Simulation of Mixed and Thermal States of One-dimensional Quantum Systems

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Introduction & Motivation

- Study properties of many-body quantum systems out-of-equilibrium with interaction to an environment
- Study static and dynamic properties of thermal states
  - Thermalization
  - Entanglement

Introduction & Motivation

Timeline:

Cazalilla, Marston
PRL 88, 256403 (2002)

Luo, Xiang, Wang
PRL 91, 049701 (2003)

Vidal
PRL 91, 147902 (2003)

Vidal
PRL 93, 040502 (2004)

White, Feiguin
condmat/0403310 (2004)

Daley, Kollath, Schollwöck, Vidal
J. Stat. Mech.: Theor. Exp. P04005 (2004)

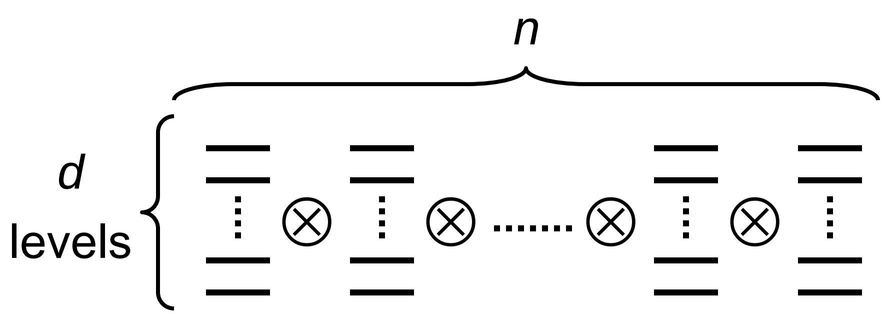
Schmitteckert
condmat/0403759 (2004)

Verstraete, Garcia-Ripoll, Cirac
condmat/0406426 (2004)

Zwolak, Vidal
condmat/0406440 (2004)

Introduction & Motivation

Starting point – one-dimensional quantum lattice systems:



with Master equation evolution

$$\dot{\rho}(t) = -i[H, \rho(t)] + \Omega[\rho(t)]$$

where H is the Hamiltonian and Ω describes some interaction to an environment

Introduction & Motivation

Interested in Hamiltonians with on-site and nearest neighbor interaction

Ex.:

- Bose-Hubbard model $H = -J\sum_l \left(b_l^\dagger b_{l+1} + h.c.\right) + \frac{U}{2}\sum_l n_l\left(n_l - 1\right) + \sum_l \varepsilon_l n_l$
- Heisenberg model $H = -B\sum_l \sigma_l^z + J\sum_l \vec{\sigma}_l \cdot \vec{\sigma}_{l+1}$

and interaction to the environment with on-site or nearest neighbor terms

Ex.:

- Dephasing $\Omega[\rho] = \gamma\sum_l \left(n_l \rho n_l - \frac{1}{2}\rho n_l^2 - \frac{1}{2}n_l^2 \rho\right)$ Environmental interaction destroys superpositions
- Amplitude Damping $\Omega[\rho] = \gamma\sum_l \left(a_l \rho a_l^\dagger - \frac{1}{2}\rho a_l^\dagger a_l - \frac{1}{2}a_l^\dagger a_l \rho\right)$ Particle losses

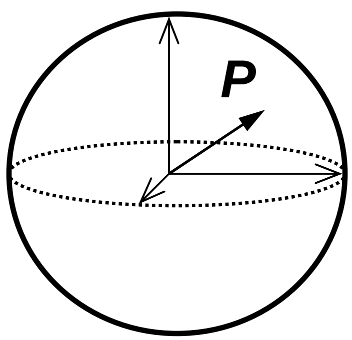
Outline

- Mixed States
- Matrix product decomposition for operators
  - Compact description of a mixed state
  - Efficient update of the decomposition
- Examples
  - Construction of thermal states
  - Mixed state simulation

Mixed States

- Take the basic description of a state as the density matrix ρ instead of the wavefunction

- As an example, the state ρ of any single spin (or any two level system) can be described by a vector ***P*** <u>in</u> the Bloch Sphere



$$\rho = \frac{1}{2}\left(\mathbf{I} + \boldsymbol{P}\cdot\boldsymbol{\sigma}\right)$$
$$= \frac{1}{2}\left(\mathbf{I} + P_x\sigma_x + P_y\sigma_y + P_z\sigma_z\right)$$

Mixed State - expansion

- For more than one spin (or lattice site), we can expand any density matrix in terms of a Pauli matrix basis (plus the identity) for each spin

$$\rho = \sum_{\mu_1 \cdots \mu_n} a_{\mu_1 \cdots \mu_n} \mu_1 \otimes \cdots \otimes \mu_n$$

$$\mu_i \in \{ \mathrm{I}, \sigma_x, \sigma_y, \sigma_z \}$$

- Thus, we can treat the density matrix itself as a vector and therefore we can have an equivalent description to the *Matrix Product State*

G. Vidal, quant-ph/0301063

Matrix Product Decomposition

- Pure State → Matrix Product State

$$\left|\Psi\right\rangle = \sum_{i_1,\ldots,i_n} \mathrm{Tr}\left(A_1^{i_1}\cdots A_n^{i_n}\right)\left|i_1\right\rangle \otimes\cdots\otimes\left|i_n\right\rangle$$

- Mixed State → Matrix Product Decomposition

$$\rho = \sum_{\mu_1,\ldots,\mu_n} \mathrm{Tr}\left(B_1^{\mu_1}\cdots B_n^{\mu_n}\right)\mu_1 \otimes\cdots\otimes \mu_n \qquad \mu_i \in \left\{\mathrm{I},\sigma_x,\sigma_y,\sigma_z\right\}$$

- For example, the completely mixed state needs only one term in the decomposition

$$\rho = \frac{I\otimes I\otimes\cdots\otimes I}{d^n} \Rightarrow \mathrm{Tr}\left(B_1^{\mu_1}\cdots B_n^{\mu_n}\right) = \prod_{\mu_j}\frac{\delta_I^{\mu_j}}{d} \qquad \left(B_j^{u_j} = \frac{\delta_I^{\mu_j}}{d}\right)$$

Simulation

- Given Master equation evolution, it is necessary to apply a (super)operator to ρ to evolve it in time. To first order:

$$\rho(t+\delta t) = \xi_{\delta t}[\rho(t)] = \rho(t) - i[H, \rho(t)]\delta t + \Omega[\rho(t)]\delta t$$

- Given a time-independent Master equation:

$$\dot{\rho}(t) = \mathcal{L}[\rho(t)] \Rightarrow \rho(t) = e^{\mathcal{L}t}\rho(0)$$

$$\left(|\dot{\Psi}(t)\rangle = -iH|\Psi(t)\rangle \Rightarrow |\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle \right)$$

Simulation

- Deal directly with the basis transformation matrices $\left\{B_i^{\mu_i}\right\}$ and use a trotter decomposition on the "time evolution superoperator"

- For local (super)operators on site *l*, only the basis transformation matrix

$$B_l^{\mu_l}$$

needs to be modified

- For nearest neighbor (super)operators on sites *l*,*l*+1, only

$$B_l^{\mu_l} \ , \ B_{l+1}^{\mu_{l+1}}$$

need to be updated, which requires $O(d^6M^3)$ operations (d^4M^2 for sparse matrices)

G. Vidal, PRL 91, 147902

Examples

- Construction of thermal states
- Mixed state evolution with dephasing
- Unequal time correlation functions

For DMRG, the decay of eigenvalues of the reduced density matrix gives an indication of how well the method is working. Here, the decay of eigenvalues of the reduced superoperator serves this purpose.

Construction of thermal states

State in thermal equilibrium:

$$\rho(\beta) = \frac{e^{-\beta H}}{\mathrm{Tr}\left(e^{-\beta H}\right)} = \frac{e^{-\beta H}}{Z}$$

At $\beta = 0$ ($T = \infty$),

$$\rho(0) = \frac{\mathbf{I}}{Z_0} \;,\; Z_0 = d^n$$

so besides normalization, the state $\rho(\beta)$ can be constructed from $\rho(0)$ by imaginary time evolution:

$$\rho(\beta) \propto e^{-\beta H} = \left(e^{-H\delta}\right)^N \mathbf{I} \;,\; N\delta = \beta$$

Construction of thermal states

Many applications
of
$e^{-H\delta}$
$\Rightarrow$

$\beta = 0$ (T = ∞)

Matrix Product Decomposition of the Completely Mixed State

$\beta \rightarrow \infty$ (T→0)

Approach ground state

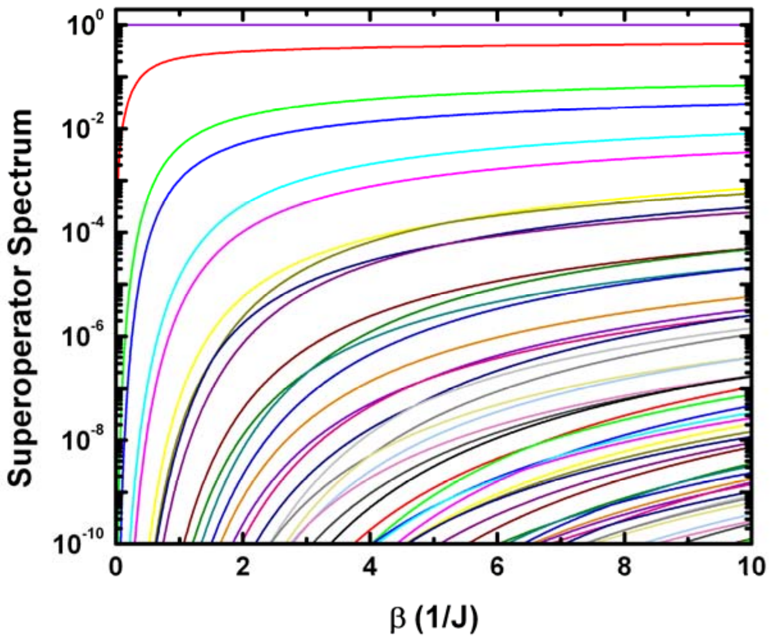
For each application of $e^{-H\delta}$ use trotter expansion to get the superoperators to be a series of on-site and nearest neighbor terms

Construction of thermal states

- Example: Critical Ising Chain (n=100)

$$H = \sum_{l=1}^{n-1} \sigma_l^x \otimes \sigma_{l+1}^x + \sum_{l=1}^{n} \sigma_l^z$$

- Superoperator spectrum for half the chain



- Rapid decay of eigenvalues
- (~50 ev's shown, M=80, which goes down to 10^{-13})

Mixed State Evolution

- Consider a fermionic system evolving according to

$$\dot{\rho}(t) = -i[H(t), \rho(t)] + \gamma \sum_l \left(n_l \rho(t) n_l - \frac{1}{2} \rho(t) n_l^2 - \frac{1}{2} n_l^2 \rho(t) \right)$$

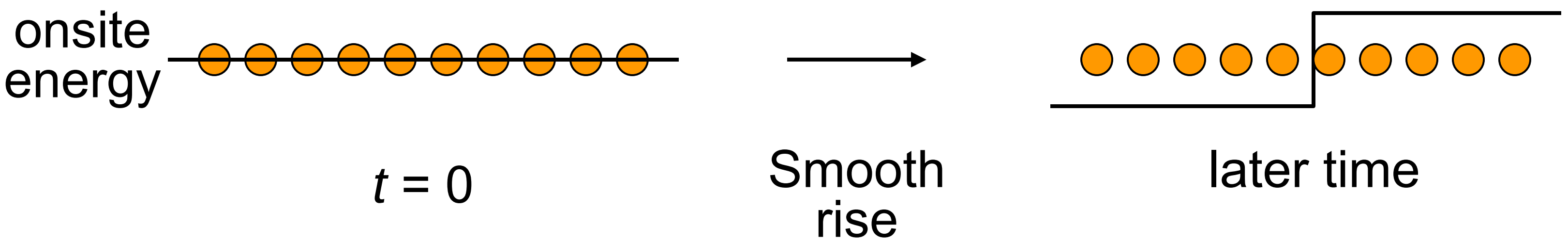
  The dephasing interaction tends to destroy states in superpositions
- Time-dependent Hamiltonian:

$$H(t) = -J \sum_{l=1}^{n-1} (a_l^\dagger a_{l+1} + h.c.) - \mu(t) \left\{ \sum_{l=1}^{n/2} n_l - \sum_{l=n/2+1}^{n} n_l \right\}$$

  with 100 lattice sites at half-filling (and J=1,γ=0.4)

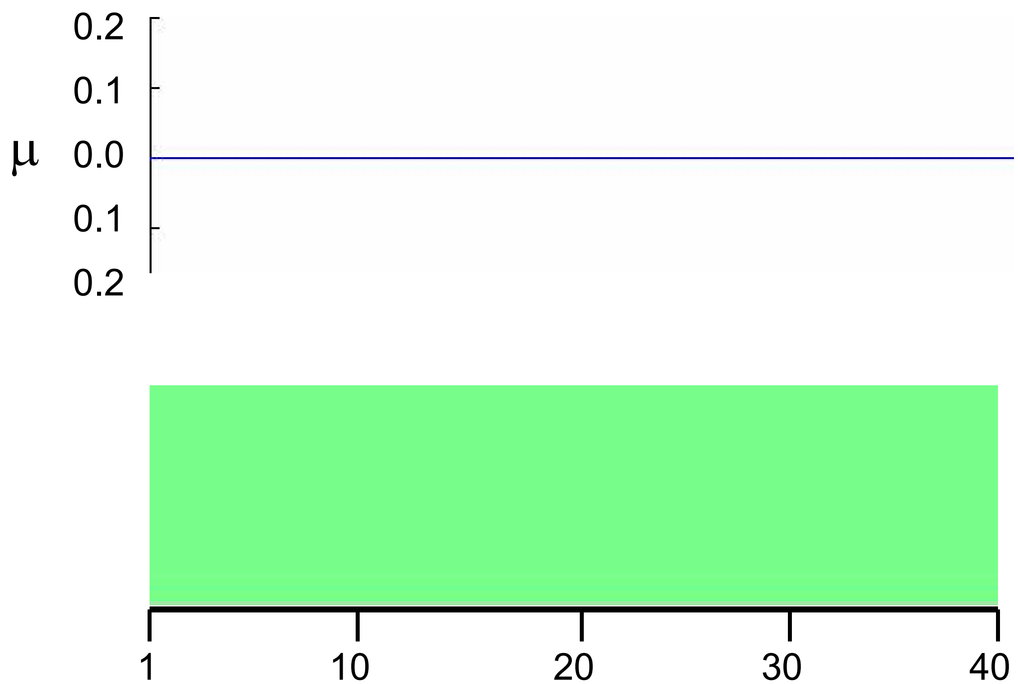
Mixed State Evolution

$\mu(t)$:



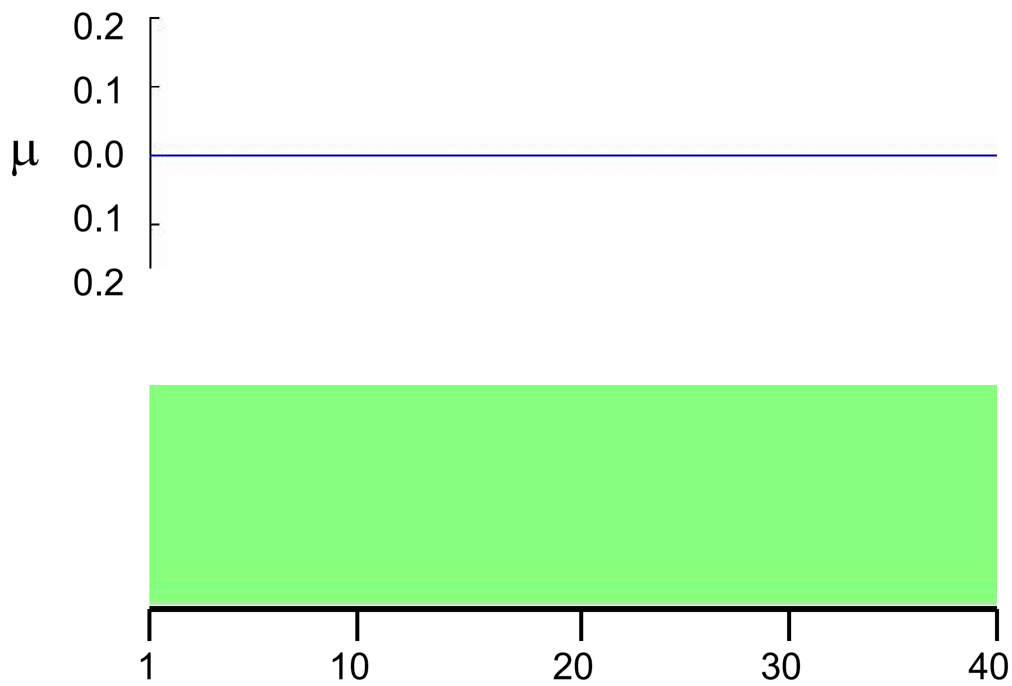
$\mu(t)$ will drive current from right to left side of the lattice

Mixed State Evolution



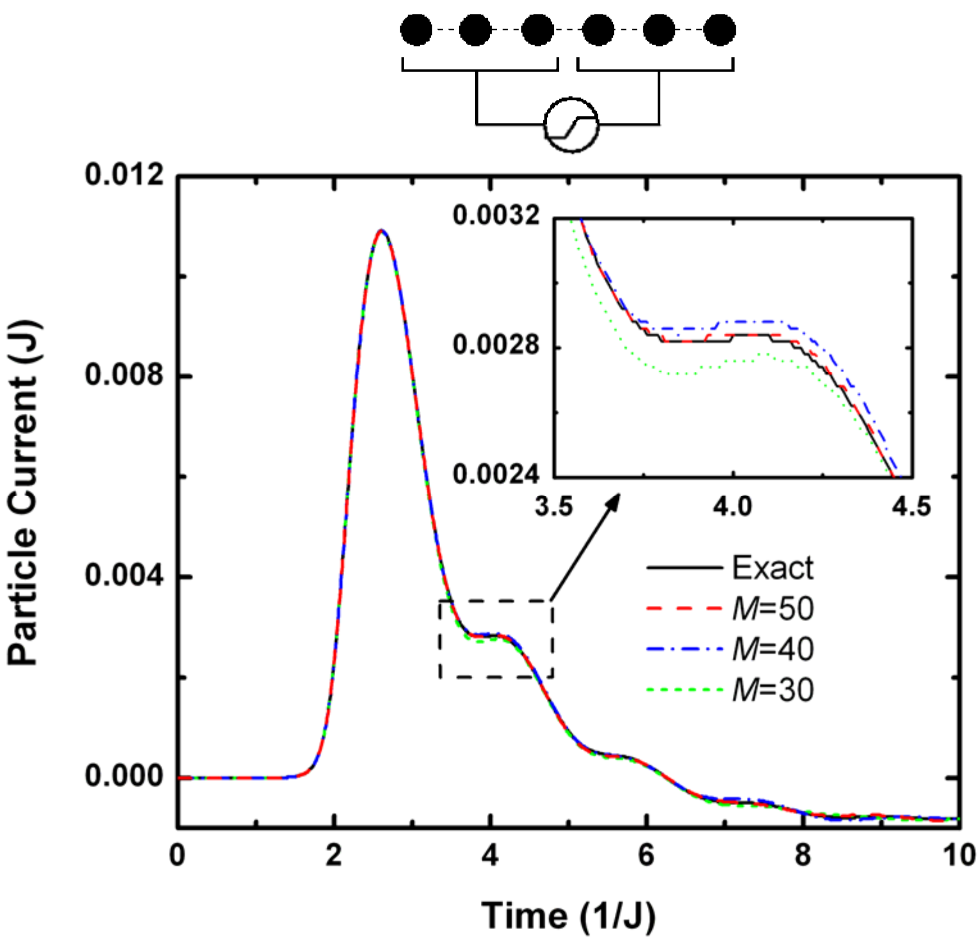
http://mike.zwolak.org/dmrg/movie1.mpg , http://mike.zwolak.org/dmrg/movie2.mpg

Mixed State Evolution



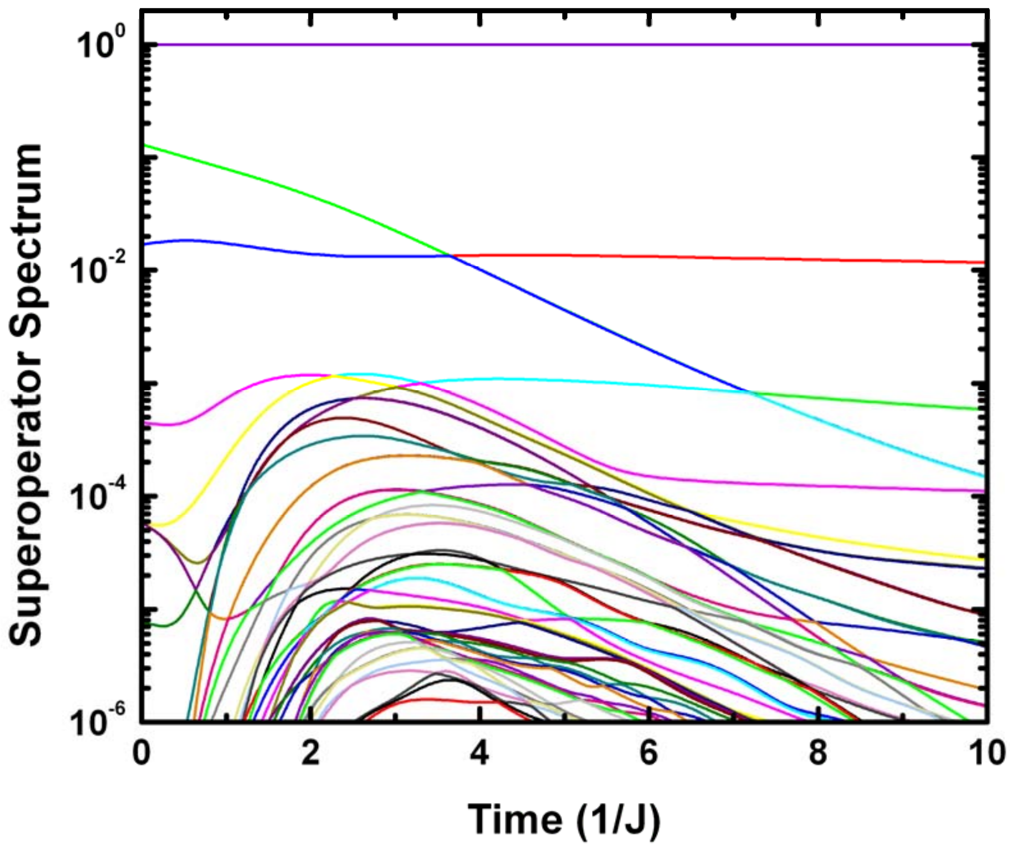
http://mike.zwolak.org/dmrg/movie3.mpg

Mixed State Evolution



M necessary for convergence is small

Mixed State Evolution



- Spectrum for *M*=50
- Eigenvalues decay exponentially

Unequal-Time Correlation Functions

Excitations propagating through the system: need unequal time correlation functions

For instance, if we destroy a fermion on one side of the chain, the correlation function

$$\left\langle a_l^\dagger(t) a_1(0) \right\rangle$$

will describe how this “hole” propagates

Unequal-Time Correlation Functions

Given the initial density matrix as a Matrix Product Decomposition

$$\rho = \rho(t = 0)$$

Act on state with a_1 at t=0

$$a_1 \rho$$

Evolve this operator to time t

$$\xi_t\left[a_1 \rho\right]$$

Act on state with $a_1^\dagger$ at time t, and compute trace

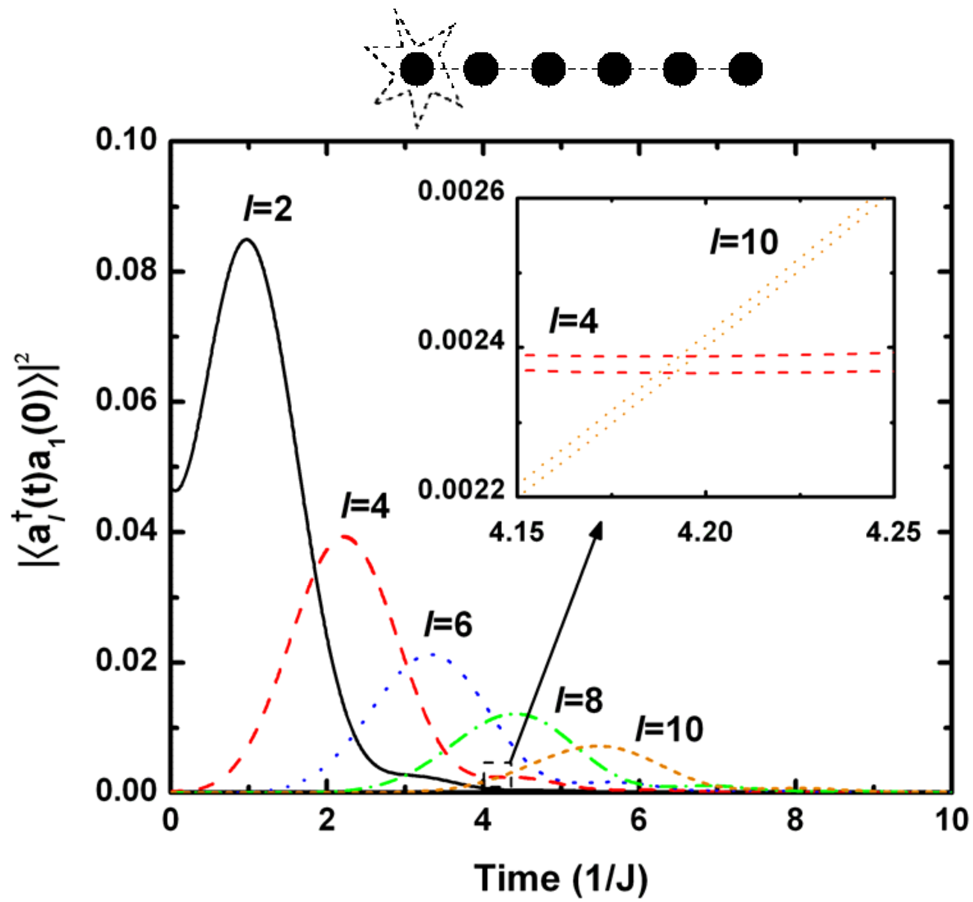
$$\left\langle a_l^\dagger(t) a_1(0) \right\rangle = \mathrm{Tr}\left(a_l^\dagger \xi_t\left[a_1 \rho\right]\right)$$

This prescription is general for any two operators

Unequal-Time Correlation Functions

$$H(t) = -J\sum_{l=1}^{n-1}(a_l^\dagger a_{l+1} + h.c.)$$

- Master Equation with dephasing (γ=0.4)
- Destroy (spinless) fermion at site 1, watch propagation
- *M*=40,50 shown in figure



Unequal-time correlation functions

Master Equation with no dephasing (γ=0.0)

http://mike.zwolak.org/dmrg/movie4.mpg

Conclusions

- The Matrix Product State can be generalized to the Matrix Product Decomposition
  - Gives a compact description of a mixed state
  - This decomposition can be efficiently updated after an application of a local operator (superoperator) allowing for simulation of real time evolution
- Simulation can be used to construct thermal states or evolve a state in time with interaction to an environment

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