^5 = 32$	$32^2 \times 32^2 = 1024 \times 1024$
6	$2^6 = 64$	$64^2 \times 64^2 = 4096 \times 4096$
7	$2^7 = 128$	$128^2 \times 128^2 = 16384 \times 16384$
⋮	⋮	⋮
n	2^n	$(2^n)^2 \times (2^n)^2 = 2^{2n} \times 2^{2n}$

⇒ more clever numerical approaches required

Unfortunately even analytical tools are scarce.

Analytically solvable prototypical examples are quadratic liouvillian models

e.g. Ising-like Hamiltonians, which are mappable to quadratic fermionic models ($\Rightarrow$ Kitaev) in 1D

$$\hat{H} = -\sum_j \left(J \hat{c}_j^\dagger \hat{c}_{j+1} + \Delta \hat{c}_j^\dagger \hat{c}_{j+1}^\dagger + h.c. \right) - 2\Gamma \sum_j \hat{n}_j$$

$\hat{c}_j^{(\dagger)}$ fermionic creation/annihilation op.

Can be diagonalized using Bogoliubov transformation

E. Lieb, T. Schultz, D. Mattis, Ann. Phys. 16, 407 (1961)

P. Pfeuty, Ann. Phys. 57, 79 (1970)

Adding dissipation, under the Lindblad formalism, is not a problem, provided $\mathcal{L}$ remains quadratic in $\hat{c}_j^{(\dagger)}$ ops.

e.g. use the following memoryless Lindblad terms:

1) $\hat{L}_j^{(e)} = \hat{c}_j$ incoherent losses

2) $\hat{L}_j^{(p)} = \hat{c}_j^\dagger$ incoherent pumping

3) $\hat{L}_j^{(d)} = \hat{n}_j = \hat{c}_j^\dagger \hat{c}_j$ dephasing bath

Cases 1-2: quadratic master equation

T. Prosen, NJP 10, 043026 (2008)

"third quantization" methods

Case 3: focusing on specific observables (es 2-point correlation functions) it is possible to write a closed set of differential equations for them

see e.g. V. Eisler, J. Stat. Mech. (2011) P06007

Finding other analytically solvable cases is hard and methods become cumbersome

Numerical Approaches

- Quantum Trajectories (wave-function Monte Carlo)

  A. Daley, Adv. Phys. 63, 77 (2014)

  H. Carmichael, "An open-system approach to quantum optics" (Springer, 1993)

- Mean-field based methods

  S. Diehl, A. Tomadin, A. Micheli, R. Fazio, P. Zoller, PRL 105, 015702 (2010)

  J. Jin, A. Biella, O. Viyuela, L. Mazza, J. Keeling, R. Fazio, DR, PRX 6, 031011 (2016)

- Refined variational & Gutzwiller MC approaches

  P. Degenfeld-Schonburg, M. Hartmann, PRB 89, 245108 (2014)

  H. Weimer, PRL 114, 040402 (2015)

  W. Casteels, R. Wilson, M. Wouters, PRA 97, 062107 (2018)

  W. Verstraelen, M. Wouters, Appl. Sci. 8, 1427 (2018)

- Perturbative methods & cluster expansions

  A. Li, F. Petruccione, J. Koch, PRX 6, 021037 (2016)

  A. Biella, J. Jin, O. Viyuela, C. Ciuti, R. Fazio, DR, PRB 97, 035103 (2018)

- Corner space renormalization method

  S. Finazzi, A. Le Baité, F. Storme, A. Baksic, C. Ciuti, PRL 115, 080604 (2015)

- Matrix-Product-Operators (MPO) for 1D systems

  ↳ Time-evolving block decimation strategies

  F. Verstraete, J. García-Ripoll, J. Cirac, PRL 93, 207204 (2004)

  M. Zwolak, G. Vidal, PRL 93, 207205 (2004)

  T. Prosen, M. Žnidarič, J. Stat. Mech. (2009) P02035

  ↳ Variational strategies for MPOs

  J. Cui, J. Cirac, M. Bañuls, PRL 114, 220601 (2015)

  E. Mascarenhas, H. Fleyac, V. Savona, PRA 92, 022116 (2015)

  A. Werner et. al. (J. Eisert, S. Montangero), PRL 116, 237201 (2016)

- Projected entangled pair operators (PEPO) for 2D systems

A. Kshetrimayum, H. Weimer, R. Orus, Nature Commun. 8, 1291 (2017)

- Variational quantum Monte-Carlo methods (neural networks)

  A. Negy, V. Savona, PRL 122, 250501 (2019)

  M. Hartmann, G. Carleo, PRL 122, 250502 (2019)

  F. Vicentini, A. Biella, N. Regnault, C. Ciuti, PRL 122, 250503 (2019)

  N. Yoshioka, R. Hamazaki, PRB 99, 214306 (2019)

- and other approaches yet...

  see, e.g., the review by H. Weimer, A. Kshetrimayum, R. Orus, arXiv: 1907.07079

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(1) Warmup method: Quantum trajectories

→ ideated in q. optics by J. Dalibard, Y. Castin, K. Mölmer, PRL 68, 580 (1992)

$$\dot{\rho} = \boxed{-i[\hat{H},\rho] - \frac{1}{2}\sum_j \gamma_j \{\hat{L}_j^\dagger \hat{L}_j, \rho\}} + \boxed{\sum_j \gamma_j \hat{L}_j \rho \hat{L}_j^\dagger}$$

effective non-Hermitian evolution $\sim -i(\hat{H}_{eff}\rho - \rho \hat{H}_{eff}^\dagger)$ | quantum jumps

where $\hat{H}_{eff} = \hat{H} - i\cdot\frac{1}{2}\sum_j \gamma_j \hat{L}_j^\dagger \hat{L}_j$ | responsible for sudden changes of the system's state

Idea: suppose initially the system is in the pure state:

$$\rho(t_0) = |\psi(t_0)\rangle\langle\psi(t_0)|$$

then, after an infinitesimal time, it evolves into

$$\rho(t_0+dt) = \underbrace{\left(1 - \sum_j dp_j\right)|\phi_0\rangle\langle\phi_0|}_{\text{ordinary (yet non-hermitian) time evolution}} + \underbrace{\sum_j dp_j |\phi_j\rangle\langle\phi_j|}_{\text{sudden jump to one of the states}}$$

ordinary (yet non-hermitian) time evolution $|\phi_0\rangle = \dfrac{e^{-i\hat{H}_{eff}dt}|\psi(t_0)\rangle}{\sqrt{1 - \sum_{j>0} dp_j}}$ with probability $1 - \sum_{j>0} dp_j$

sudden jump to one of the states $|\phi_j\rangle = \dfrac{\hat{\tilde{L}}_j|\psi(t_0)\rangle}{\|\hat{\tilde{L}}_j|\psi(t_0)\rangle\|}$ with probability $dp_i = \langle\psi(t_0)|\hat{\tilde{L}}_i^\dagger \hat{\tilde{L}}_i|\psi(t_0)\rangle\cdot dt$

$\left(\hat{\tilde{L}}_j \equiv \sqrt{\gamma_j}\, \hat{L}_j \right)$

Algorithm:

① start from a given pure state $|\psi(t_0)\rangle$ and pick up a random number $\varepsilon \in (0,1]$ (or from the updated state at the previous iteration)

② if $\varepsilon < \sum_{j>0} dp_j$, perform a "quantum jump" to the state:

$$|\psi(t_0+dt)\rangle = \begin{cases} |\phi_1\rangle & \text{if} \quad 0 < \varepsilon \leq dp_1 \\ |\phi_2\rangle & \text{if} \quad dp_1 < \varepsilon \leq dp_1 + dp_2 \\ \vdots & \vdots \\ |\phi_n\rangle & \text{if} \quad dp_{n-1} < \varepsilon \leq \sum_{j=1}^{n} dp_j \end{cases}$$

(n is the number of Lindblad jump operators)

③ if $\varepsilon > \sum_{j>0} dp_j$, evolve to $|\psi(t_0+dt)\rangle = |\phi_0\rangle \sim e^{-i\hat{H}_{\text{eff}}\, dt} |\psi(t_0)\rangle$

At each time step dt, these steps have to be ITERATED, picking up a new random number $\varepsilon \in (0,1]$

The expectation value of a given observable $\hat{A}$ on the quantum state $\rho(t)$ can be reconstructed after averaging in time a single (or many) trajectory, for a long enough time:

$$\langle \hat{A} \rangle \equiv \mathrm{Tr}\left[\rho(t)\, \hat{A} \right] \simeq \lim_{T \to +\infty} \frac{1}{T} \int_0^T \langle \psi(t) | \hat{A} | \psi(t) \rangle \, dt$$

↳ stochastic unraveling of the master equation

In practice one always deals with pure states, so it is possible to adapt numerical methods for the time evolution of pure states into the context of mixed states (e.g. TEBD methods: MPO for open systems ...)

Unfortunately the algorithmic complexity keeps being exponential ...

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② A standard approximation which drastically reduces the

A standard approximation which drastically reduces the complexity of the problem is a **mean-field** treatment.

In its simplest form, the many-body Hamiltonian is decoupled site-by-site, thus reducing it to a single-site problem.

Let's take an example: $\hat{H} = -\frac{J}{z}\sum_{\langle ij\rangle}\hat{b}_i^\dagger\hat{b}_j + U\sum_j \hat{n}_j^2 + \Omega\sum_j\left(\hat{b}_j^\dagger + \hat{b}_j\right)$

this is the term connecting many sites

decoupling: $\hat{b}_j = \langle\hat{b}_j\rangle + (\delta\hat{b}_j)$ ⇒ ($\delta\hat{b}_j$ small)

$$\hat{b}_i^\dagger\hat{b}_j = \left(\langle\hat{b}_i^\dagger\rangle + \delta\hat{b}_i^\dagger\right)\left(\langle\hat{b}_j\rangle + \delta\hat{b}_j\right) =$$

$$= \langle\hat{b}_i^\dagger\rangle\langle\hat{b}_j\rangle + \langle\hat{b}_i^\dagger\rangle\delta\hat{b}_j + \langle\hat{b}_j\rangle\delta\hat{b}_i^\dagger + \delta\hat{b}_i^\dagger\delta\hat{b}_j =$$

$$= \langle\hat{b}_i^\dagger\rangle\hat{b}_j + \langle\hat{b}_j\rangle\hat{b}_i - \langle\hat{b}_i^\dagger\rangle\langle\hat{b}_j\rangle$$

($\delta\hat{b}_i^\dagger\delta\hat{b}_j$: negligible)

$$\Rightarrow \hat{H}_{MF} \sim \left\{\left(\Omega - J\langle\hat{b}\rangle\right)\hat{b}^\dagger + h.c.\right\} + U\hat{n}^2$$

is now a single-site Hamiltonian!

renormalized driving field: $\Omega \to (\Omega - J\langle\hat{b}\rangle)$

↳ single-site dissipative problem, with a Lindblad m.e. given by:

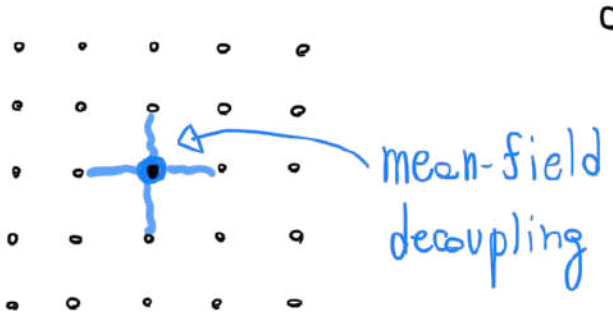
$$\frac{d\rho^{single}}{dt} = -i\left[\hat{H}_{MF}, \rho^{single}\right] + \mathcal{D}_j\left[\rho^{single}\right]$$

($\mathcal{D}_j$: this accounts for the dissipative terms, which are usually single-site)

Gutzwiller ansatz:

$$\rho_{MF}(t) = \prod_j \rho_j^{single}(t)$$

inter-site correlations & entanglement are completely NEGLECTED



Algorithm:

① Start from a given initial state $\rho^{single}(0)$ and integrate the above single-site m.e. for a small time step dt

(driven-dissipative), if the long-time stationary state is sought, just find the eigenvector of $\mathcal{L}(\rho^{single})$ associated to the zero eigenvalue

note: the mean-field value is: $\langle \hat{b} \rangle = Tr[\rho^{single}(0)\,\hat{b}]$

② Recalculate the expectation value self-consistently:

$$\langle \hat{b} \rangle(dt) = Tr[\rho^{single}(dt)\,\hat{b}]$$

③ Substitute such value $\langle \hat{b} \rangle(dt)$ into the single-site m.e. and iterate from step ①, now starting from $\rho^{single}(dt)$

⇒ steady-state solution: long-time limit starting from a generic initial state

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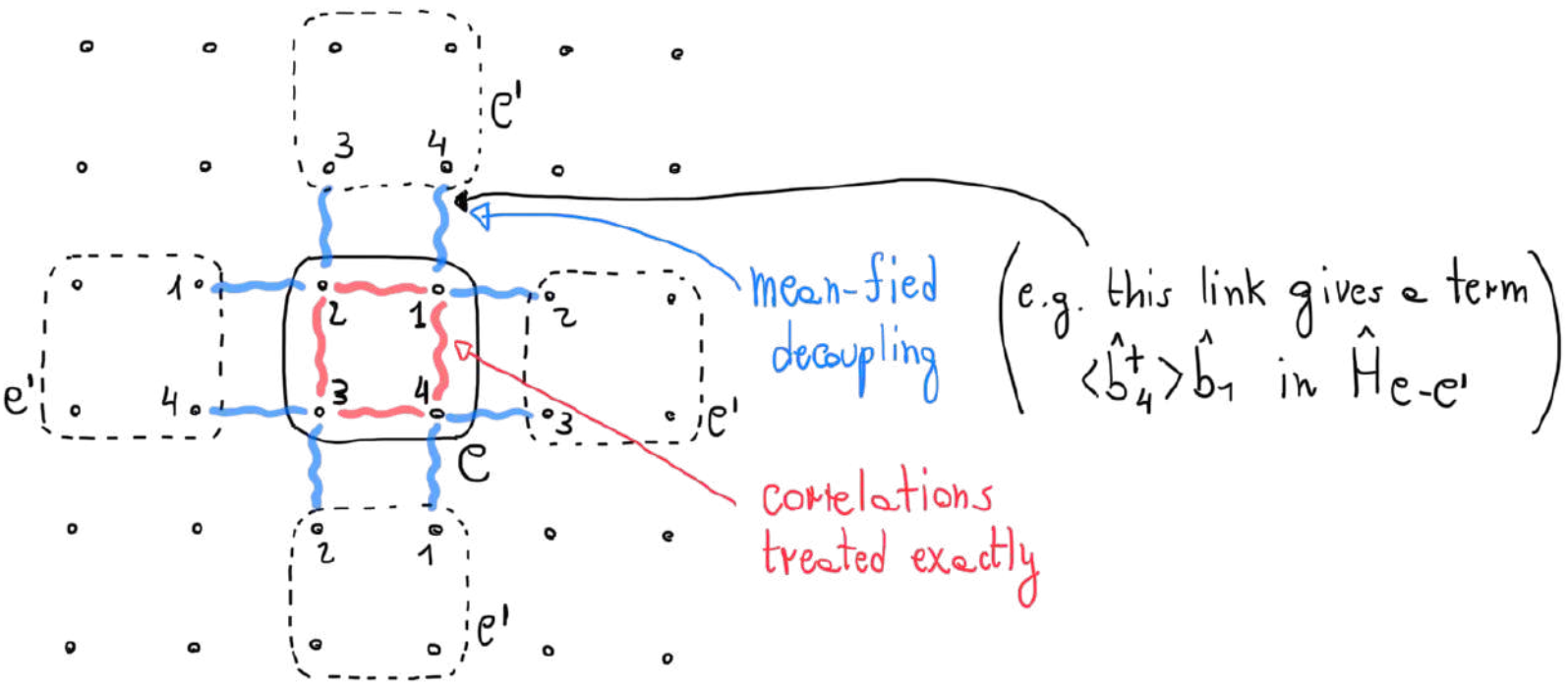
2b Improving mean field: cluster mean field

$$\hat{H}_{CMF} = \hat{H}_c + \hat{H}_{e\text{-}e'}$$

$\hat{H}_c$: exact Hamiltonian of a cluster of sites

$\hat{H}_{e\text{-}e'}$: interaction between neigboring clusters, treated at a mean-field level



The whole lattice is thus decoupled into a lattice structure:

$$\rho_{CMF}(t) = \bigotimes_e \rho_e(t)$$

In the above example, the master equation to be manipulated is for an ensemble of $2\times 2 = 4$ sites ($\Rightarrow$ Liouvillian is of size $16^2 \times 16^2$)

- Cluster mean-field methods can be easily integrated with other approaches as quantum trajectories and tensor networks

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A refined Variational, pseudo mean-field, approach:

The true stationary state is approximated by a variational density matrix, found by minimizing a suitable norm of the full master equation:

$$\left\| \frac{d\rho}{dt} \right\| = \left\| -i[\hat{H},\rho] + \mathcal{D}[\rho] \right\| \quad \leftarrow = \|\mathcal{L}[\rho]\| \text{ to be minimized}$$

one good norm is the trace norm $\|\hat{A}\| = \mathrm{Tr}[|\hat{A}|]$

As for M.F., the simplest variational state is a product of single-site density matrices, but this can be extended to states which include n.n. correlations and so on...

→ In practice one parametrizes the system state with a set of variational parameters: $\rho = \rho(\{\alpha_i\})$ and tries to get the best choice of $\{\alpha_i\}$ which minimizes $\|\mathcal{L}[\rho]\|$.

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③ Corner-space renormalization:

extension of Wilson's numerical renormalization group to open quantum systems (K. Wilson, Rev. Mod. Phys. 47, 773 (1975))

→ Wilson's RG: a real-space blocking procedure in lattice systems

consider, e.g., 1D quantum chains

A) Break the chain into finite identical blocks

$B(n,m)$ n: # sites in each block
m: # states used to describe the block

B) Build up the block Hamiltonian using m states (initially $m = 2^n$)

c) Join it with a nearby block and form $\hat{H}_{B\text{-}B}$ using m^2 states

D) Diagonalize $\hat{H}_{B\text{-}B}$ and order eigenstates $\{|u_\alpha\rangle\}_{\alpha=1\dots m^2}$

such that $E_1 \leq E_2 \leq E_3 \leq \dots E_{m^2}$

E) Change basis to represent the $\hat{H}$

E) Change basis representation of $H_{B\text{-}B}$ and truncate it to m states

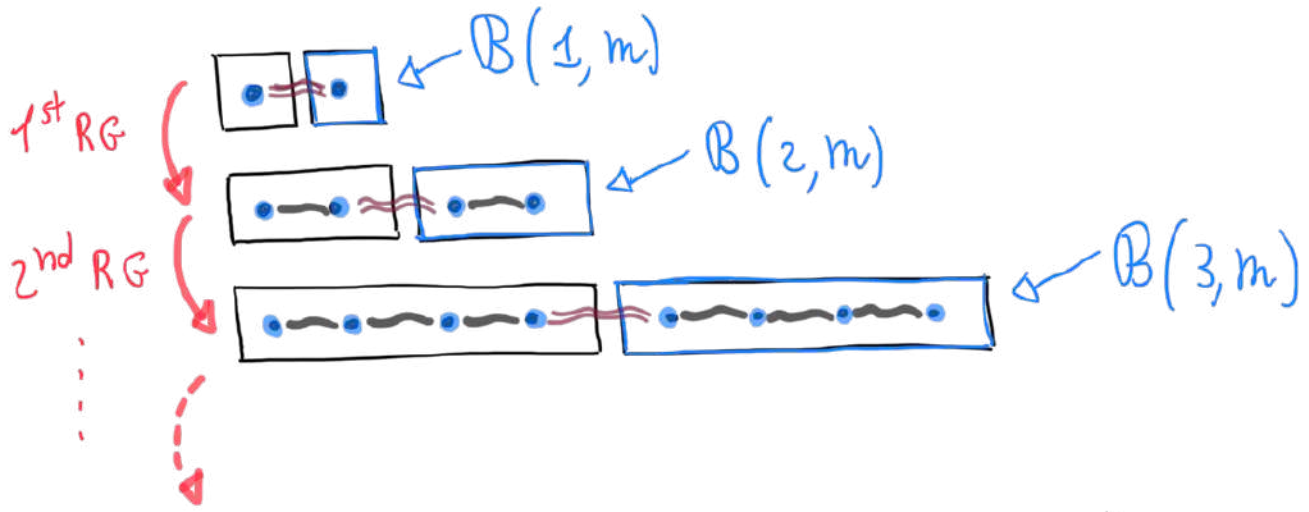
for this purpose, construct $\hat{O}_{B\text{-}B\to B'} = \left(|u_1\rangle \; |u_2\rangle \; \dots \; |u_m\rangle \right)$

a $(m^2 \times m)$ isometric matrix $\left(\hat{O}^\dagger \hat{O} = \hat{\mathbb{1}}_{m\times m} \right)$

and update all the relevent operators, such as the Hamiltonian, as

$$\hat{H}_{B\text{-}B} \to \hat{H}_{B'} = \hat{O}^\dagger_{B\text{-}B\to B'} \, \hat{H}_{B\text{-}B} \, \hat{O}_{B\text{-}B\to B'}$$

F) Repeat steps C-D-E using the new block $B'(2n, m)$.



Q big problem (especially for closed systems):

the selected eigenvectors $\{|u_\alpha\rangle\}_{\alpha=1\dots m}$ are NOT optimal,

since $\hat{H}_{B\text{-}B}$ contains no connections with the rest of the lattice.

⇒ The adaptive basis would only catch states having nodes at the boundaries of previously uncoupled blocks.

Solution: some kind of "environment" would be needed in order to frame $\boxed{B}\text{-}\boxed{B}$ into a larger system

⇒ DMRG for closed systems [S. White, PRL 69, 2863 (1992)]

But for OPEN systems this trouble is not so crucial

→ Corner space RG:

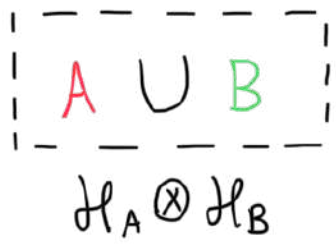
A) Find the steady-state density matrix for a small subsystem

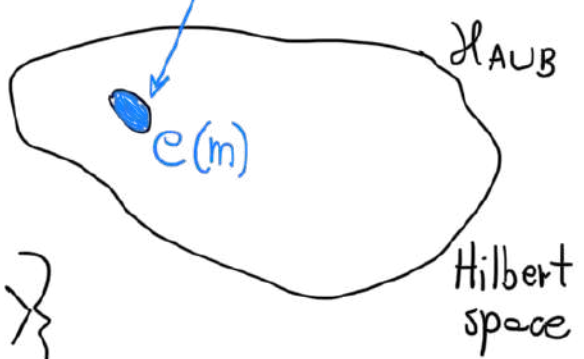
$\mathcal{H}_A \qquad \mathcal{H}_B$

$$\rho^{(A)} = \sum_r p_r^{(A)} \, |\phi_r^{(A)}\rangle\langle\phi_r^{(A)}|$$

$$\rho^{(B)} = \sum_{r'} p_{r'}^{(B)} \, |\phi_{r'}^{(B)}\rangle\langle\phi_{r'}^{(B)}|$$

B) Merge the two lattices & select the m most probable pairs of states ⟶ choose them by maximizing $p_r^{(A)} \times p_{r'}^{(B)}$

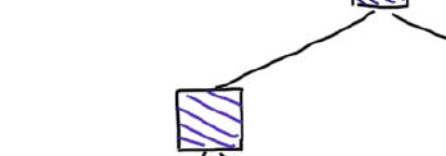




$$\mathcal{C}(m) = \mathrm{Span}\left\{ |\phi_{r_1}^{(A)}\rangle |\phi_{r_1'}^{(B)}\rangle, \dots, |\phi_{r_m}^{(A)}\rangle |\phi_{r_m'}^{(B)}\rangle \right\}$$

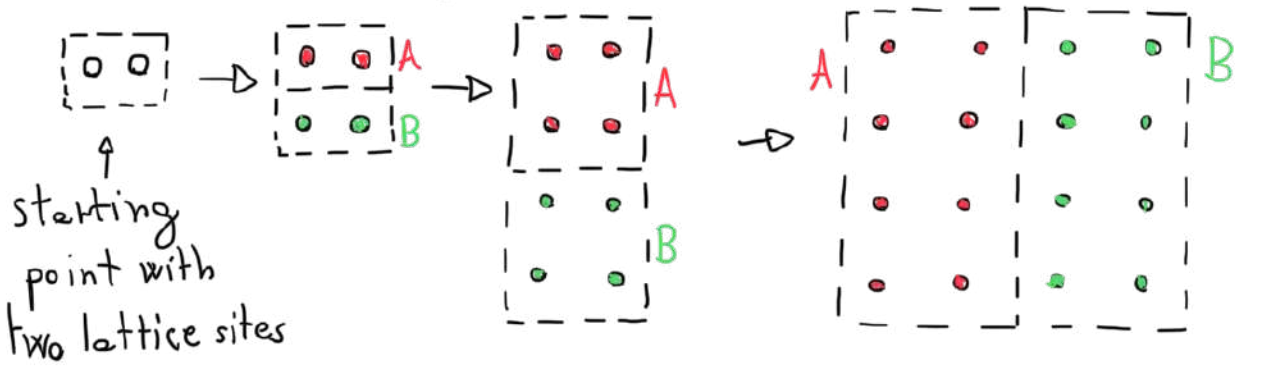
C) Find the steady-state solution of the master equation restricted to the corner space

D) Increase the dimension m of the corner space (if needed) until convergence is reached:



$$\mathrm{Tr}[\rho \hat{A}] \to \mathrm{Tr}[\rho_{\mathrm{EXACT}} \hat{A}]$$

E) Repeat this procedure such to increase the dimension of the lattice → go back to step B & iterate



and so on... (example for a 2D lattice)

- The description of the various blocks composing the full lattice can be optimized in a variational fashion, going back and forth in the grouping of the various blocks (analogously as for tensor networks / finite-system DMRG or NRG)

corner space ~ tree tensor network (TTN)

TTN structure for a 1D lattice

(it can be generalized to other geometries)

but there are more suitable tensor-network structures (or other variational ansatzes) to study the emerging many-body physics. let us see them ...

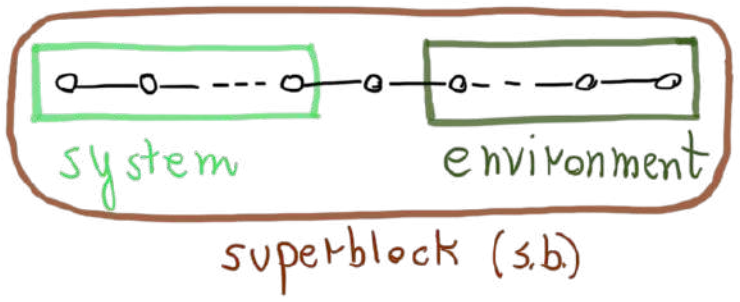
Let us come back to unitary systems, for a moment.

Wilson's numerical RG was found to be NON optimal,
so a new RG scheme has been put forward by S. White (1992):

Density matrix renormalization group (DMRG)

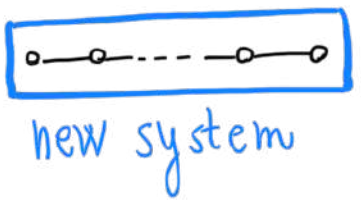
Core of the algorithm:

Construct a portion of the system, then enlarge it,
until the desired size is reached.
At each step truncate the Hamiltonian basis,
so to keep the Hilbert space size manageable



system m states
new system 2m states

⇓ Truncation: keep only the most relevant (m states)
according to $\rho = Tr_{env}\left[|\psi_{GS}\rangle_{s.b.}\langle\psi_{GS}|\right]$
i.e. diagonalize ρ and go in the basis of it,
throwing away the less significant eigenstates
(order them using the corresponding eigenvalues)


new system

Then iterate the procedure ...

DMRG is equivalent to a (quasi-variational) optimization
of a particular tensor-network structure:

in 1D: MATRIX PRODUCT STATE (MPS)
in 2D: PROJECTED ENTANGLED PAIR STATE (PEPS)

see Roman's lectures...

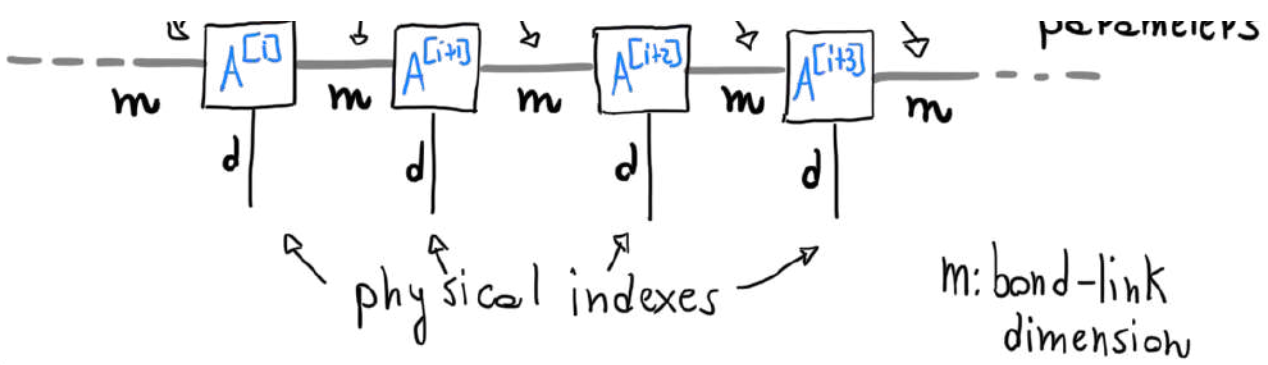
---

(4) In 1D MPS have been routinely employed in a dissipative setting (MPS → MATRIX PRODUCT OPERATORS)

MPS

$O(N \times d \times m^2)$

(closed systems)

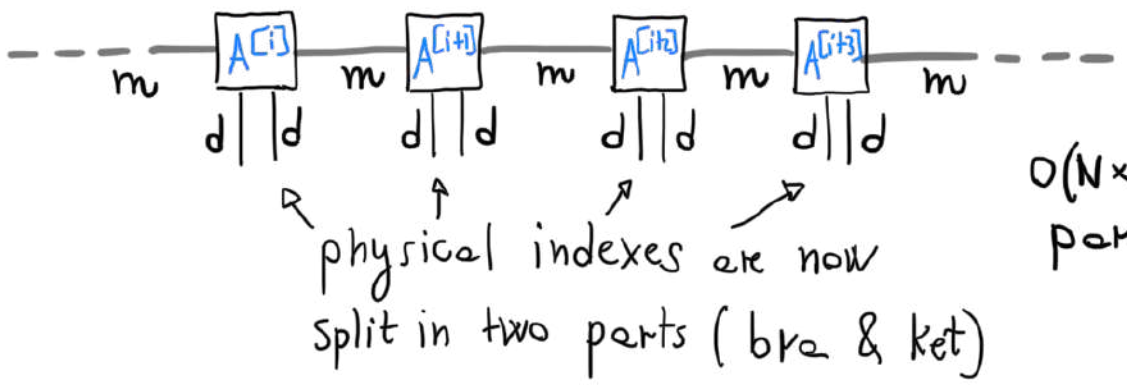


→ Q "corner" of the full Hilbert space is targeted !?

m: bond-link dimension

d: local Hilbert space dim. (d=2 for spins-½)

MPO (open systems)



$O(N \times d^2 \times m^2)$ parameters

MPOs can be used for open systems, by means of a

super-operator formalism:

every linear operator $\hat{A}$ acting on the Hilbert space $\mathcal{H}$ (let $\{|i\rangle\}_{i=1\dots d}$ be a basis)

can be associated with a vector in a superoperator space

$$\mathbb{B}(\mathcal{H}) \to \mathcal{H} \otimes \mathcal{H}$$

↓ linear operators acting on $\mathcal{H}$

↘ this is characterized by a basis $\{|i,j\rangle\}_{\substack{i=1\dots d \\ j=1\dots d}}$

$$\hat{A} = \sum_{i,j} A_{ij} |i\rangle\langle j| \quad \Rightarrow \quad |A\rangle\rangle = \sum_{ij} A_{ij} |i\rangle \otimes |j\rangle$$

"super-ket" $|i,j\rangle\rangle$

defining the identity $|\mathbb{1}\rangle\rangle = \sum_i |i\rangle \otimes |i\rangle$,

one can see that: $(\hat{B} \otimes \hat{\mathbb{1}})|\mathbb{1}\rangle\rangle = (\hat{\mathbb{1}} \otimes \hat{B}^T)|\mathbb{1}\rangle\rangle = |B\rangle\rangle$

$$\Rightarrow |AB\rangle\rangle = (\hat{A}\hat{B} \otimes \hat{\mathbb{1}})|\mathbb{1}\rangle\rangle = (\hat{A} \otimes \hat{\mathbb{1}})(\hat{B} \otimes \hat{\mathbb{1}})|\mathbb{1}\rangle\rangle = (\hat{A} \otimes \mathbb{1})|B\rangle\rangle = (\hat{\mathbb{1}} \otimes \hat{B}^T)|A\rangle\rangle$$

$$\Rightarrow |ABC\rangle\rangle = (\hat{A} \otimes \hat{C}^T)|B\rangle\rangle$$

where the scalar product is defined by:

$$\langle\langle \mathbb{1}|B\rangle\rangle = \sum_i B_{ii} = Tr[\hat{B}]$$

$$\langle\langle A|B\rangle\rangle = \sum_{ij} A_{ij}^* B_{ij} = Tr[\hat{A}^\dagger \hat{B}]$$

If we now consider the Liouvillian $\mathcal{L}[\rho]$,

this can be seen as a superoperator acting on the super-ket $|\rho\rangle\rangle$

$$\mathcal{L}|\rho\rangle\rangle = \left\{ \left(-i\hat{H} - \sum_j \gamma_j \hat{L}_j^\dagger \hat{L}_j\right) \otimes \hat{\mathbb{1}} + \hat{\mathbb{1}} \otimes \left(i\hat{H}^T - \sum_j \gamma_j \hat{L}_j^T \hat{L}_j^*\right) + \sum_j \gamma_j \hat{L}_j \otimes \hat{L}_j^* \right\} |\rho\rangle\rangle$$

$$\Rightarrow \quad \boxed{\frac{d|\rho\rangle\!\rangle}{dt} = \mathcal{L}\,|\rho\rangle\!\rangle} \quad \text{so that} \quad |\rho(t)\rangle\!\rangle = e^{\mathcal{L}t}\,|\rho(0)\rangle\!\rangle$$

The easiest strategy to "integrate" the master equation using the MPO formalism is thus to use a TIME EVOLVING BLOCK DECIMATION (TEBD) strategy and follow the time evolution with a Trotter decomposition of $\mathcal{L}$:

$$\mathcal{L} = \sum_j \mathcal{L}_{j,j+1} \quad \Rightarrow \quad e^{\mathcal{L}t} = \exp\left\{ \sum_j \mathcal{L}_{j,j+1}\, t \right\}$$

the state $|\rho(t)\rangle\!\rangle$ should be kept in the form of a MPO (similarly to what one does for closed 1D systems → MPS):

$$|\rho\rangle\!\rangle = \sum_{\substack{i_1 \dots i_N \\ j_1 \dots j_N}} \mathrm{Tr}\left[A^{[1]i_1,j_1} A^{[2]i_2,j_2} \cdots A^{[N]i_N,j_N} \right] |i_1,j_1\rangle\!\rangle \otimes |i_2,j_2\rangle\!\rangle \otimes \dots \otimes |i_N,j_N\rangle\!\rangle$$

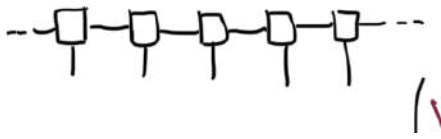
Issue: TEBD is usually associated to a bond-link growth in time of the MPS (or MPO).

- For closed systems (MPS) this growth is controlled by the increase of bipartite entanglement $S(\rho_{A|B})$: roughly speaking, $m \sim \exp(S(t))$
- For open systems (MPO) one should instead look at the bipartite operator-space entanglement entropy (OSEE). Unfortunately this has no physical meaning, thus the range of validity of a TEBD+MPO approach for dissipative systems is still debated ...

(4b) For 2D systems one can generalize such construction as in closed-system scenarios:

closed, 1D

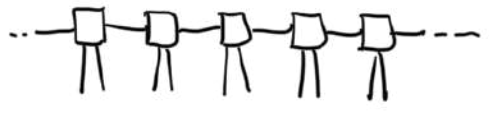
Matrix Product States (MPS)



(Vidal, Cirac, ...)

open, 1D

Matrix Product Operators (MPO)

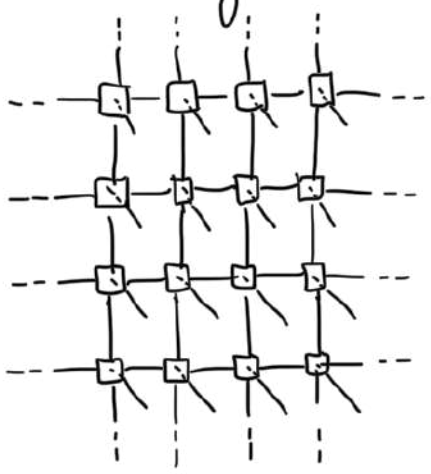


(Vidal, Zwolak, ...)

(Verstraete...)

closed, 2D

Projected Entangled Pair States (PEPS)

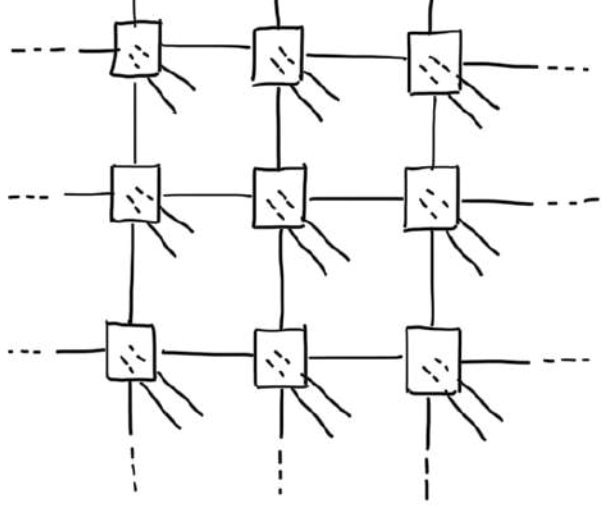


(F. Verstraete, J. Cirac, cond-mat/0407066)

(Cirac, ...)

open, 2D

Projected Entangled Pair Operators (PEPO)



(A. Kshetrimayum, A. Weimer, R. Orus, 2017)

Another possible issue with TEBD methods:

Positivity of $\rho(t)$ is generally NOT guaranteed

→ one could directly target the ground state of the Hermitian and positive semidefinite operator

$\mathcal{L}^\dagger \mathcal{L}$

(e.g. by imaginary time evol. or by Variational DMRG methods)

Unfortunately this is highly NON-LOCAL ⇒ typically creates troubles...

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5 An arguably promising approach:

Variational Monte-Carlo for open systems

Idea: use a variational wave function which corresponds to a RESTRICTED BOLTZMANN MACHINE (RBM)

→ neural-network simulations

(G. Carleo, M. Troyer, SCIENCE 355, 602 (2017))

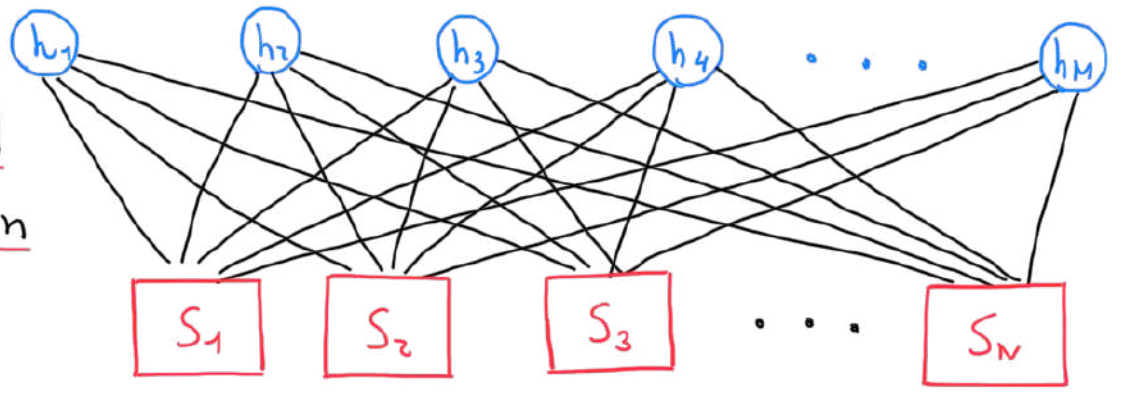
- FOR CLOSED SYSTEMS:

represent the w.f. $|\psi(t)\rangle$ in terms of an "artificial neural network" specified by a set of internal parameters W.

Such parameters are optimized by Monte-Carlo meth...

(either Variational MC (sampling or time-dependent VMC).
↳ reinforcement learning

Restricted Boltzmann Machine



Consider a quantum system with N discrete-valued degrees of freedom (e.g. spins, occupation numbers, ...)

$$S = (S_1, S_2, \dots, S_N)$$

Ψ is a mapping of S to exponentially many complex numbers which fully specify the state: $\Psi(S)$

RBM: take a visible layer of (N) nodes
corresponding to the physical variables in a chosen basis
[e.g. spins 1/2, with $S_j = \sigma_j^z \quad \forall j = 1 \dots N$]

then take a single hidden layer of (M) auxiliary variables
[e.g. spin variables $(h_1, \dots, h_M)$]

(*) $$\Psi_M(S, W) = \sum_{\{h_i\}} \exp\left\{ \sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z \right\}$$

$h_i = \{-1, +1\}$
hidden variables

network parameters
$W \equiv \{a_j, b_i, W_{ij}\}_{\substack{j=1\dots N \\ i=1\dots M}}$

(*) Specifies the response of the network to a given input state S.

RBM: No intralayer connections ⇒ it is easy to trace out the hidden variables:

$$\Psi_M(S, W) = e^{\sum_j a_j \sigma_j^z} \cdot \prod_{i=1}^{M} F_i(S)$$

where
$$F_i(S) = 2\cosh\left[b_i + \sum_j W_{ij} \sigma_j^z \right]$$

the "control parameter", which takes the role of the bond link, is the density of hidden variables $\alpha = \frac{M}{N}$

Remark: although the physical variables (DO NOT) interact directly, in the RBM, correlations are induced by hidden variables and are intrinsically NON-LOCAL in space.

⇒ systems in arbitrary dimension (and not only in 1D) are, in principle, reliably treatable with RBMs.

(A) Ground-state search:

minimize the energy cost function $E(W) = \dfrac{\langle \psi_M | \hat{H} | \psi_M \rangle}{\langle \psi_M | \psi_M \rangle}$ with respect to the network weights W.

- At the k-th iteration, realize a MC sampling of $|\Psi_M(S, W_k)|^2$
- obtain stochastic estimates of energy gradient
- use such estimates to propose a next set of weights W_{k+1}, with an improved gradient-descent optimization

(B) Unitary dynamics:

define time-dependent weights $W(t)$ that, at each time, are "trained" to best reproduce the quantum dynamics.

→ minimize $R[\dot{W}(t)] = \text{dist}\left(\partial_t \Psi, -i\hat{H}\Psi\right)$

e.g. by sampling $|\Psi_M(S, W(t))|^2$ at each time and provide the best stochastic estimate of the $\dot{W}(t)$ that minimizes $R^2(t)$

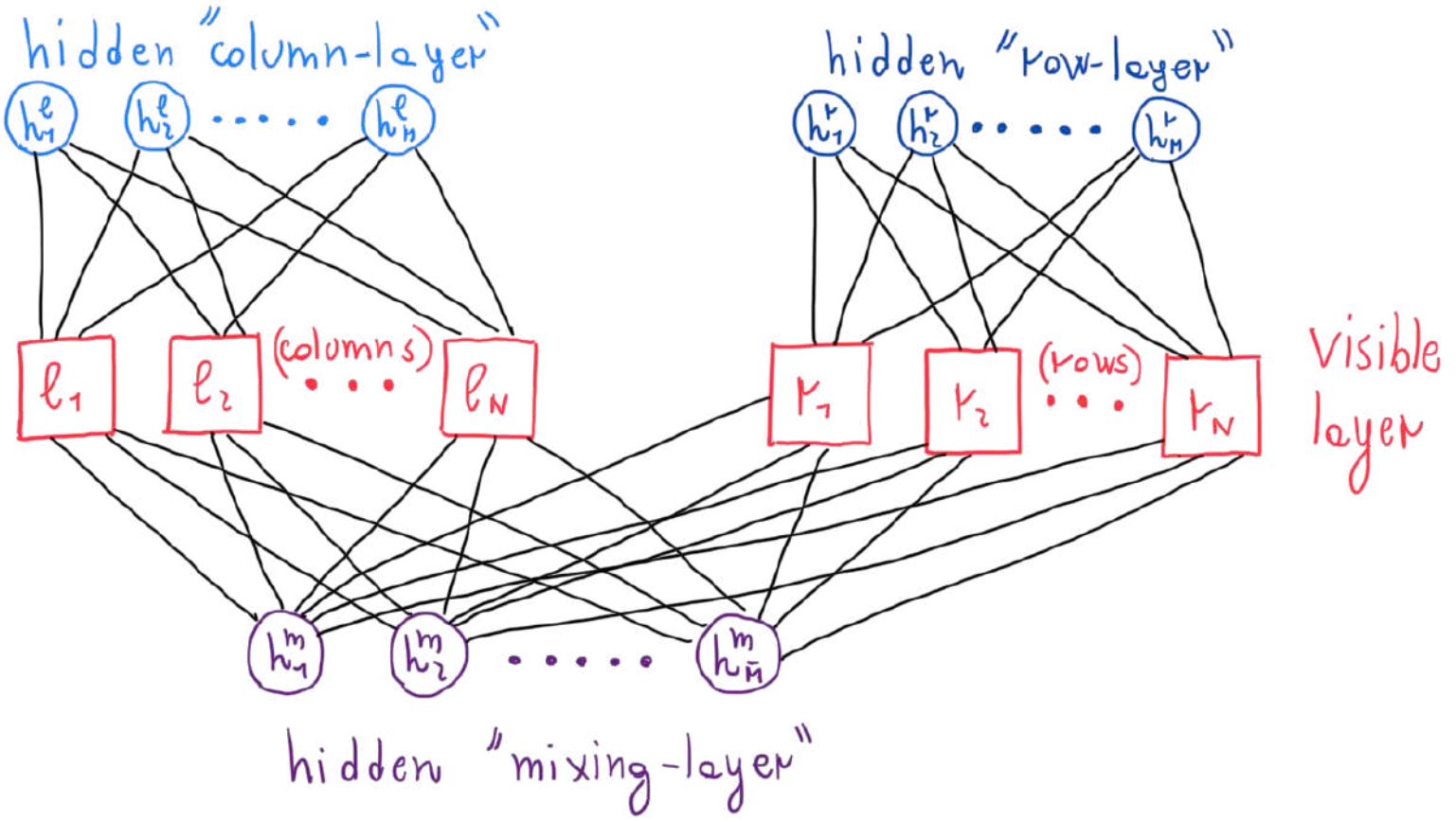
Once time derivatives are obtained, use them to obtain the full time evolution after time integration.

- FOR OPEN SYSTEMS:

a more complicated RBM should be invoked, for example considering three sets of hidden units:

$h^{(e)}$ $h^{(h)}$ $h^{(m)}$

Correlations btw column d.o.f. of ρ | Correlations btw row d.o.f. of ρ | mixed correlations between the two



then use the following parametrization for the density matrix:

$$\rho_{\vec{e},\vec{r}} = \exp\left\{ \sum_{j=1}^{N} \left(a_j e_j + a_j^* r_j \right) \right\} \cdot \prod_{k=1}^{M} \chi_k \cdot \prod_{p=1}^{\bar{M}} y_p$$

with

$$\chi_k = \cosh\left[b_k + \sum_{j=1}^{N} W_{kj} e_j \right] \cdot \cosh\left[b_k^* + \sum_{j=1}^{N} W_{kj}^* r_j \right]$$

$$y_p = \cosh\left[c_p + c_p^* + \sum_{j=1}^{N} \left(U_{pj} e_j + U_{pj}^* r_j \right) \right]$$

network parameters: $W = \{ a_j, b_k, W_{kj}, U_{pj} \}$ $j=1\dots N$, $k=1\dots M$, $p=1\dots \bar{M}$

$\vec{e} = (e_1, e_2, \dots, e_N)$ left indices of ρ

$\vec{r} = (r_1, r_2, \dots, r_N)$ right indices of ρ

analogously as for pure states, here $M, \bar{M}$ play the role of the bond links (number of auxiliary variables)

→ The approximate dynamics of the master equation can be cast as a variational optimization problem (use time-dependent VMC)

Write ρ as a super-ket $|\rho\rangle\!\rangle$ so that $\partial_t |\rho\rangle\!\rangle = \mathcal{L} |\rho\rangle\!\rangle$

According to ⊛, $|\rho\rangle\!\rangle$ is parametrized by $(N+1)(M+\bar{M})+N$ complex variables

now, using the notation $\vec{\alpha}$ to indicate the ensemble of these variational parameters (both real and imaginary parts are treated independently) we can express

$$\partial_t |\rho\rangle\!\rangle = \sum_k \dot{\alpha}_k \hat{O}_k |\rho\rangle\!\rangle \quad \text{where } \hat{O}_k \text{ is a diagonal matrix with entries } [\hat{O}_k]_{\vec{e}_r,\vec{e}_r} = \frac{\partial \log \rho_{\vec{e}_r}}{\partial \alpha_k}$$

To approximate the dynamics of $|\rho(t)\rangle\!\rangle$, one finds a closed eq. of motion for the $\alpha_k(t)$, $\forall k$.

i.e. minimize $\delta = \left\| \sum_k \dot{\alpha}_k \hat{O}_k |\rho\rangle\!\rangle - \hat{\mathcal{L}} |\rho\rangle\!\rangle \right\|_2^2$ Hilbert-Schmidt norm $\|\hat{A}\|_2^2 = \mathrm{Tr}|\hat{A}|^2 = \sum_{ij} |A_{ij}|^2$

with respect to $\dot{\alpha}_k$, using VMC sampling.

[see, e.g., M. Hartmann, G. Carleo, PRL 122, 250502 (2019)

alternative approaches are proposed in:

A. Nagy, V. Savona, PRL 122, 250501 (2019)

F. Vicentini, A. Biella, N. Regnault, C. Ciuti, PRL 122, 250503 (2019)

N. Yoshioka, R. Hamazaki, PRB 99, 214306 (2019)