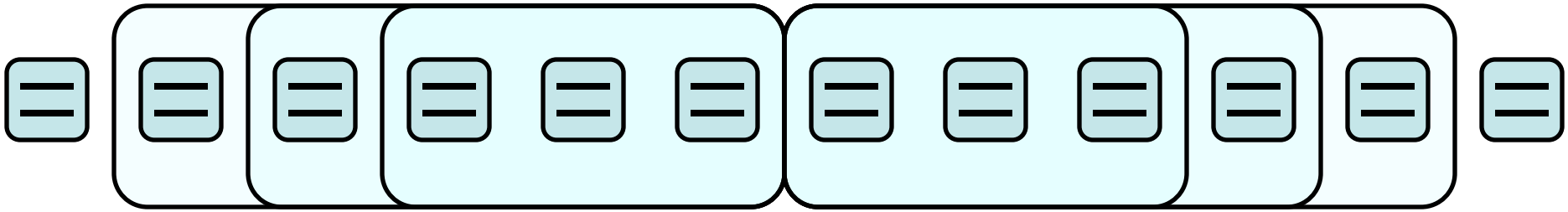
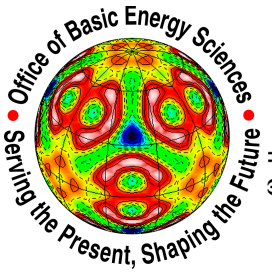
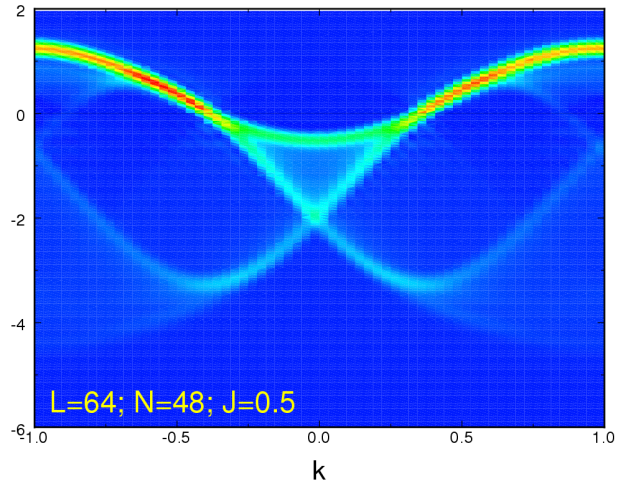
The time-dependent DMRG and its applications

Adrian Feiguin







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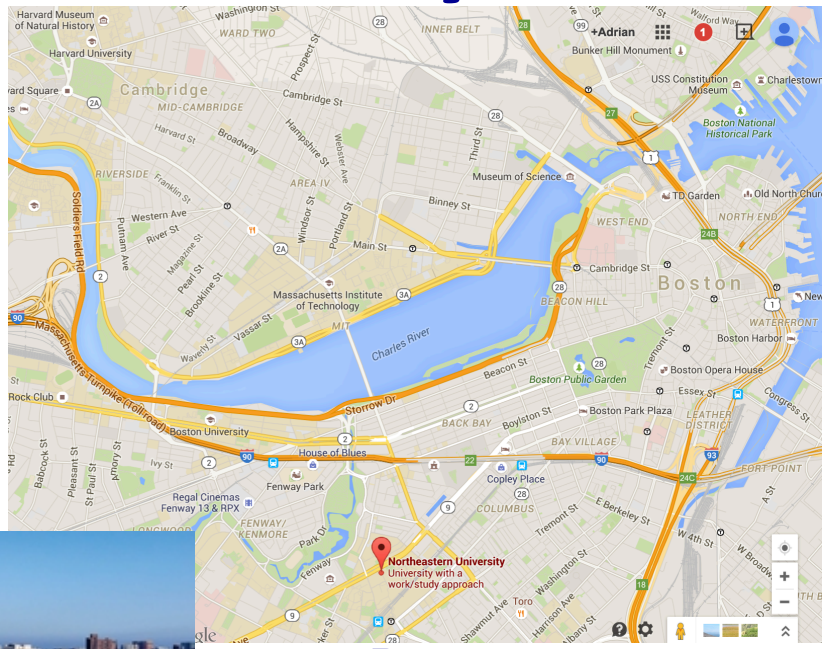


Boston

Some literature

- G. Vidal, PRL 93, 040502 (2004)
- S.R.White and AEF, PRL 93, 076401 (2004)
- Daley et al, J. Stat. Mech.: Theor. Exp. P04005 (2004)
- AEF and S.R.White, PRB 020404 (2005)
- U. Schollwoeck and S.R. White, arXiv:cond-mat/0606018
- AEF, Vietri school lecture notes (AIP proceedings)
- AEF, “Strongly correlated systems: Numerical methods”, Springer.

Solving the t-d Schrödinger Equation

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = H\left|\Psi(t)\right\rangle \rightarrow \left|\Psi(t)\right\rangle = e^{-itH}\left|\Psi(t=0)\right\rangle$$

Let us assume we know the eigenstates of H

$$\left|\Psi(t=0)\right\rangle = \sum_n c_n\left|\psi_n\right\rangle$$

$$\left|\Psi(t)\right\rangle = e^{-itH}\left|\Psi(t=0)\right\rangle \rightarrow \left|\Psi(t)\right\rangle = \sum_n c_n e^{-itE_n}\left|\psi_n\right\rangle$$

In reality, we work in some arbitrary basis

$$\left|\Psi(t=0)\right\rangle = \sum_k d_k\left|\varphi_k\right\rangle$$

$$\rightarrow \left|\Psi(t)\right\rangle = \sum_k d_k e^{-itH}\left|\varphi_k\right\rangle$$

$$= \sum_k d_k \sum_n a_{kn} e^{-itE_n}\left|\psi_n\right\rangle$$

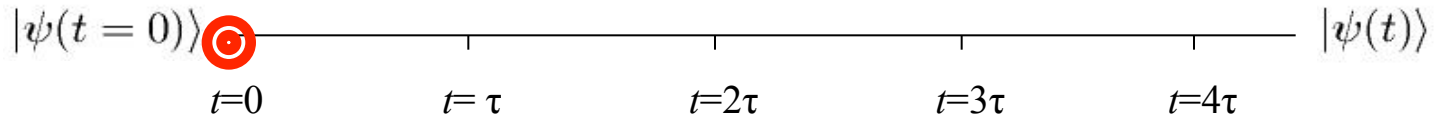
$$= \sum_k d_k(t)\left|\varphi_k\right\rangle \text{ with } d_k(t) = d_k\sum_n a_{kn}e^{-itE_n}$$

Mixture of excited states with oscillating terms with different frequencies

Typically we avoid high freq. oscillations by adding a phase $e^{-itH} \rightarrow e^{-it(H-E_0)}$

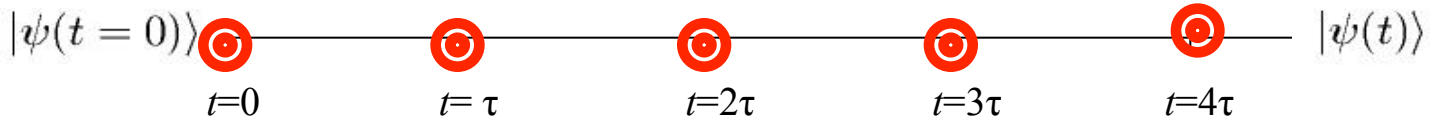
Time evolution and DMRG: First attempts

- Cazalilla and Marston, PRL 88, 256403 (2002) use the infinite system method to find the ground state, and evolved in time using this fixed basis without sweeps. This is not quasi-exact. However, they found that works well for transport in chains for short to moderate time intervals.



- Luo, Xiang and Wang, PRL 91, 049901 (2003) showed how to target correctly for real-time dynamics. They target

$$\psi(t{=}0),\ \psi(t{=}\tau)\ ,\ \psi(t{=}2\tau)\ ,\ \psi(t{=}3\tau)\ldots$$



This is quasiexact as $\tau \to 0$ if you add sweeping.

The problem with this idea is that you keep track of all the history of the time-evolution, requiring large number of states m. It becomes highly inefficient.

The Density Matrix Renormalization Group. "Classical" analogy

Image compression algorithms (e.g. Jpeg)

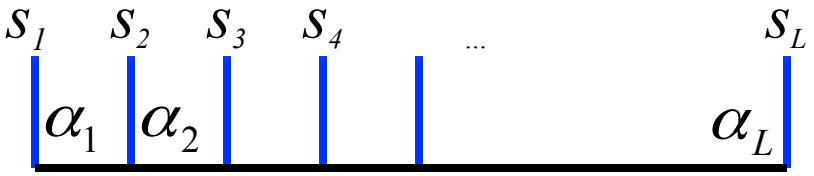
We want to achieve "lossless compression"
… or at least minimize *the loss of information*

Density Matrix Renormalization Group

A variational method that follows the principles of exact diagonalization and NRG.

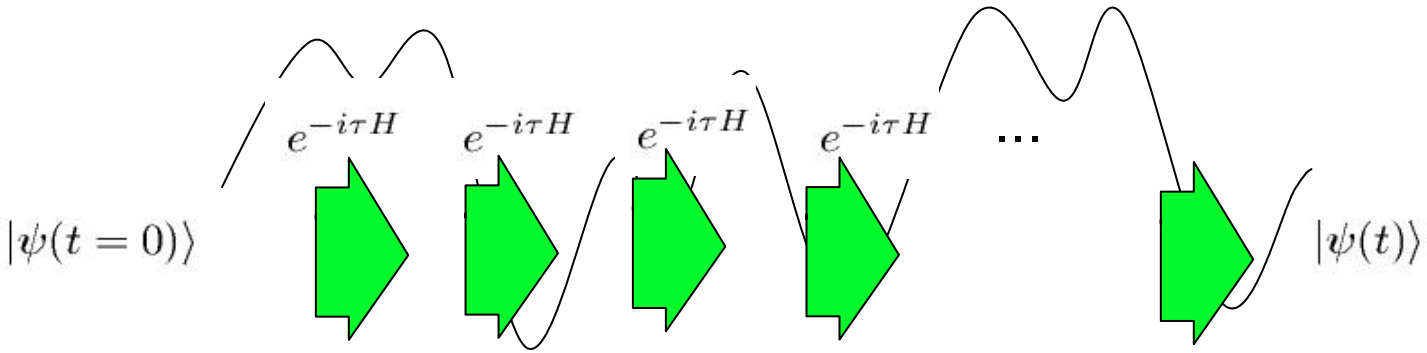
- *Similar capabilities as exact diagonalization, but able to study larger systems.*
- *Yields variational solution in the form of a matrix-product state.*

$$|\psi\rangle = \sum_{\{s\}} A[s_1]_{\alpha_1} A[s_2]_{\alpha_1,\alpha_2} \ldots A[s_2]_{\alpha_{L-1},\alpha_L} A[s_L]_{\alpha_L} \, | \, s_1 \ldots s_L \rangle$$

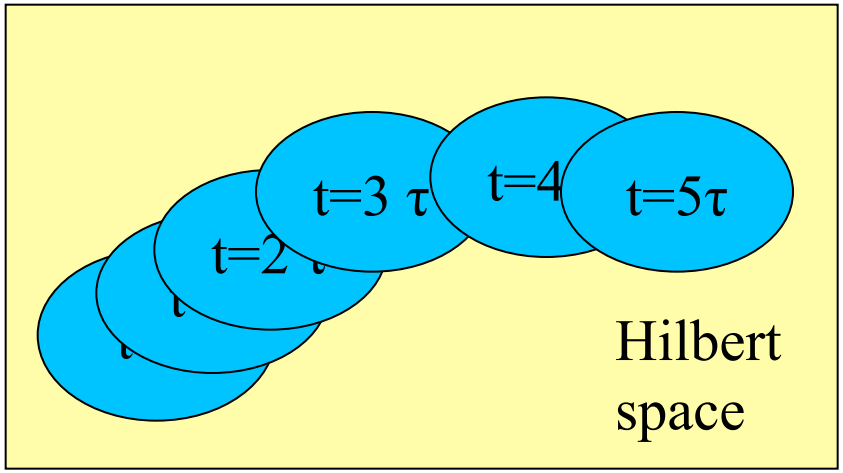


- *No a-priori assumptions about the physics.*
- *Can calculate properties of very large systems (1D and quasi-2D) with unprecedented accuracy.*
- *Results are variational, but "quasi-exact": Accuracy is finite, but under control*

Adaptive Time-dependent DMRG:



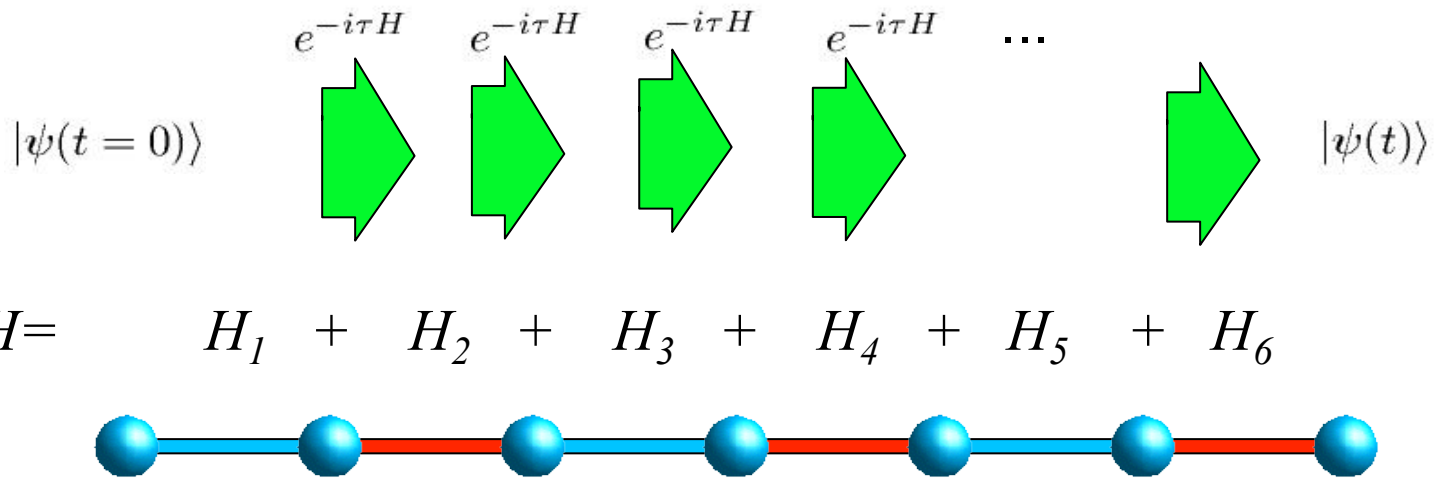
In a truncated basis:



We need to "follow" the state in the Hilbert space adapting the basis at every step

S.R.White and AEF, PRL (2004), Daley et al, J. Stat. Mech.: Theor. Exp. (2004); AEF and S.R.White, PRB (2005), Rapid Comm. Based on TEBD ideas by G. Vidal, PRL (94).

Evolution operator



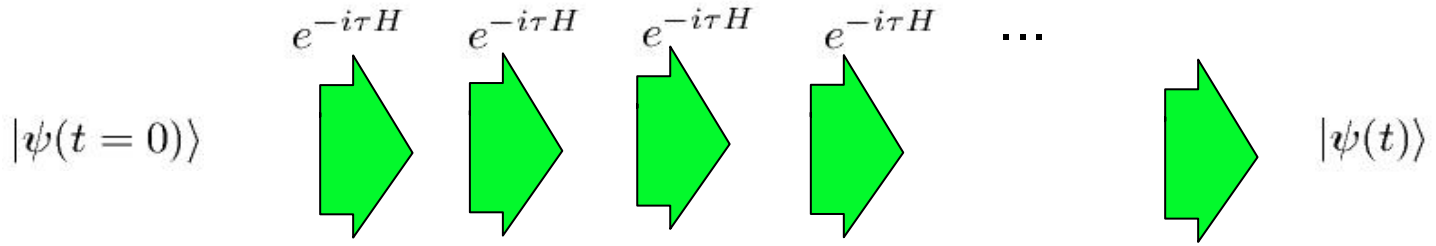
We would feel tempted to do something like:

$$e^{-i\tau H} = e^{-i\tau(H_1+H_2+H_3+H_4\ldots)} \approx e^{-i\tau H_1} e^{-i\tau H_2} e^{-i\tau H_3} e^{-i\tau H_4} \ldots$$

But it turns out that $e^{-i\tau(H_1+H_2)} \neq e^{-i\tau H_1} e^{-i\tau H_2}$ because $[H_1, H_2] \neq 0$

This actually would give you an error of the order of τ^2, similar to a 1st order S-T expansion…

Suzuki-Trotter approach



$$H = H_1 + H_2 + H_3 + H_4 + H_5 + H_6$$

$$H_A = H_2 + H_4 + H_6$$

$$H_B = H_1 + H_3 + H_5$$

$$e^{-i\tau(H_A+H_B)} = e^{-i\tau H_A} e^{-i\tau H_B} e^{i\frac{\tau^2}{2}[H_A,H_B]} = e^{-i\tau H_A} e^{-i\tau H_B} e^{O(\tau^2)}$$

Suzuki-Trotter expansions

We want to write

$$e^{(A+B)h+C_2h^2+C_3h^3+C_4h^4+O(h^5)} = \prod_{p=1}^{P} e^{a_pAh} e^{b_pBh}$$

with $C_2 = \alpha(\{a_p, b_p\})[A, B]$;

$$C_3 = \beta(\{a_p, b_p\})[A,[A,B]] + \gamma(\{a_p, b_p\})[B,[B,A]]$$

We want to choose the a's and b's such that they kill the first K coefficients C_K, minimizing the number of factors P for a given order, to obtain

$$e^{(A+B)h+O(h^{K+1})} = \prod_{p=1}^{P} e^{a_pAh} e^{b_pBh}$$

We will impose the conditions that the operators enter symmetrically in the decomposition and $\sum_p a_p = \sum_p b_p = 1.$

I.P Omelyan et al., Comp. Phys. Commmun. 146, 188 (2002) and references therein.

Suzuki-Trotter expansions

First order:

$$e^{(A+B)h+O(h^2)} = e^{Ah}e^{Bh}$$

Second order:

$$e^{(A+B)h+\alpha(a,b)[A,B]h^2+O(h^3)} = e^{aAh}e^{bBh}e^{(1-a)Ah}e^{(1-b)Bh}$$

$$e^{aAh}e^{bBh}e^{(1-a)Ah}e^{(1-b)Bh} \approx e^{(aA+bB)h}e^{((1-a)A+(1-b)B)h}$$

$$\approx e^{(A+B)h+\frac{1}{2}ab[A,B]h^2+\frac{1}{2}(1-a)(1-b)[A,B]h^2+\frac{1}{2}a(1-b)[A,B]h^2-\frac{1}{2}(1-a)b[A,B]h^2}$$

$$= e^{(A+B)h+(ab-b+1/2)[A,B]h^2}$$

We kill the second order term by choosing a=1/2; b=1

$$e^{(A+B)h+O(h^3)} = e^{Ah/2}e^{Bh}e^{Ah/2}$$

Suzuki-Trotter expansions

Fourth order:

$$e^{(A+B)h+O(h^5)} = e^{a_1 Ah} e^{b_1 Bh} e^{a_2 Ah} e^{b_2 Bh} e^{a_2 Ah} e^{b_3 Bh} e^{(1-a_1-a_2-a_3)Ah} e^{(1-b_1-b_2-b_3)Bh}$$

One solution (the most convenient expression) has the form (Forest-Ruth formula)

$$e^{(A+B)h+O(h^5)} = e^{Ah\theta/2} e^{B\theta h} e^{(1-\theta)Ah/2} e^{(1-2\theta)Bh} e^{(1-\theta)Ah/2} e^{\theta Bh} e^{\theta Ah/2}$$

with $\theta = 1/(2-\sqrt[3]{2})$

Evolution using Suzuki-Trotter

1st order Suzuki-Trotter decomposition:

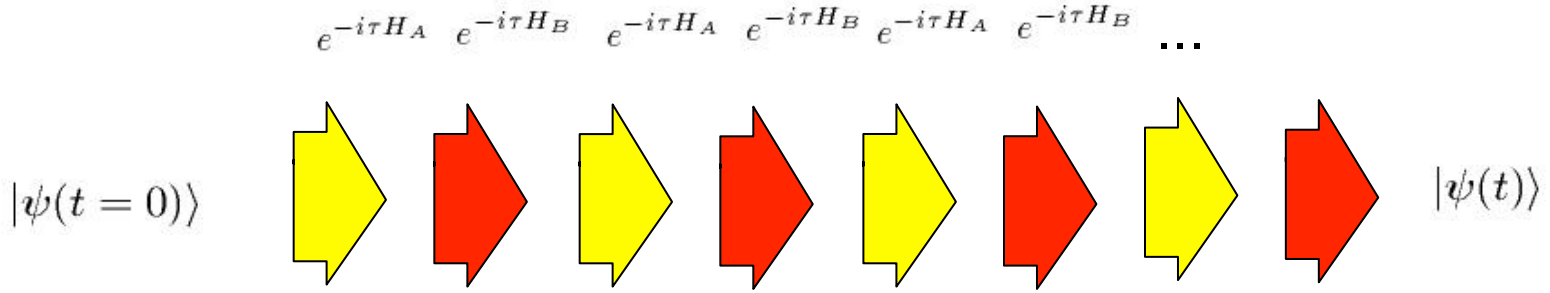
$$e^{-i\tau H} \approx e^{-i\tau H_A} e^{-i\tau H_B}$$

where $H = H_A + H_B$. Here we make A the even bonds and B the odd, 1D only. The individual link-terms $\exp(-i\tau H_j)$ (coupling sites j and $j+1$) within H_A or H_B commute. Thus

$$e^{-i\tau H_B} = e^{-i\tau H_1} e^{-i\tau H_3} e^{-i\tau H_5} \ldots$$

No error introduced!

So the time-evolution operator is a product of individual link terms.
Each link term only involves two-sites interactions => small matrix, easy to calculate!



The two-site evolution operator

Example: Heisenberg model (spins)

$$H = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} \quad \text{with} \quad \vec{S}_i \cdot \vec{S}_{i+1} = S_i^z S_{i+1}^z + \frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right)$$

The two-site basis is given by the states

$$|\sigma\sigma'\rangle = \{|\uparrow\uparrow\rangle; |\uparrow\downarrow\rangle; |\downarrow\uparrow\rangle; |\downarrow\downarrow\rangle\}$$

We can easily calculate the Hamiltonian matrix:

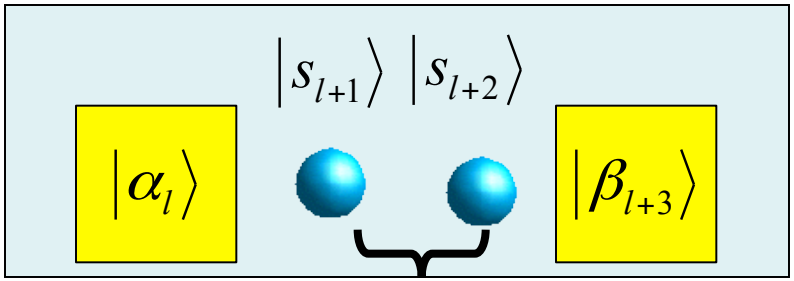
$$H = \begin{pmatrix} 1/4 & & & 0 \\ & -1/4 & 1/2 & \\ & 1/2 & -1/4 & \\ 0 & & & 1/4 \end{pmatrix}$$

Exercise: Exponentiate (by hand) the matrix by following these steps:

1. Diagonalize the matrix and calculate eigenvalues and eigenvectors
2. Calculate the exponential of *H* in the diagonal basis
3. Rotate back to the original basis

Evolving the wave-function

We want to apply the evolution operator between the two central sites:



$e^{-i\tau Hij}$

As we've seen before, the link evolution operator can be written as

$$e^{-itH_{l+1,l+2}} = U^{s_{l+1},s_{l+2}}_{s'_{l+1},s'_{l+2}} \left| s_{l+1} s_{l+2} \right\rangle \left\langle s'_{l+1}\, s'_{l+2} \right|$$

And the wave function after the transformation:

$$e^{-itH_{l+1,l+2}} \left|\psi\right\rangle = \sum_{\alpha_l, s_{l+1}, s_{l+2}, \beta_{l+3}} \varphi(\alpha_l, s_{l+1}, s_{l+2}, \beta_{l+3}) \left|\alpha_l\right\rangle \otimes \left|s_{l+1}\right\rangle \otimes \left|s_{l+2}\right\rangle \otimes \left|\beta_{l+3}\right\rangle$$

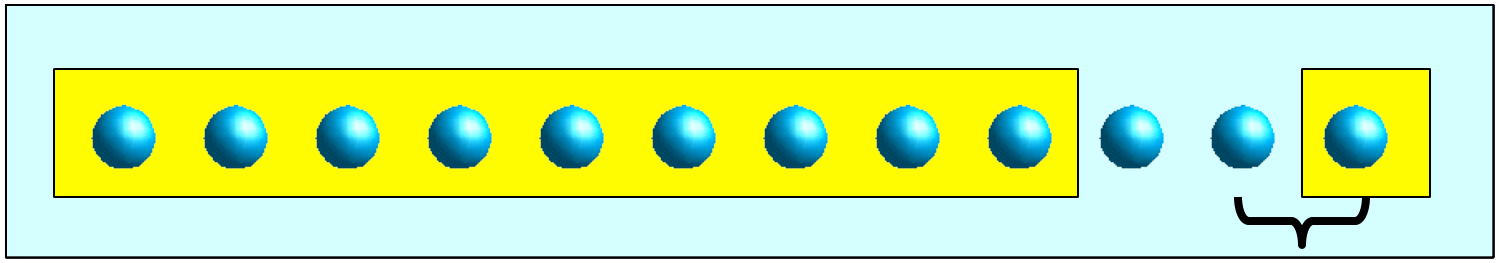
$$\text{with } \varphi(\alpha_l, s_{l+1}, s_{l+2}, \beta_{l+3}) = \sum_{s'_{l+1}, s'_{l+2}} U^{s_{l+1},s_{l+2}}_{s'_{l+1},s'_{l+2}} \psi(\alpha_l, s_{l+1}, s_{l+2}, \beta_{l+3})$$

tDMRG: The algorithm

S.R.White and A.E. Feiguin, PRL (2004), Daley et al, J. Stat. Mech.: Theor. Exp. (2004)

We turn off the diagonalization and start applying the evolution operator

We move to the end to start time-evolution



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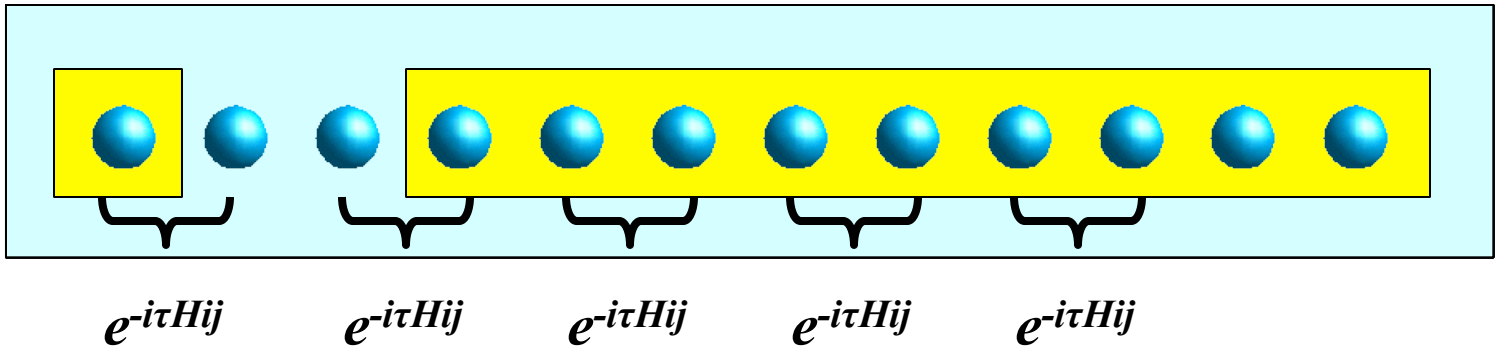


Depending on the S-T break-up, a few sweeps evolve a time step

Each link term only involves two-sites interactions: small matrix, easy to calculate! Much faster than Lanczos!

Time-step targeting method

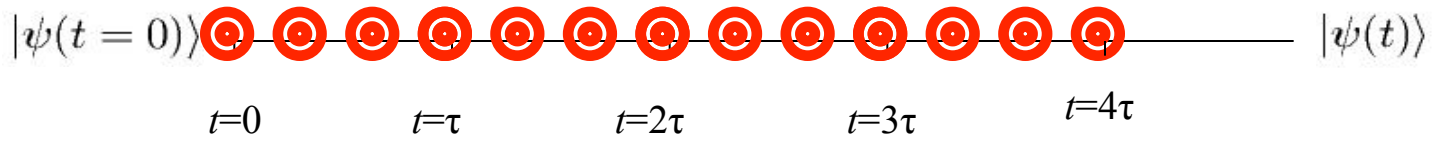
What if we don't have a "nice" Hamiltonian, and S-T cannot be applied

The time-evolution can be implemented in various ways:

1) Krylov basis: Calculate Lanczos (tri-diagonal) matrix, and exponentiate. (time consuming)
2) Runge-Kutta. (non-unitary!)

- We target one time step accurately, then we move to the next step.

- We keep track of intermediate points between t and $t+\tau$



AEF and S. R.White, PRB (05). See also P. Schmitteckert, PRB 70, 121302(2004)

Recall the fourth order Runge-Kutta method for integrating $y'(t) = f(y,t) = f(y)$:

$$k_1 = \tau f(y); \quad k_2 = \tau f(y + k_1/2); \quad k_3 = \tau f(y + k_2/2); \quad k_4 = \tau f(y + k_3);$$

Then

$$y(t+\tau) \approx y(t) + \frac{1}{6}(k_1 + 2(k_2 + k_3) + k_4)$$

Using Mathematica, we find that to $O(\tau^4)$,

$$y(t+\tau/3) \approx y(t) + \frac{1}{162}(31k_1 + 14(k_2 + k_3) - 5k_4)$$

$$y(t+2\tau/3) \approx y(t) + \frac{1}{81}(16k_1 + 20(k_2 + k_3) - 2k_4)$$

The recipe is:

- Each half-sweep is one time step. At each step of the half-sweep, do one RK step, but without advancing $t \to t + \tau$.
- At each step, target $\psi(t)$, $\psi(t + \tau/3)$, $\psi(t + 2\tau/3)$, and $\psi(t + \tau)$.
- At the last step, when the basis fully represents the states of the time step, advance to $t + \tau$ more accurately using 10 RK steps with step $\tau/10$.

Sources of error

- **Suzuki-Trotter error:** Can be controlled by using higher order expansions, or smaller time-steps. If we use a p^{th} order S-T decomposition, the accumulated error after n steps is

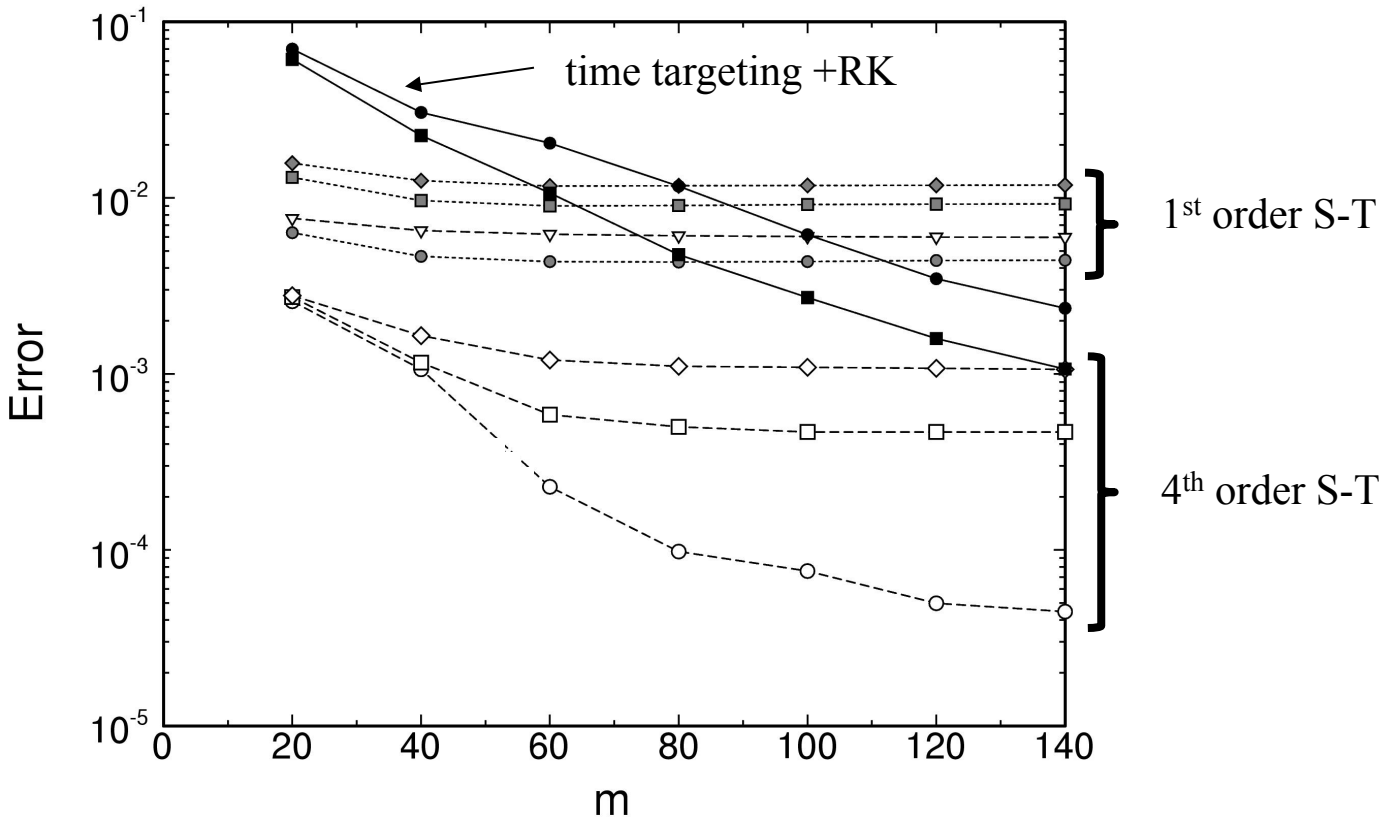
$$\varepsilon(t) = nh^{p+1} = \frac{t}{h} h^{p+1} = th^{p}$$

- **Truncation error:** In principle it can be controlled by keeping more DMRG states as the entanglement grows. Caveat: only works for "well-behaved" problems, since typically the entanglement grows uncontrollably.
- **Runge-Kutta/Krylov:** the error is dominated by the truncation error.

Recipe: instead of fixing the number of states for the simulation, we fix the truncation error, and we let the algorithm determine the optimal number of states… until the basis grows too large and the simulation breaks down. Hopefully this will enable us to go to large times…

S=1 Heisenberg chain (*L*=32; *t*=8)

$$E(t) = \sqrt{\frac{1}{L}\sum_{x=1}^{L}\left(S^z(x,t) - S^z_{Exact}(x,t)\right)^2},$$



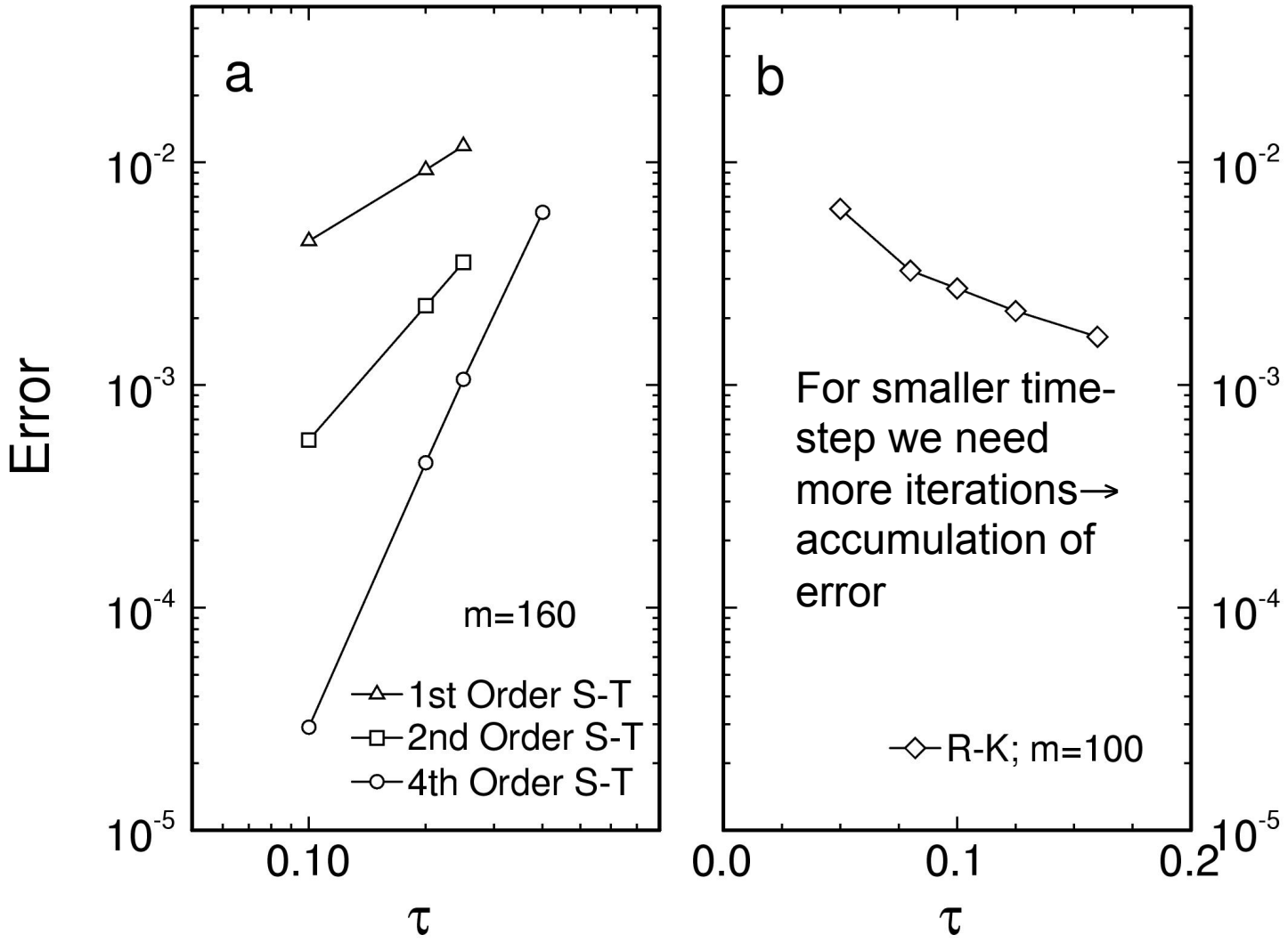


FIG. 3: Error $E(t = 8)$ for the Haldane chain for different time steps τ: a) 1st, 2nd, and 4th order Suzuki-Trotter break-ups and $m = 160$; b) Runge-Kutta and $m = 100$.

Fixed error, variable number of states

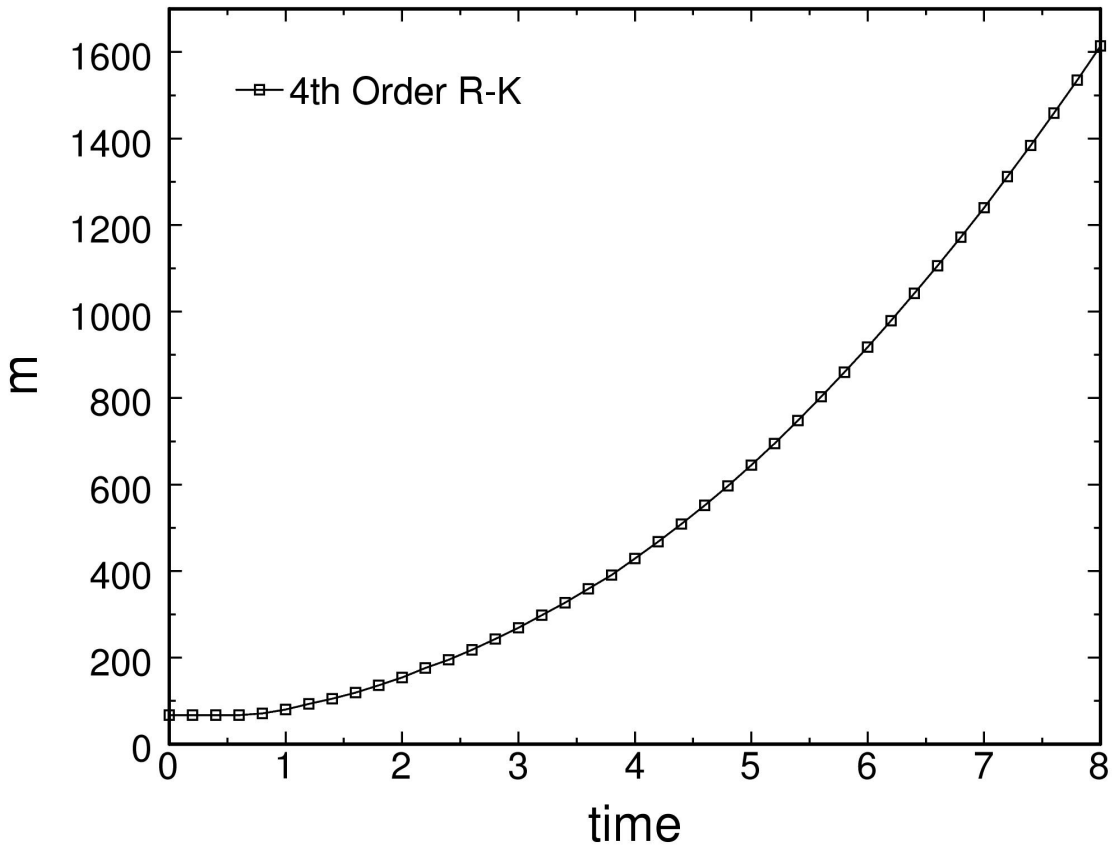


FIG. 4: Number of states required to keep a truncation error of 10^{-8}, as a function of time. The results correspond to a R-K simulation of a Haldane chain with $L = 32$.

Comparing S-T and time step targeting

- S-T is fast and efficient for one-dimensional geometries with nearest neighbor interactions
- S-T error depends strongly on the Trotter error but it can be reduced by using higher order expansions.
- Time step targeting (Krylov,RK) can be applied to ladders and systems with long range interactions
- It has no Trotter error, you can use a larger time-step, but it is more time consuming and you need more DMRG states.
- In RK simulations it is a good practice to do an intermediate sweep without evolving in time to improve the basis.
- Time evolution using RK is non-unitary (dangerous!). Krylov expansion is the right choice.

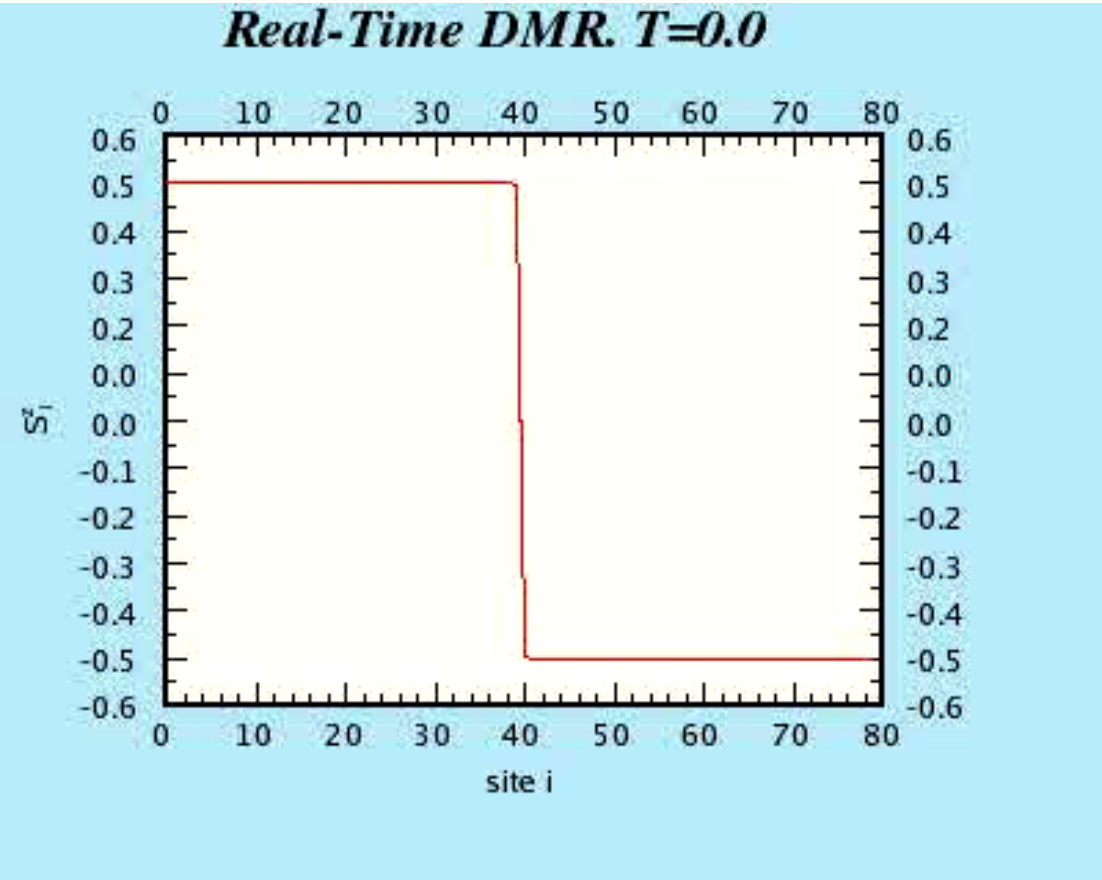
Applications

1. Transport in nano-structures
2. Spectral properties, optical conductivity…
3. Systems driven out of equilibrium, quenches.
4. Time-dependent Hamiltonians.
5. Decoherence: Free induction decay, Hahn echo, Rabi oscillations, pulse sequences…

…

Spin transport

Example: half polarized spin S=1/2 chain



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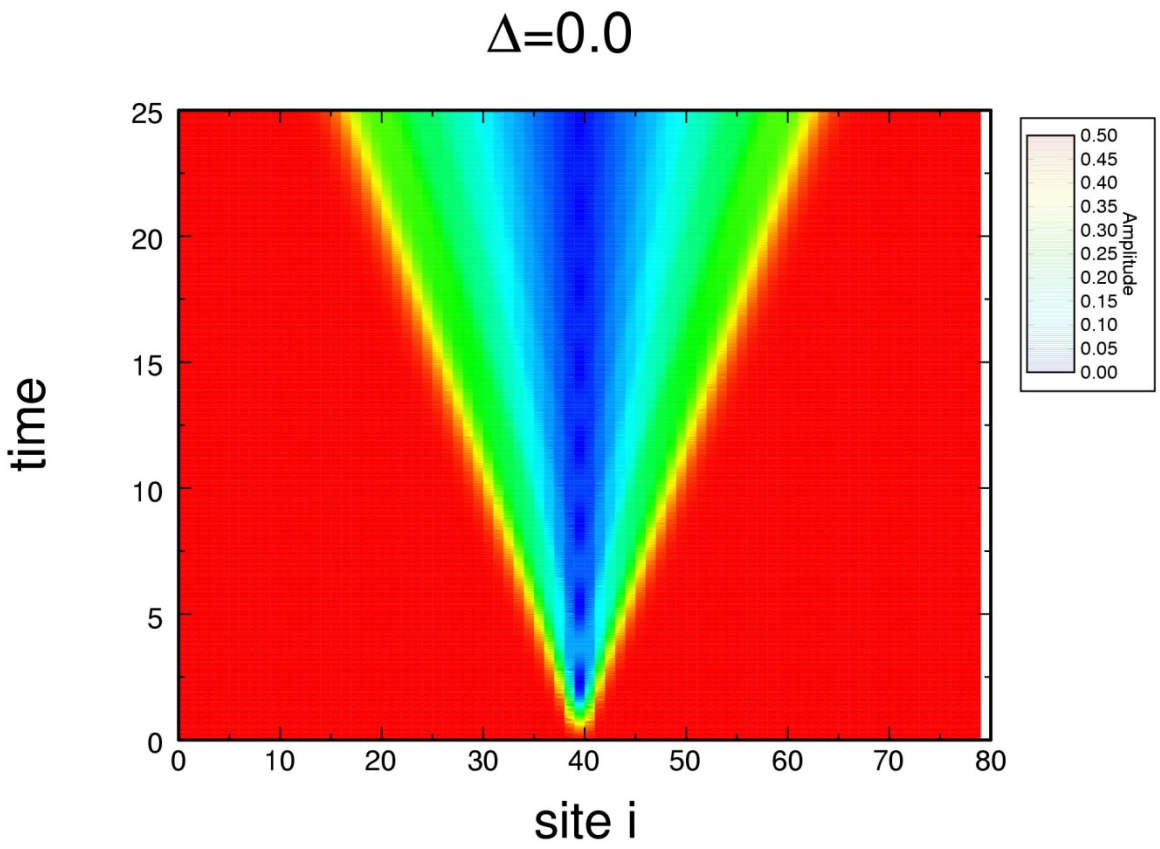


The enemy: Entanglement growth

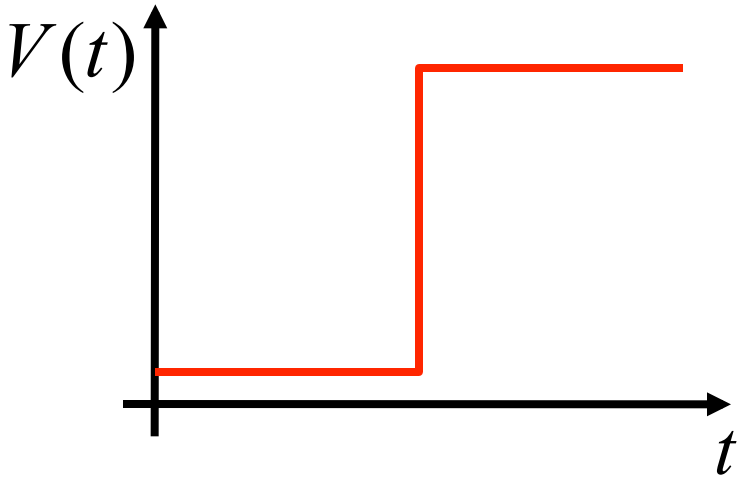
We have seen that the truncation error, or the number of state that we need to keep to control it, depends fundamentally on the entanglement

$$S = S(t)$$

We need to understand this behavior if we want to learn how to fight it!

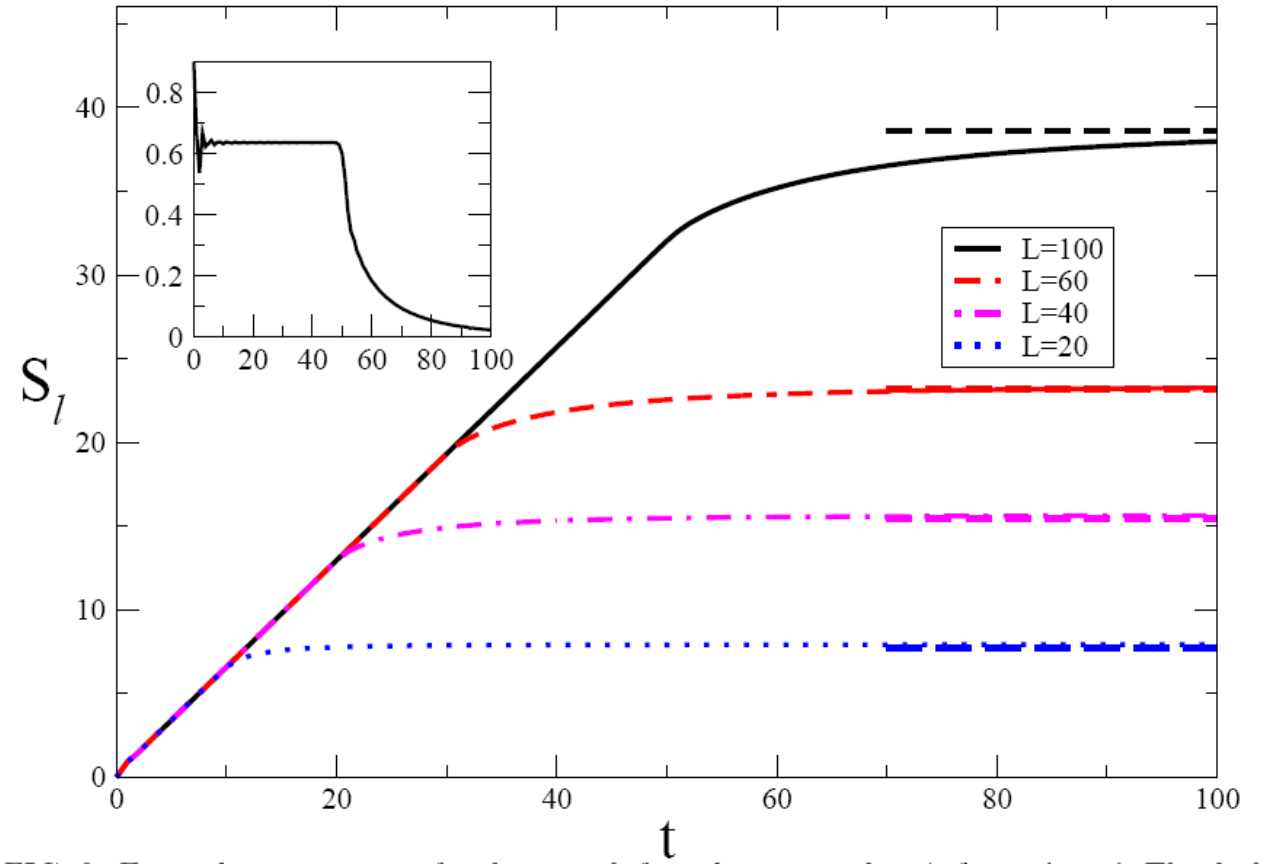
Possible scenarios:

- Global quench
- Local quench
- Periodic quench
- Adiabatic quench
- …



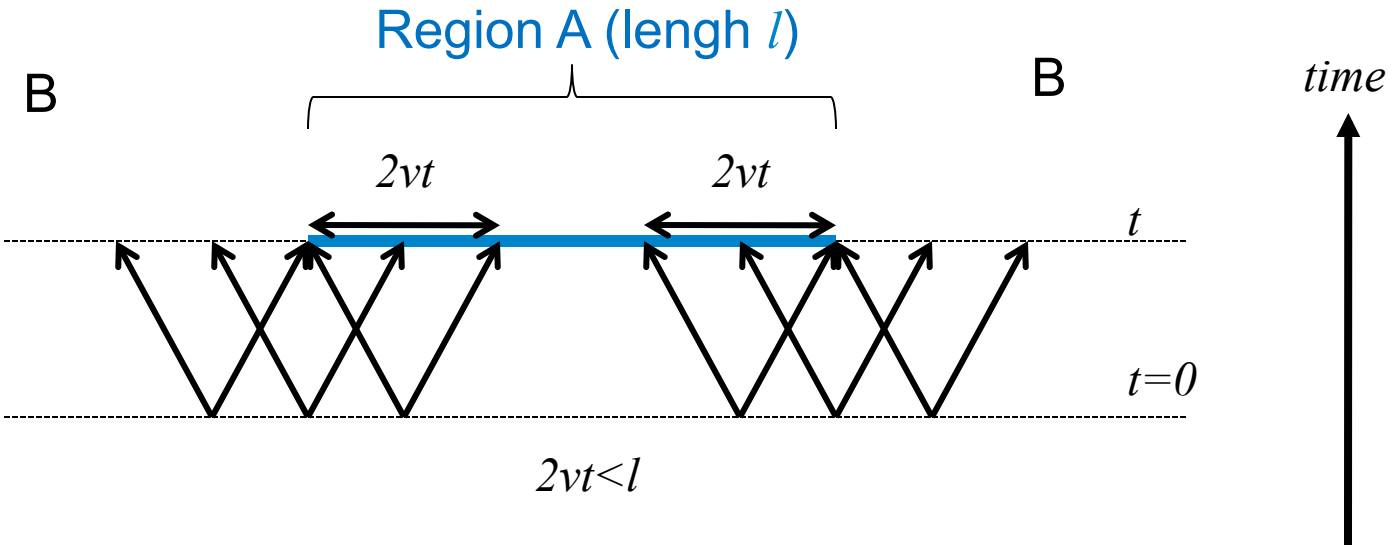
All of a sudden, we are no longer in the ground-state, but some high energy state. Important questions: thermalization vs. integrability

E-growth: global quench



Calabrese and Cardy, JStatM (05)

Global quench: qualitative picture

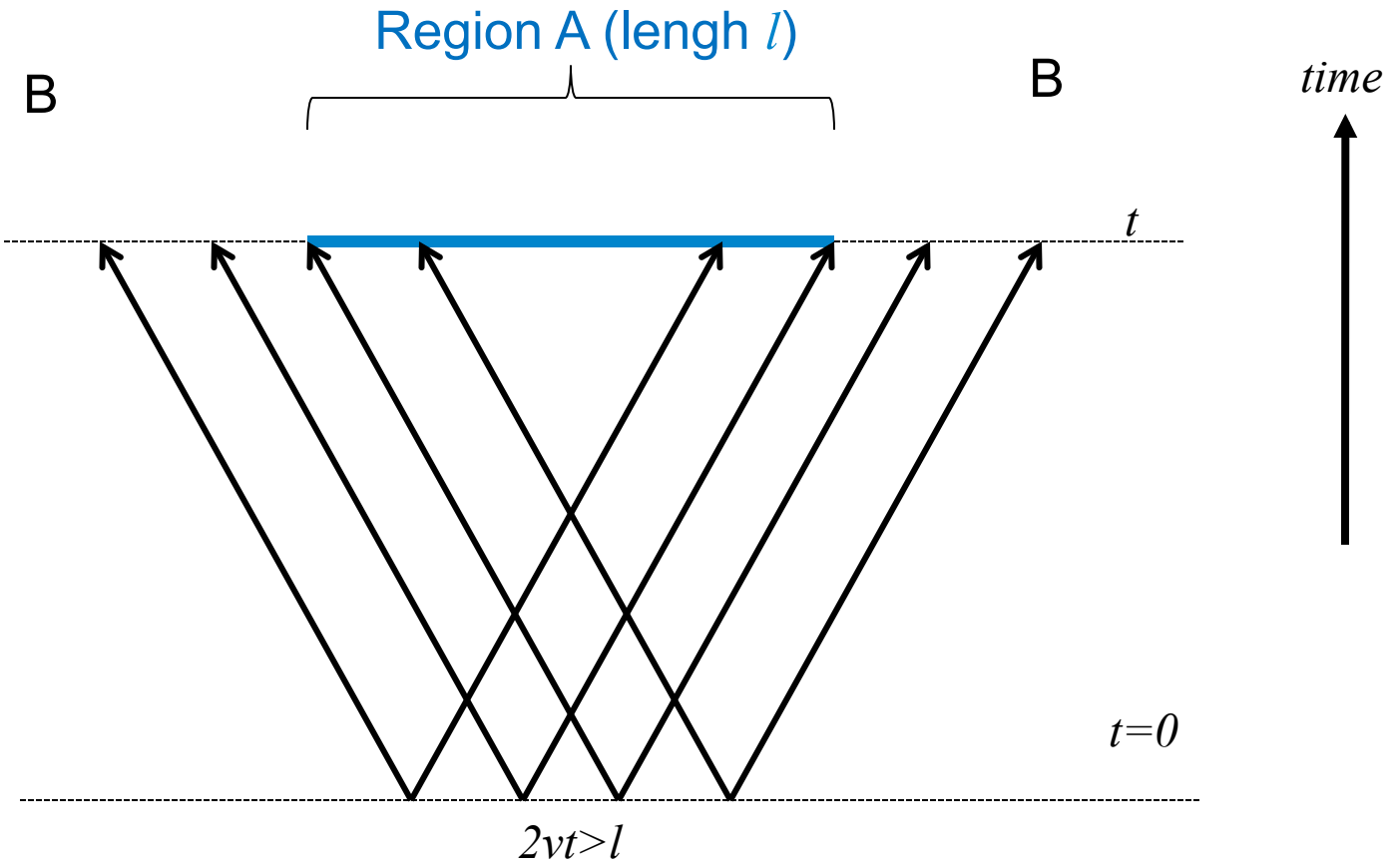


We assume that entangled pairs of quasi-particles are created at t=0, and they propagate with maximum velocity

$$\Rightarrow S = S_0 + ct$$

Calabrese and Cardy, JStatM (05)

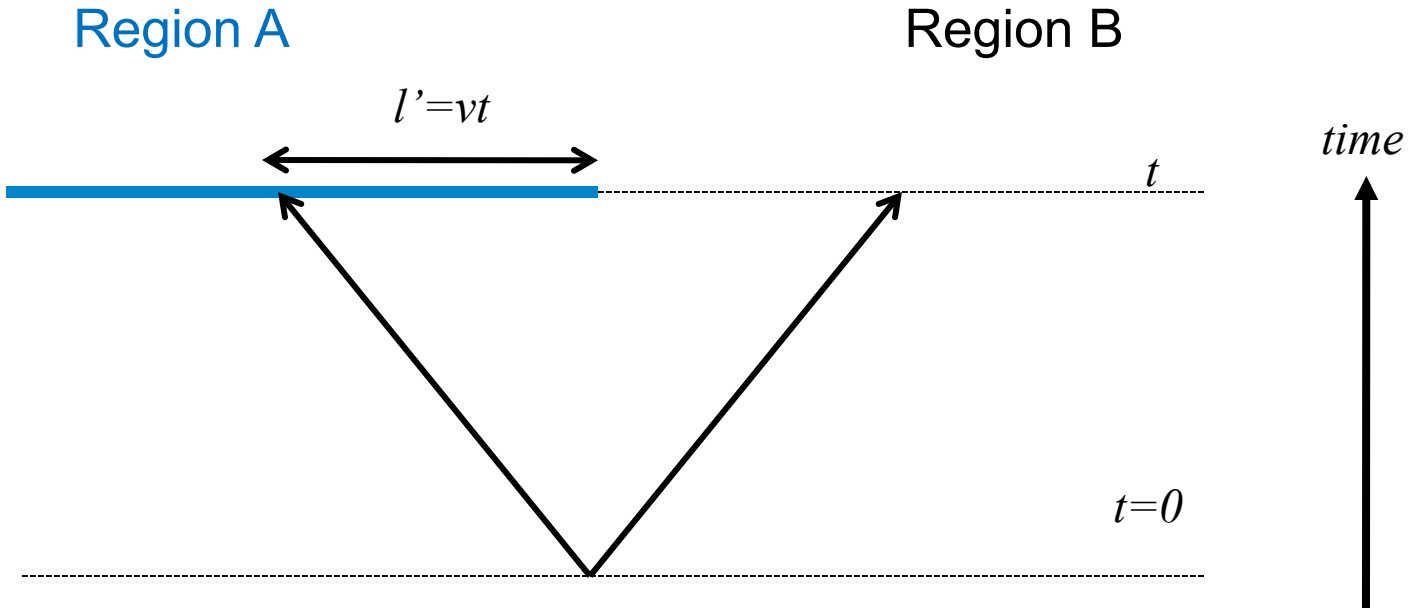
Global quench: qualitative picture



The number of entangled pairs saturates

Calabrese and Cardy, JStatM (05)

Local quench: qualitative picture



The perturbation propagates from the center, splitting the system into two pieces, inside and outside of the light-cone

$$\Rightarrow S = S_0 + c' \log(l') = S_0 + c' \log(vt)$$

Calabrese and Cardy, JStatM (07)

Computational cost

Global quench:

$$S \approx ct \rightarrow m \approx \exp(S) = \exp(ct)$$

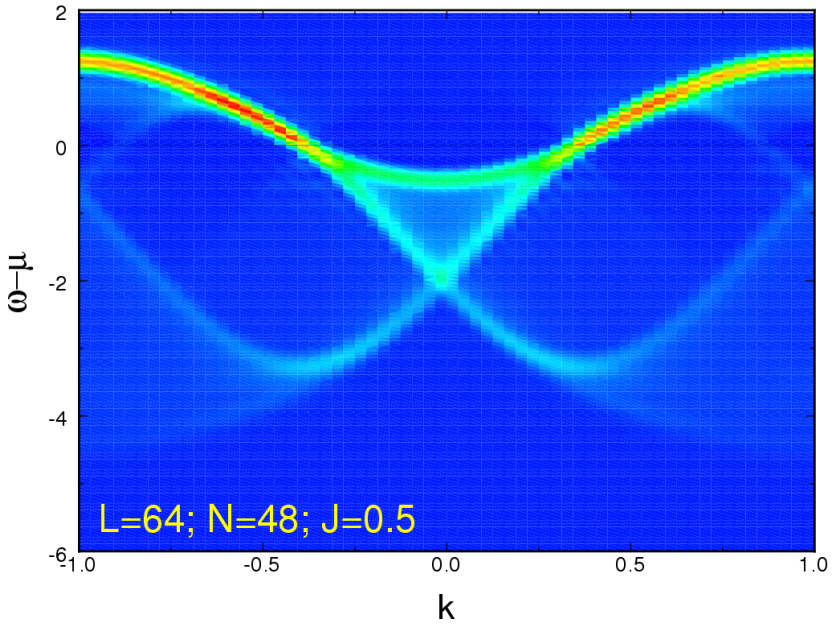
Local quench:

$$S \approx \log(vt) \rightarrow m \approx \exp(S) = t^{\text{const.}}$$

Adiabatic quench:

$$S \approx \text{const.} \rightarrow m \approx \text{const.}$$

Time-dependent correlation functions – Spectral properties



References: AEF and SR White (05)

Calculating spectral functions

To get spectral functions, we Fourier transform a time dependent Green's function such as

$$G(t) = \langle \phi | B(t) A(0) | \phi \rangle$$

where ϕ is the ground state. Here is the recipe:

- Use standard DMRG to get $|\phi\rangle = |\phi(t=0)\rangle$. Turn off Davidson/Lanczos.
- During a half sweep, apply A to $|\phi\rangle$, $|\psi(t=0)\rangle = A|\phi\rangle$, targetting both ϕ and ψ, and doing the wavefunction step-to-step transformation.
- Start the sweeps to time evolve, applying the link operators, on both $\phi(t)$ and $\psi(t)$.
- Measure $G(t)$ as

$$G(t) = \langle \phi(t) | B | \psi(t) \rangle$$

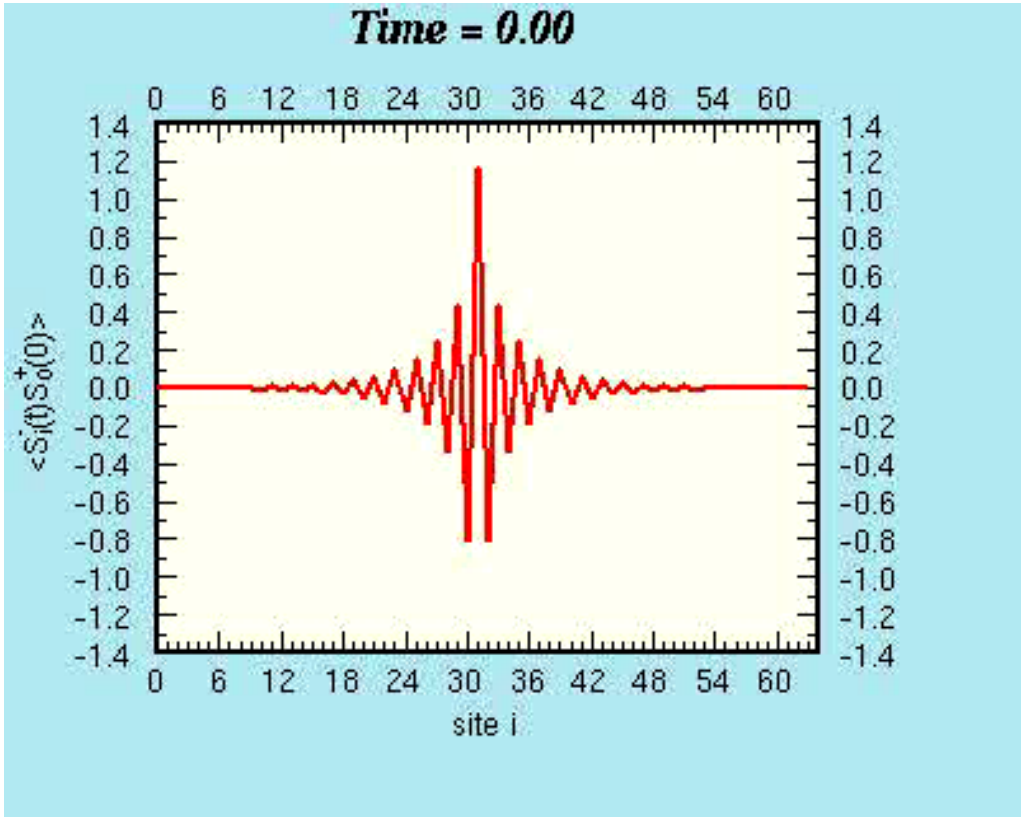
To get all momenta at once, let A be, e.g., S_i^+ for the center site i, and measure with $B = S_j^-$ for all sites j as you sweep. This gives you, for example

$$G(i-j,t) = \langle \phi | S^-(j,t) S^+(i,0) | \phi \rangle$$

This we can Fourier transform in both space and time to get $G(k,\omega)$.

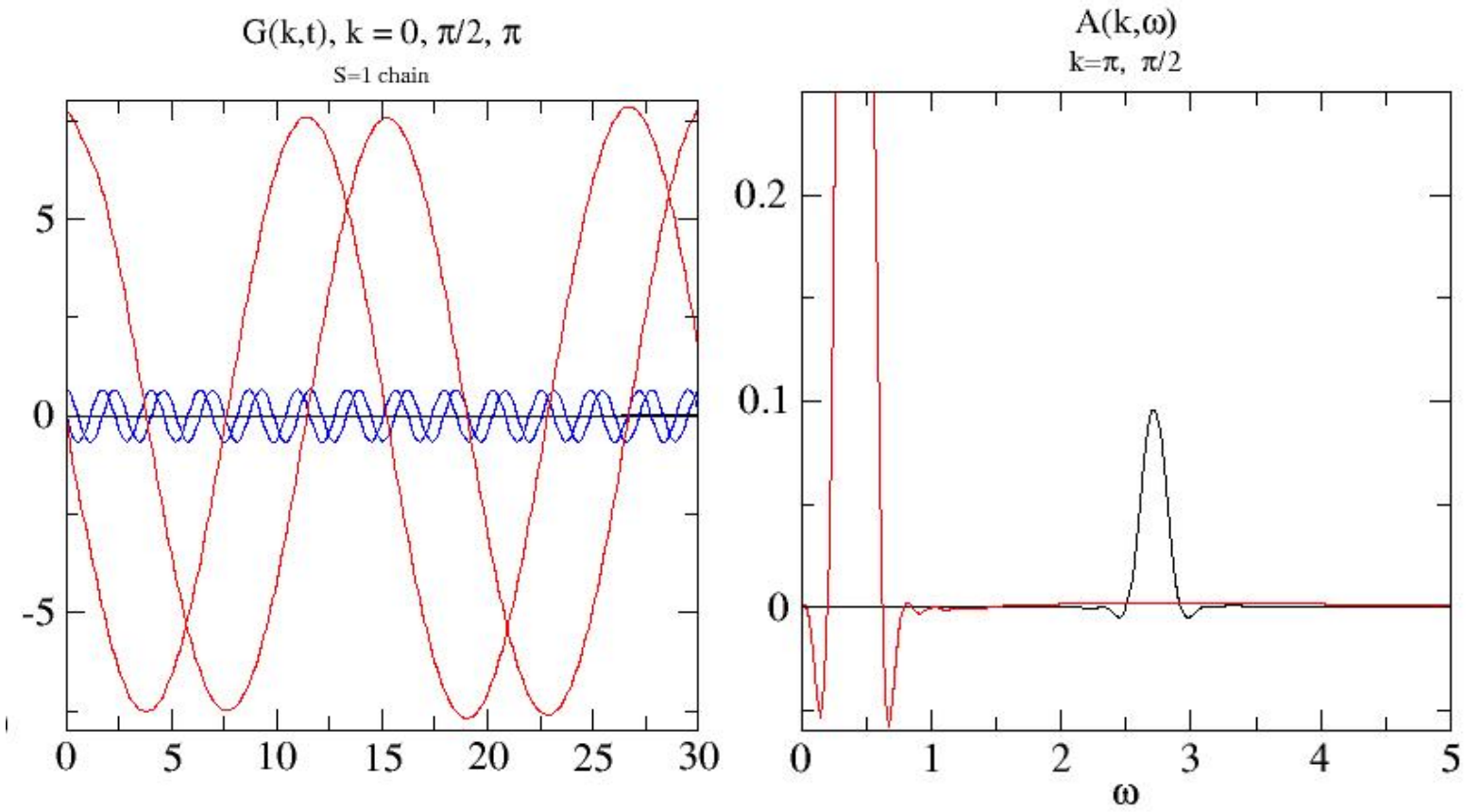
Time dependent correlation functions

S=1 Heisenberg chain



$$G(x,t) = -i\langle\phi|T[S_x^-(t)S_0^+(0)]|\phi\rangle$$

Fourier transform to k and ω

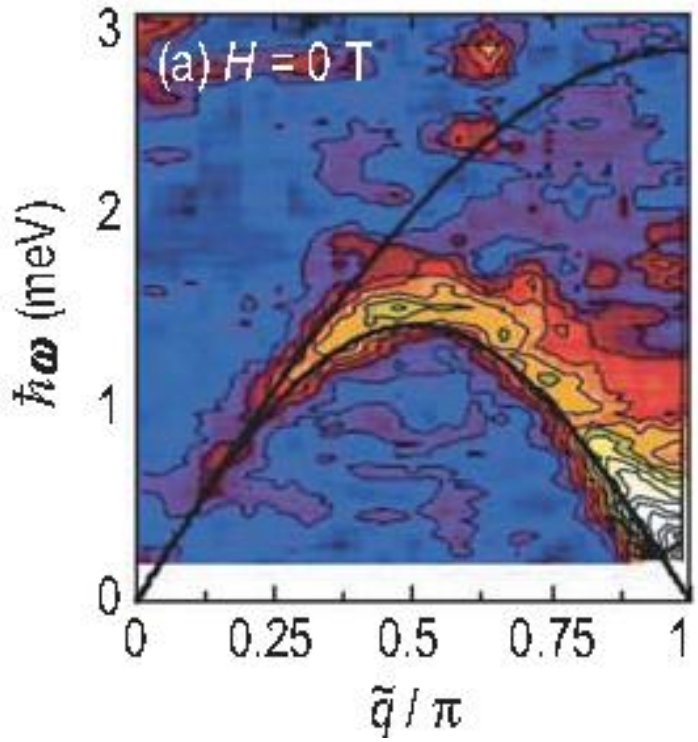


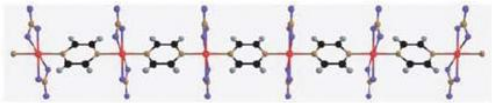
$$G(k,\omega) = 2\int_0^\infty dt \cos\omega t \sum_x \cos kx G(x,t)$$

Courtesy, SR White.

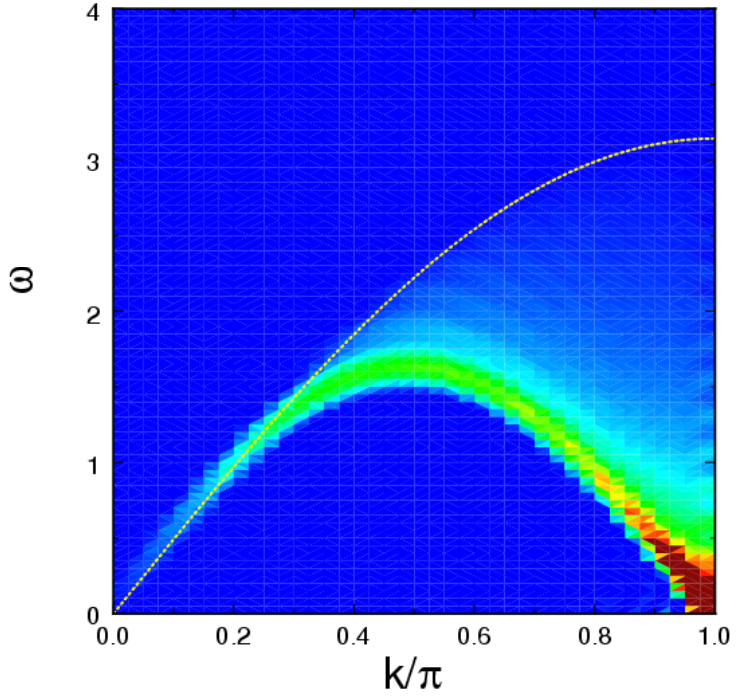
S=1/2 Heisenberg chain

$Cu(C_4H_4N_2)(NO_3)_2$



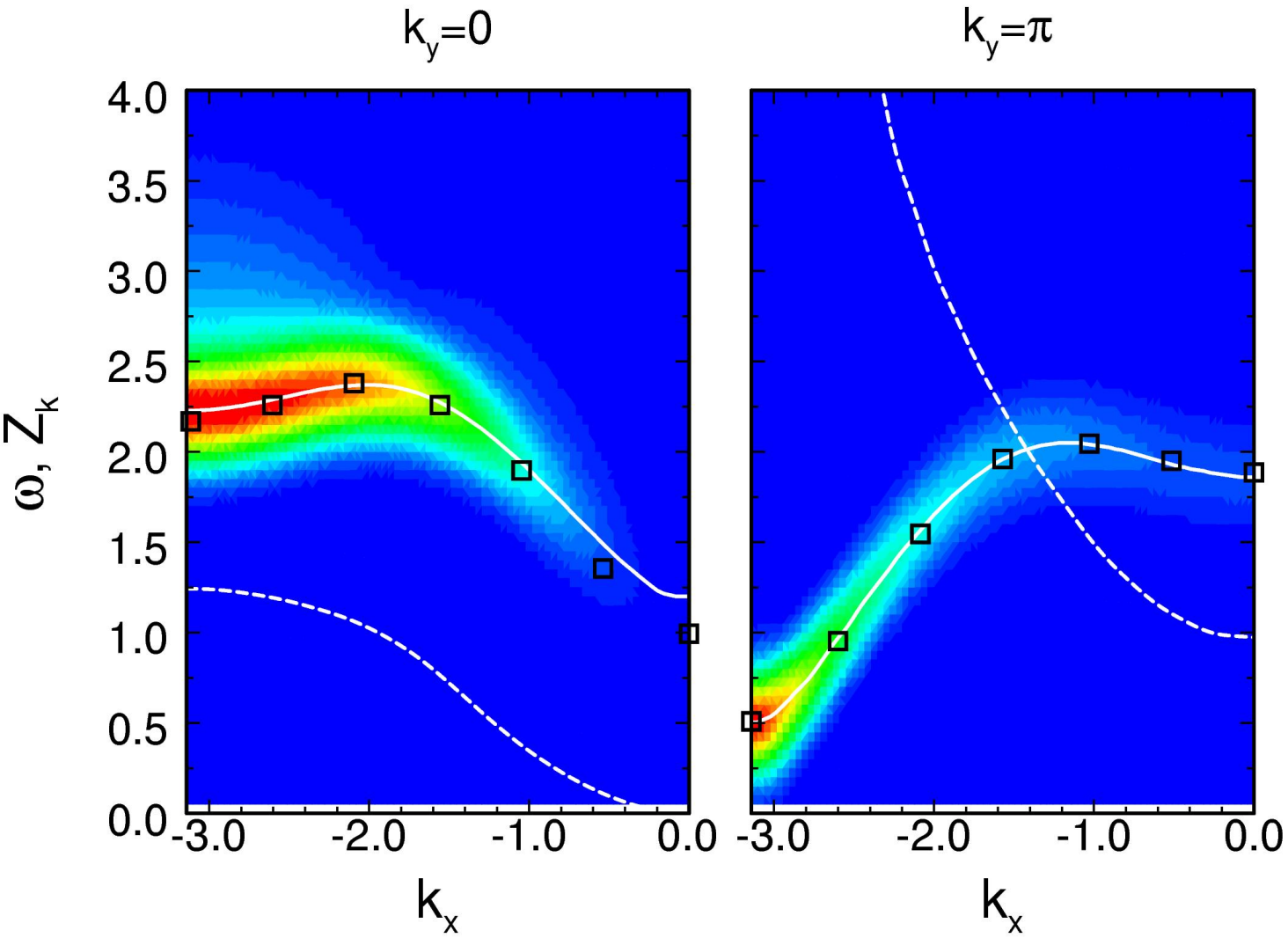


tDMRG



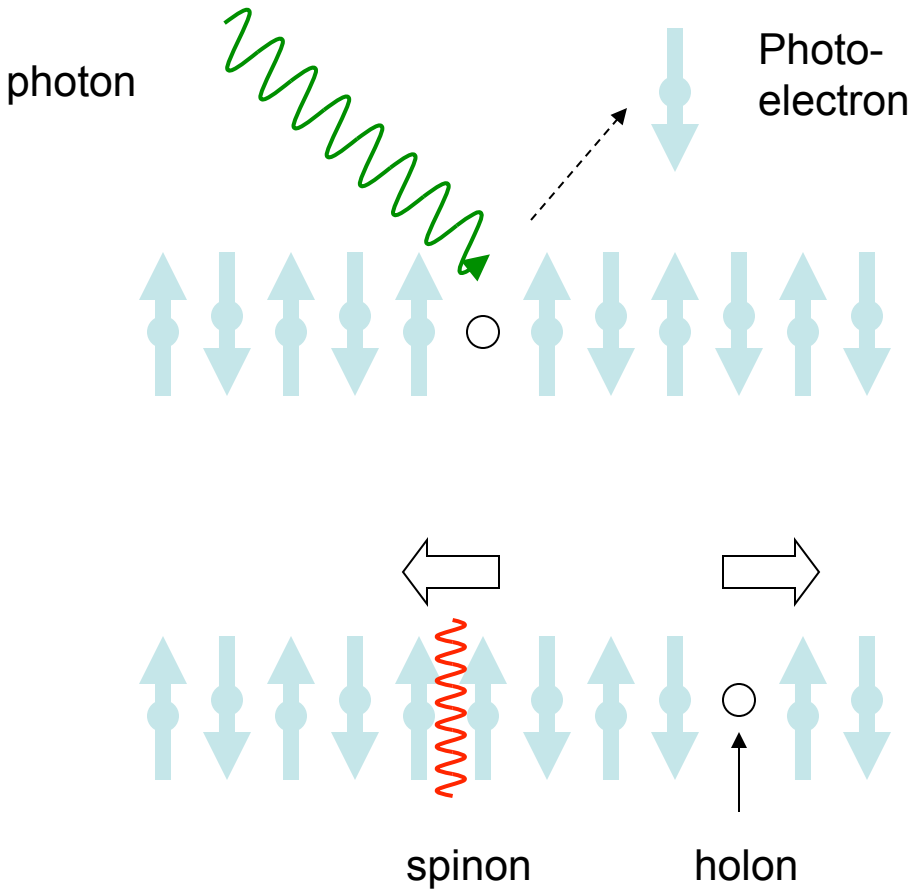
L=80; *m*=200; τ=0.1

S=1/2 **Heisenberg ladder** 2x*L* (*L*=32)



Spin-charge separation

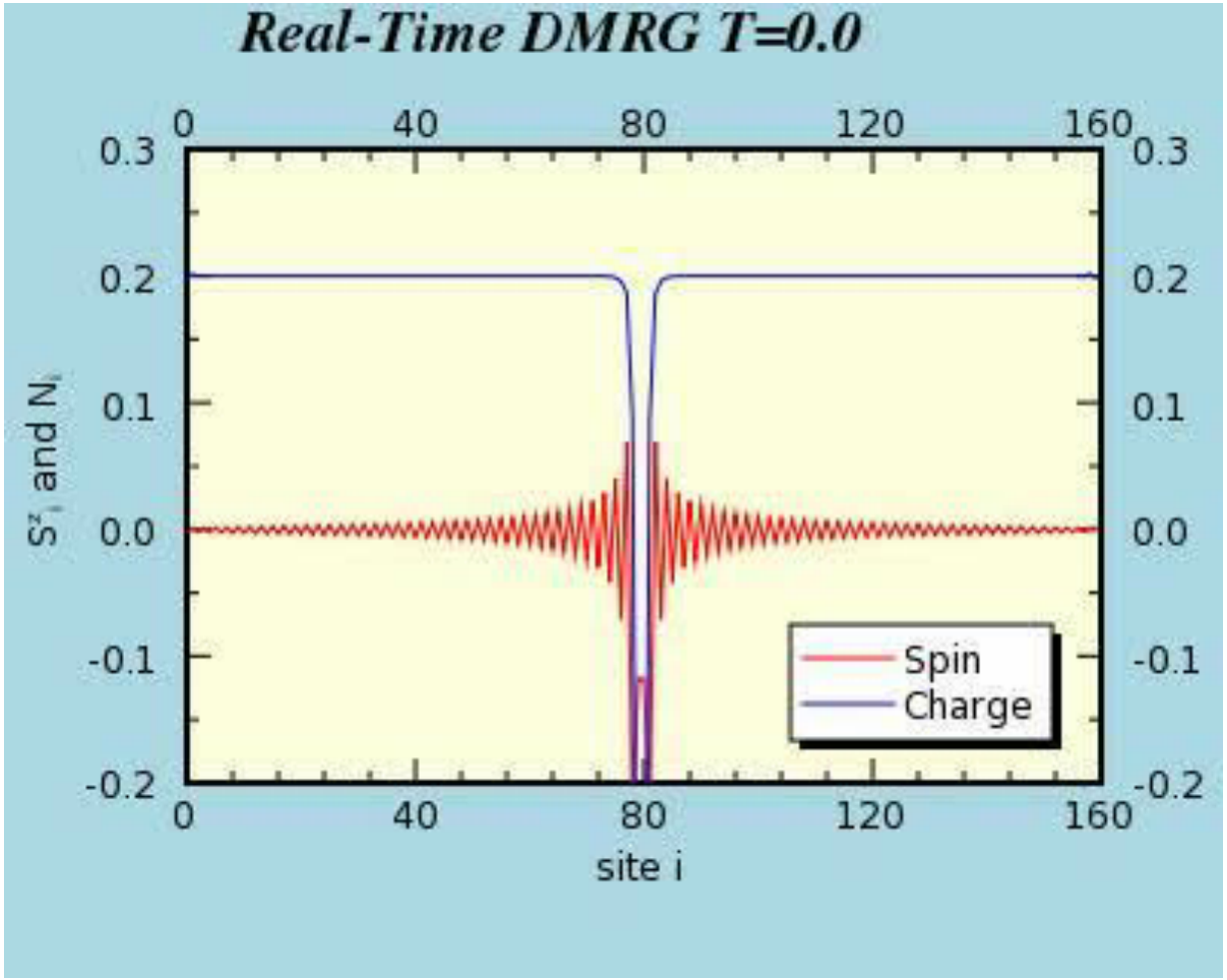
(seen in photoemission – ARPES)



The excitations don't carry the same quantum numbers as the original electron
→ zero quasi-particle weight

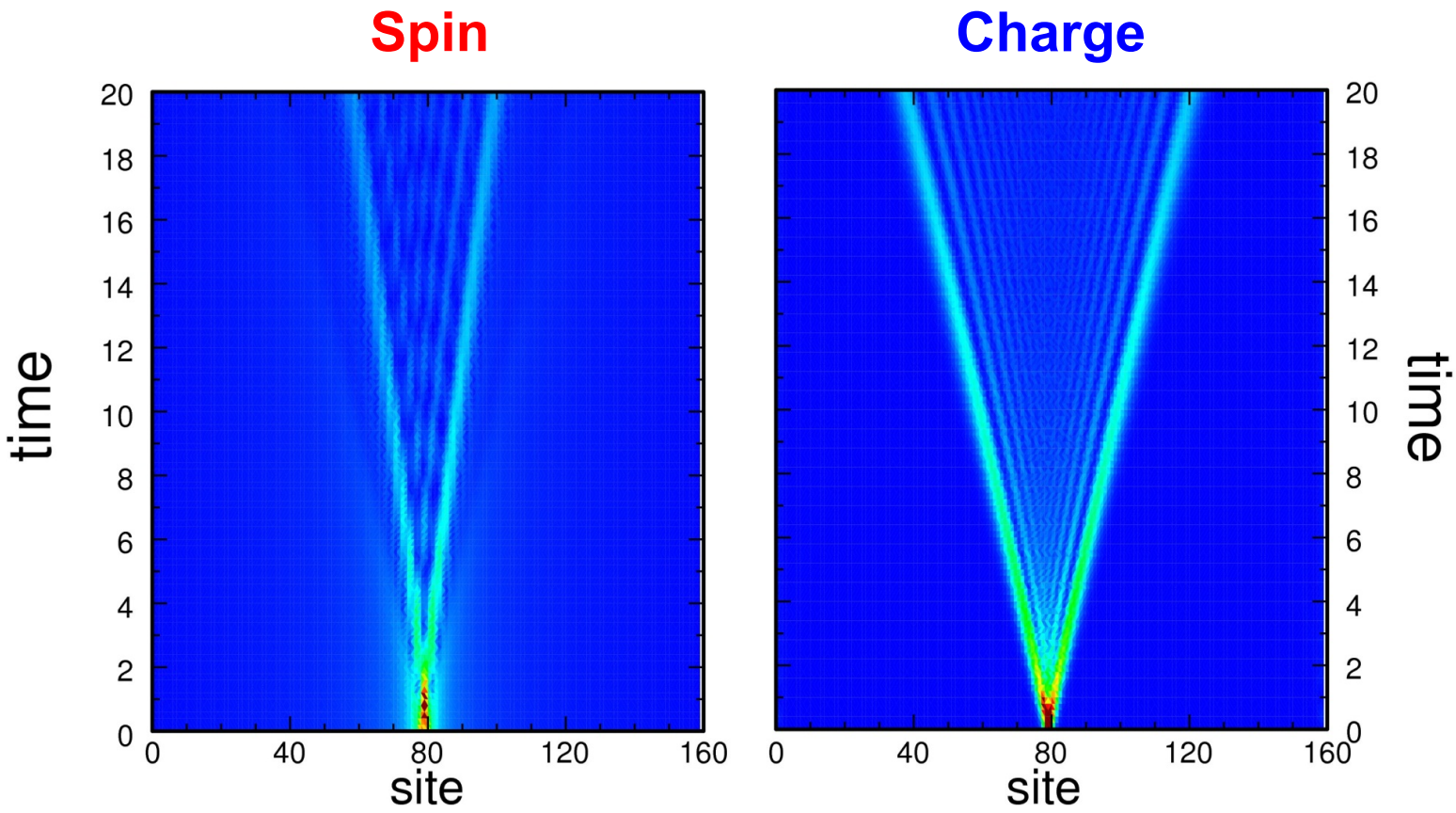
Real-time simulation

Half-filled Hubbard model (L=160, U=4)



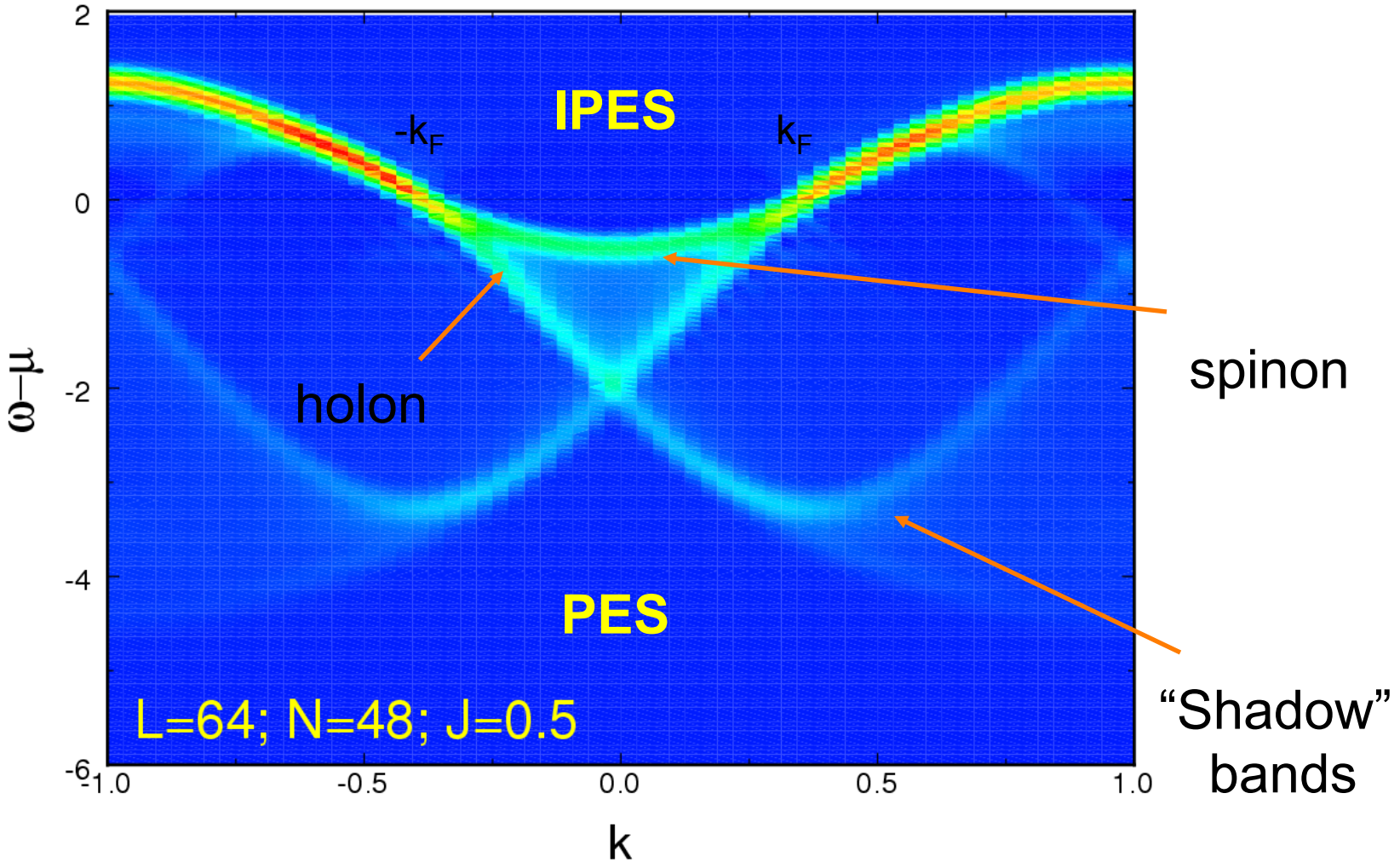
S.R.White and AEF, PRL (2004), Daley et al, J. Stat. Mech.: Theor. Exp. (2004); AEF and S.R.White, PRB (2005), Rapid Comm.

Lightcones



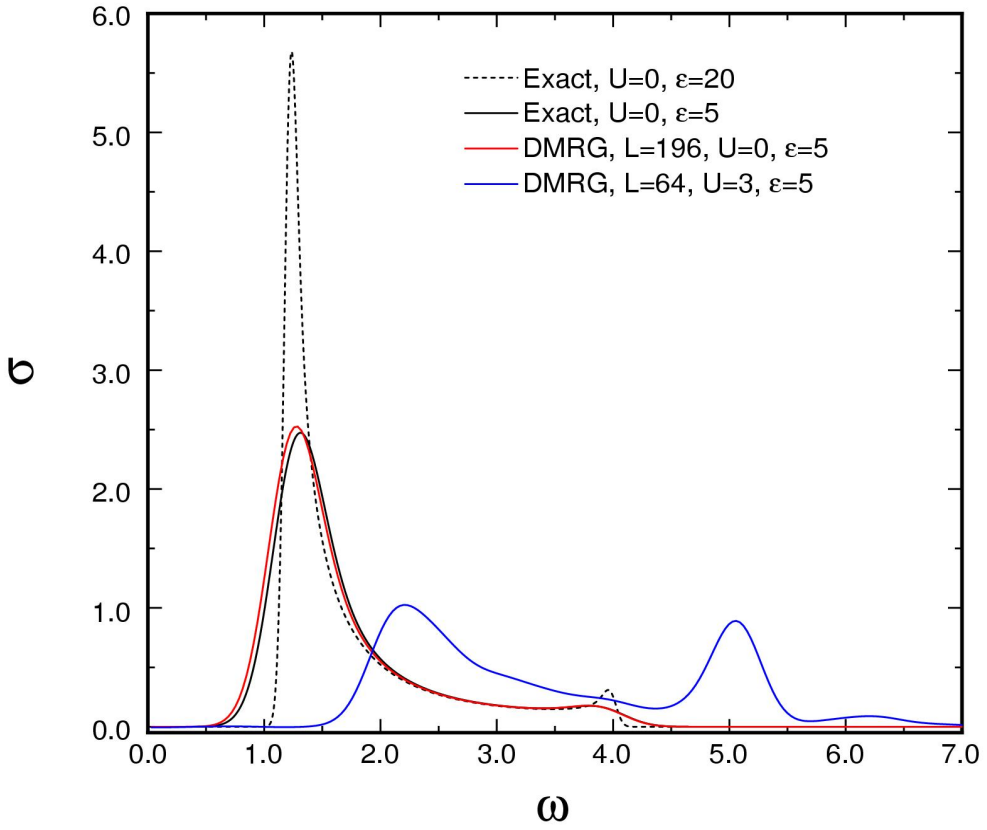
Spin and charge propagate at different velocities

ARPES at T=0; J=0.5



Optical conductivity: Peierls-Hubbard model

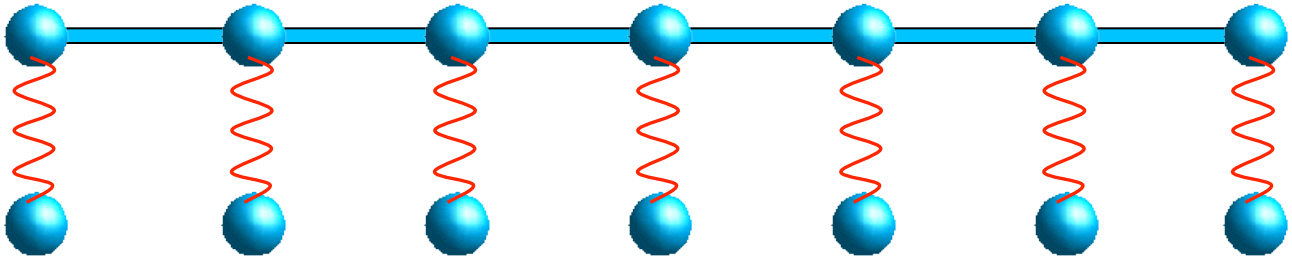
$$H = T + U \sum_{l=1}^{N} \left(n_{l,\uparrow} - \frac{1}{2} \right) \left(n_{l,\downarrow} - \frac{1}{2} \right) \qquad T = -\sum_{l;\sigma} \left(t - (-1)^l \frac{\Delta}{2} \right) \left(c^+_{l,\sigma} c_{l+1,\sigma} + c^+_{l+1,\sigma} c_{l,\sigma} \right) .$$



$$\sigma_1(\omega) = \frac{\pi}{N a \omega} \lim_{\eta \to 0} \mathrm{Im}\, G_J(\hbar\omega + i\eta)$$
$$= \frac{\pi}{N a \omega} \sum_n |\langle \psi_0 | J | \psi_n \rangle|^2 \, \delta(\hbar\omega + E_0 - E_n)$$

$$J = \frac{iae}{\hbar} \sum_{l;\sigma} \left(t - (-1)^l \frac{\Delta}{2} \right) \left(c^+_{l,\sigma} c_{l+1,\sigma} - c^+_{l+1,\sigma} c_{l,\sigma} \right)$$

Finite-temperature DMRG



References: AEF and S. R. White, PRB, Rapid (05)

Liouville representation

Consider an operator

$$A = \sum_{jk} a_{jk} \left| j \right\rangle \left\langle k \right|$$

If the dimension of the Hilbert space is *d*, we need dxd entries to define A

Another way to define the operator is by working in Liouville space: we recast it in the form

$$\left| A \right\rangle\!\right\rangle = \sum_{jk} a_{jk} \left| jk \right\rangle\!\right\rangle$$

Were

$$\left| jk \right\rangle\!\right\rangle \equiv \left| j \right\rangle \left\langle k \right|$$

Liouville representation (cont.)

If the operator is the density matrix then we can write the equation of motion as

$$\frac{d\rho}{dt} = -i\left[H, \rho\right]$$

It can be rearranged as

$$\frac{d\rho_{jk}}{dt} = -i\sum_{m}\left[H_{jm}\rho_{mk} - \rho_{jm}H_{mk}\right] = -i\sum_{mn} L_{jk,mn}\rho_{mn}$$

Were

$$L_{jk,mn} = H_{jm}\delta_{kn} - H^{*}_{kn}\delta_{jm}$$

The Liouvillian L is a superoperator with d^2xd^2 entries

$$\frac{d\left|\rho\right\rangle\!\right\rangle}{dt} = -iL\left|\rho\right\rangle\!\right\rangle$$

analogous to the Schroedinger equation

From Liouville to Thermo Field representation

We need dxd entries to define an operator, so we can define an "ancillary" space, which is a duplicate of our Hilbert space

$$\mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H}'$$

For each state $|x\rangle$ in H, we define a "tilde" state $|\tilde{x}\rangle$ living in the ancillary space ("thermo-field double").

Now, we can define a **"quantum"** state

$$|\psi_A\rangle = \sum_{jk} a_{jk} |j\rangle |\tilde{k}\rangle$$

This state encodes the operator A, and the dxd amplitudes contain all the information.

Takahashi and Umezawa, Collect Phenom. 2, 55 (1975)

Thermo Field representation

If the operator is the density matrix, once again we see $\left|\psi_\rho\right\rangle = \sum_{jk} \rho_{jk} \left| j \right\rangle \left| \tilde{k} \right\rangle$

$$\frac{d\left|\psi_\rho\right\rangle}{dt} = -i\left(H - \tilde{H}\right)\left|\psi_\rho\right\rangle \quad \rightarrow \quad \left|\psi_\rho(t)\right\rangle = e^{-it\left(H-\tilde{H}\right)}\left|\psi_\rho(t=0)\right\rangle$$

with $\tilde{H} = H^+$ acting on the ancillary states

It is easy to verify that: $\frac{d\rho_{jk}}{dt} = -i\sum_m \left[H_{jm}\rho_{mk} - \rho_{jm}H_{mk}\right]$

But we work with quantum states and Hamiltonians, instead of operators and superoperators. All the machinery of many-body, Green's function, numerics, can be seamlessly generalized to solve the non equilibrium problem!

Finite temperature

Problem: we want to calculate a thermal average:

$$\langle A \rangle = Z^{-1}(\beta)\mathrm{Tr}\{Ae^{-\beta H}\}, \quad Z(\beta) = \mathrm{Tr}\{e^{-\beta H}\}.$$

as an average using a wave function instead of density matrices:

$$\langle A \rangle = \frac{\langle \psi_\rho(\beta) | A | \psi_\rho(\beta) \rangle}{\langle \psi_\rho(\beta) | \psi_\rho(\beta) \rangle} = \frac{1}{Z(\beta)} \sum_n e^{-\beta E_n} \langle n | A | n \rangle$$

with

$$Z(\beta) = \langle \psi_\rho(\beta) | \psi_\rho(\beta) \rangle$$

AEF and S. R. White, PRB, Rapid (05), Verstraete PRL 2004, Zwolak PRL 2004

Finite temperature

Let's consider a two-level system

$$\rho = \rho_{00}|0\rangle\langle 0| + \rho_{01}|0\rangle\langle 1| + \rho_{10}|1\rangle\langle 0| + \rho_{11}|1\rangle\langle 1|$$

or

$$|\psi_\rho\rangle = \rho_{00}|0\rangle|\tilde{0}\rangle + \rho_{01}|0\rangle|\tilde{1}\rangle + \rho_{10}|1\rangle|\tilde{0}\rangle + \rho_{11}|1\rangle|\tilde{1}\rangle$$

At ***infinite temperature***

$$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$$

$$|\psi_\rho(\beta = 0)\rangle = \frac{1}{2}|0\rangle|\tilde{0}\rangle + \frac{1}{2}|1\rangle|\tilde{1}\rangle$$

We can perform a "particle-hole" transformation an rewrite it as:

$$|\psi_\rho(\beta = 0)\rangle = \frac{1}{2}\left(|0\rangle|\tilde{1}\rangle + |1\rangle|\tilde{0}\rangle\right) \equiv \frac{1}{2}\left(|\uparrow\rangle|\tilde{\downarrow}\rangle + |\downarrow\rangle|\tilde{\uparrow}\rangle\right)$$

Note: The sign does not matter, we can also use the singlet as the maximally entangled state

Example: single spin

We introduce and auxiliary spin (ancilla)

$$|I_0\rangle = |\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle$$

↑: "physical" spin

↓: "ancilla"

We trace over ancilla:

$$\rho = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The density matrix corresponds to the physical spin at infinite temperature!

Takahashi and Umezawa, Collect Phenom. 2, 55 (1975), Verstraete PRL 2004, Zwolak PRL 2004

Evolution in imaginary time

Now, let's prove that the thermal state is equivalent to evolving the maximally entangled state in imaginary time.

$$e^{-\beta H/2}\left|\psi(\beta=0)\right\rangle = e^{-\beta H/2}\sum_{\text{all states } n}\left|n,\tilde{n}\right\rangle$$

Since this expression does not depend on the choice of basis, we can assume that the configurations *n* are actually eigenstates of *H*

$$\sum_n e^{-\beta H/2}\left|n,\tilde{n}\right\rangle = \sum_n e^{-\beta E_n/2}\left|n,\tilde{n}\right\rangle$$

$$\rightarrow \left\langle\psi(\beta)\right|\hat{A}\left|\psi(\beta)\right\rangle = \sum_{n,m} e^{-\beta(E_n+E_m)/2}\left\langle m,\tilde{m}\right|\hat{A}\left|n,\tilde{n}\right\rangle$$

$$= \sum_{n,m} e^{-\beta(E_n+E_m)/2}\left\langle m\right|\hat{A}\left|n\right\rangle\left\langle\tilde{m}\right|\left.\tilde{n}\right\rangle$$

$$= \sum_n e^{-\beta E_n}\left\langle n\right|\hat{A}\left|n\right\rangle$$

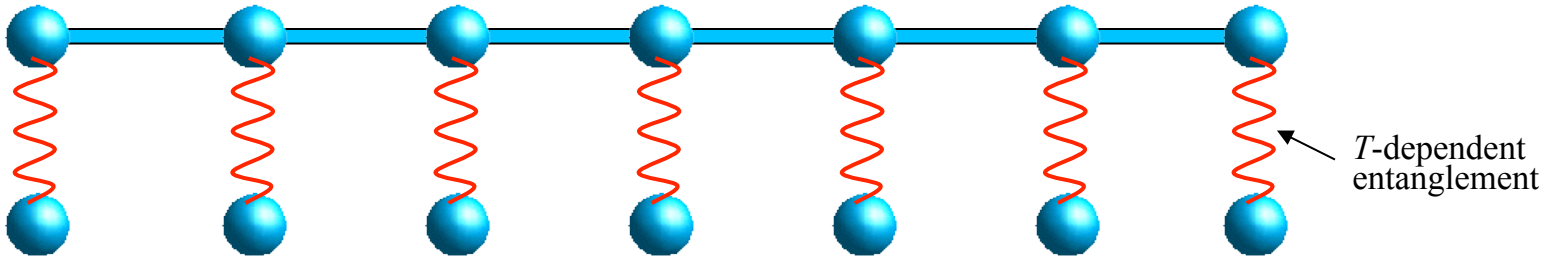
Similarly:

$$\left\langle\psi(\beta)\right|\left.\psi(\beta)\right\rangle = \sum_n e^{-\beta E_n} = Z(\beta)$$

Evolution in imaginary time

The thermal state is equivalent to evolving the maximally mixed state in imaginary time.

$$\frac{d}{d\beta}|\psi(\beta)\rangle = -\frac{H}{2}|\psi(\beta)\rangle \Rightarrow |\psi(\beta)\rangle = \exp\left(-\frac{H}{2}\right)|\psi(\beta=0)\rangle$$



- The ancillas and the real sites do not interact!
- The **global** state is modified by the action of the Hamiltonian on the real sites, that are entangled with the ancillas.
- The mixed state can be written as a pure state in an enlarged Hilbert space (ladder-like or bi-layer-like in 2D).
- The thermal state is the “square root” of the density matrix.

Maximally mixed state for β=0 (T=∞)

CM: thermofield representation, QI: mixed state purification

$$|I\rangle = \sum |n,\tilde{n}\rangle$$ (auxiliary field $\tilde{n}$ is called ancilla state)

with $|n\rangle = |s_1\, s_2\, s_{3\ldots} s_N\rangle$ 2^N states!!!

$$|I\rangle = |\uparrow\uparrow,\uparrow\uparrow\rangle + |\downarrow\downarrow,\downarrow\downarrow\rangle + |\uparrow\downarrow,\uparrow\downarrow\rangle + |\downarrow\uparrow,\downarrow\uparrow\rangle$$

each term can be re-written as a product of local "site-ancilla" states:

$$|I\rangle = |\uparrow,\uparrow\rangle|\uparrow,\uparrow\rangle + |\downarrow,\downarrow\rangle|\downarrow,\downarrow\rangle + |\uparrow,\uparrow\rangle|\downarrow,\downarrow\rangle + |\downarrow,\downarrow\rangle|\uparrow,\uparrow\rangle$$

after a "spin-reversal" (flip) transformation on the ancilla we get

$$|I\rangle = |I_0\rangle|I_0\rangle \text{ with } |I_0\rangle = |\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle$$

Exercise: prove that the maximally mixed state $|I\rangle = \sum |n,\tilde{n}\rangle$ does not depend on the choice of basis or representation

Initial state

We have found that the initial state:

$$|I\rangle = \sum |n, \tilde{n}\rangle$$

Can be written as:

$$|I\rangle = \prod_{\text{sites } i} |I_0\rangle_i \quad \text{with} \quad |I_0\rangle_i = \sum_s |s, \tilde{s}\rangle_i$$

The maximally entangled state between system and ancillas is a product state (totally disentangled) of spin-ancilla pairs!!

The initial state in DMRG language looks like:

$$|I\rangle = |I_L\rangle |I_0\rangle_{N/2} |I_0\rangle_{N/2+1} |I_R\rangle,$$

In this basis, left and right block have only one state!

As we evolve in time, the size of the basis will grow.

Purification

We have found that the initial state is:

$$|\psi(\beta=0)\rangle = \sum_n |n\rangle|\tilde{n}\rangle$$

It is easy to see that it can be written as:

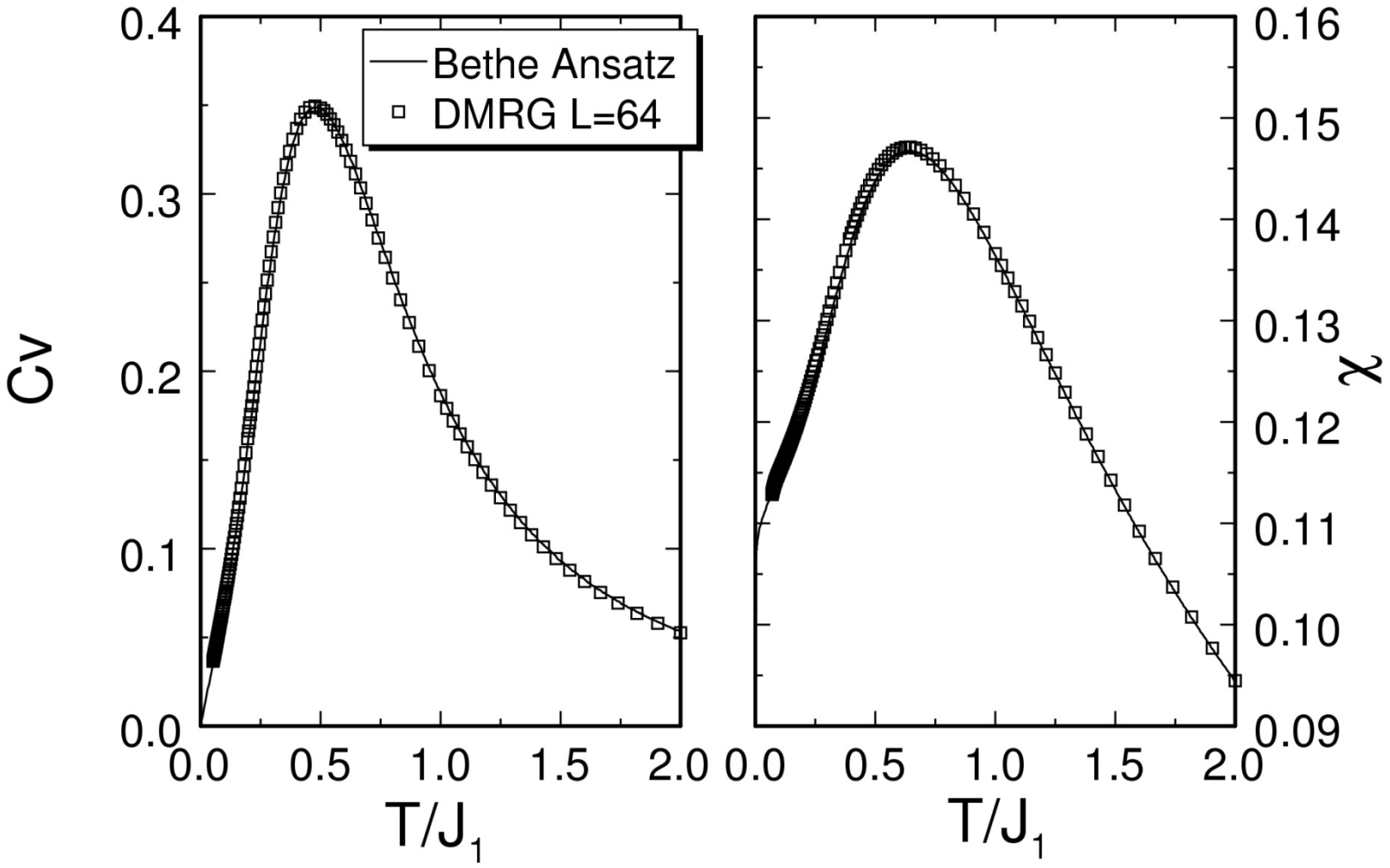
$$|\psi(\beta=0)\rangle = \prod_{\text{sites } l} |\psi_{0l}\rangle \text{ with } |\psi_{0l}\rangle = \sum_s |s,\tilde{s}\rangle_l$$

The maximally entangled state between system and ancillas is a product state (totally disentangled) of spin-ancilla pairs!!

At T=0, the system "decouples" from the ancilla: they become totally disentangled, meaning

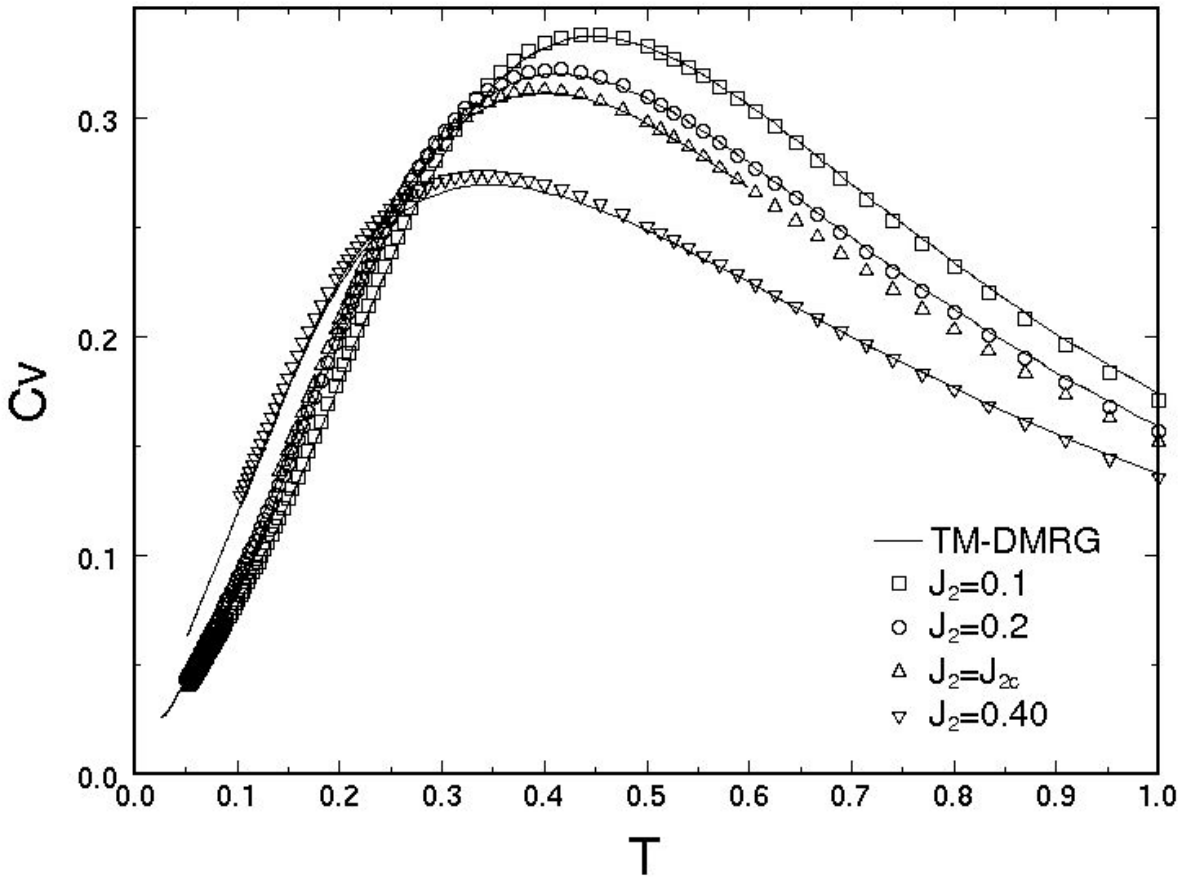
$$|\psi(\beta=\infty)\rangle = |\text{g.s.}\rangle \otimes |\text{ancillas}\rangle$$

Thermodynamics of the spin-1/2 chain



Frustrated Heisenberg chain

$$H = \sum_i J_1 \mathbf{S}_i.\mathbf{S}_{i+1} + J_2 \mathbf{S}_i.\mathbf{S}_{i+2}.$$



* TM-DMRG results from Wang and Xiang, PRB 97; Maisinger and Schollwoeck, PRL 98.

Frustrated Heisenberg chain

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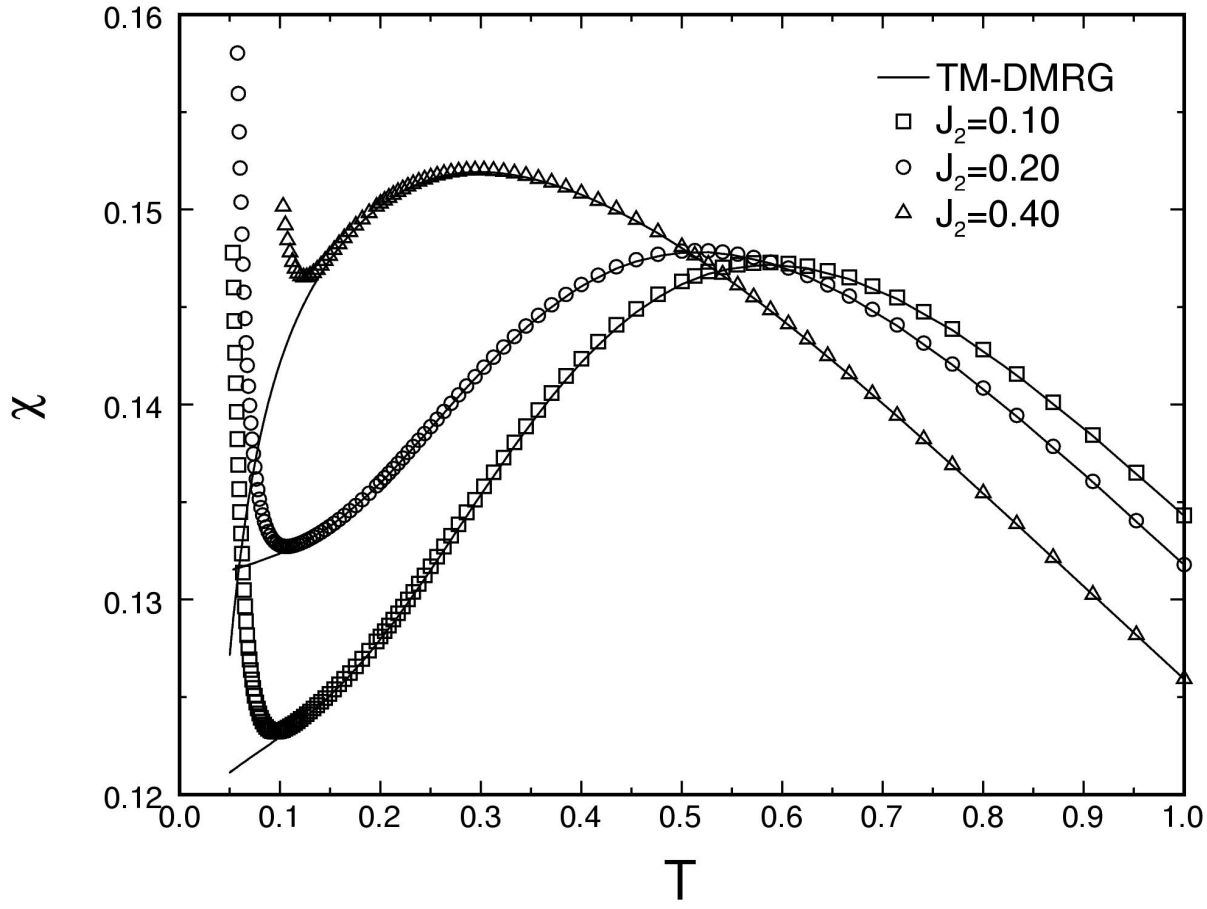


* TM-DMRG results from Wang and Xiang, PRB 97; Maisinger and Schollwoeck, PRL 98.

The maximally mixed state in the canonical ensemble

We need to generate a state: $|I\rangle = \sum |n, \tilde{n}\rangle$

Where the n states are configurations with fixed total S^z, or fixed number of particles N

The previous example was in the ***grand canonical***, all spin projections contribute:

$$|I\rangle = |\uparrow\uparrow, \uparrow\uparrow\rangle + |\downarrow\downarrow, \downarrow\downarrow\rangle + |\uparrow\downarrow, \uparrow\downarrow\rangle + |\downarrow\uparrow, \downarrow\uparrow\rangle$$

The maximally mixed state in the ***canonical*** with $S^z = 0$ would look:

$$|I\rangle = |\uparrow\downarrow, \uparrow\downarrow\rangle + |\downarrow\uparrow, \downarrow\uparrow\rangle$$

The maximally mixed state in the canonical ensemble (contd.)

Let us focus on the physical spins. Let us generate the symmetric superposition of all the spin configurations with $S^z = 0$:

$$|S\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$$

It is a and eigenstate of the operator S^2 with $S = 1$

In general, we can prove that the symmetric superposition of all spin configurations is an eigenstate of S^2 **with maximum spin** S.

Therefore, if we want to generate this state, we calculate the ground state of the Hamiltonian in desired S^z subspace

$$H = -S^2 = -\sum_{i,j} \vec{S}_i \cdot \vec{S}_j$$

For fixed with S^z this becomes (except for a constant)

$$H = -\sum_{i \neq j} S_i^+ S_j^- + S_i^- S_j^+$$

The maximally mixed state in the canonical ensemble (contd.)

Now, we need to add the ancilla, so we use:

$$H = -\sum_{i \neq j} \left(S_i^+ \tilde{S}_i^- \right)\left(S_j^- \tilde{S}_j^+ \right) + \left(S_i^- \tilde{S}_i^+ \right)\left(S_j^+ \tilde{S}_j^- \right)$$

Recipe:

1) We prepare the state at infinite temperature as the ground state of an artificial Hamiltonian acting on an enlarged Hilbert space coupling physical spins and ancillas.
2) We evolve the state in imaginary time, using the time-dependent DMRG

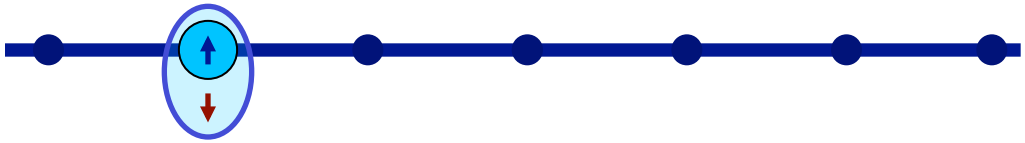
AEF, G. Fiete, PRB (2010)

The maximally mixed state in the canonical ensemble (contd.)

For fermions:

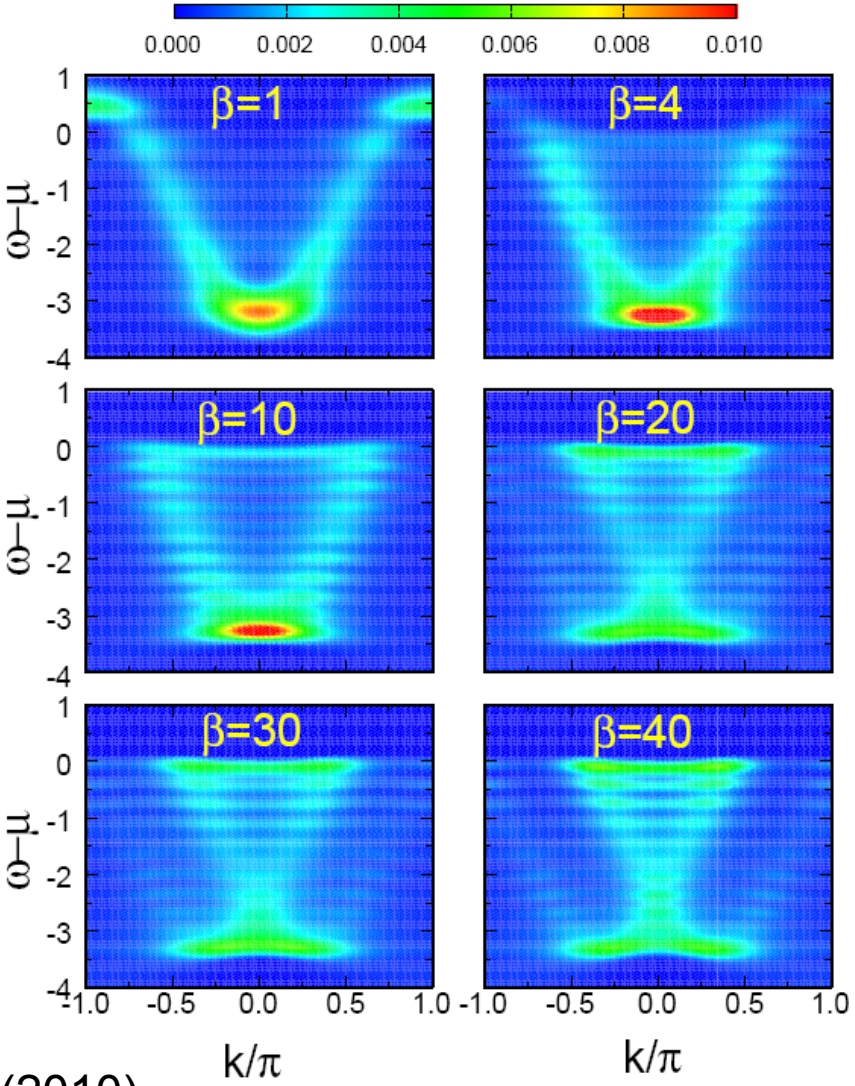
$$H = -\sum_{i \neq j} \left(\Delta_i^\dagger \Delta_j + \text{h.c.} \right)$$

fermion-ancilla pair



ARPES at finite T

t-J chain: L=32. N=24. J=0.05



AEF and G. Fiete, PRB (2010)