Title: Quantum Many-body Dynamics with Matrix Product States

Date: Feb 24, 2014 11:00 AM

URL: http://pirsa.org/14020156

Abstract: The talk is divided into two parts: in the first, I will talk about dynamics of far-from equilibrium initial states in different lattice models. I will present results of quench dynamics of the XXZ-Heisenberg magnet, where interesting physics emerges after quenching the system. Then I will present results for scattering of solitonic objects in different integrable and non-integrable lattice models. In the second part, I will talk about dynamics of impurity systems. There I will talk about how impurity spectral functions can be calculated using the Chebyshev technique, and how MPS can serve as a high resolution impurity solver for Dynamical Mean-Field Theory. Finally, I will show some results for steady-state currents through a quantum dot device.

Outline

- **Methods**: Matrix Product States and Operators
  - Definitions, Basics, Approximations
  - Dynamics with MPS
- **Applications I**: Many-body dynamics
  - Quenches in the XXZ Heisenberg model
  - Solitonic excitations in lattice models
- **Applications II**: Dynamical correlation functions

  Single Impurity Anderson Model

  DMFT
- **Applications III**: I-V characteristics of the SIAM

Matrix Product States (MPS)

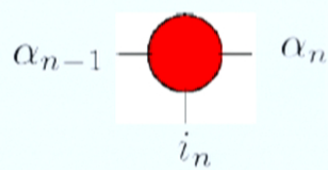
- Consider 1-d systems
- Wave function representation with matrix products:

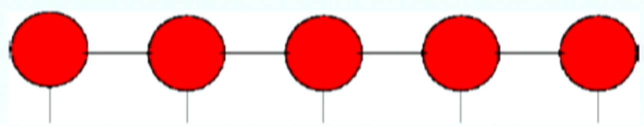
$$|\psi\rangle = \sum_{\{i_1 \ldots i_N\}} c_{i_1 \ldots i_N} |i_1 \ldots i_N\rangle$$

$$c_{i_1 \ldots i_N} = \vec{A}^{i_1} A^{i_2} \ldots A^{i_{N-1}} \vec{A}^{i_N}$$

- A^{i_n}: site-dependent $\chi \times \chi$ matrices,

  $|i_n\rangle$: local d-dimensional basis at site n

- Graphically: $A^{i_n}_{\alpha_{n-1}\alpha_n} =$ 

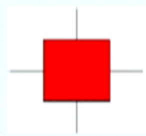
$c_{i_1 \ldots i_N} =$ 

Matrix Product Operators (MPO)

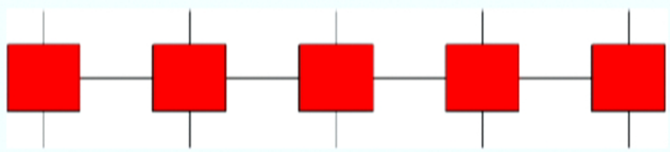
- Similar representation for operators, e.g. Hamiltonian:

$$\hat{O} = \sum_{i_1 \ldots i_N} M^{i_1 i'_1} \ldots M^{i_N i'_N} \left| i_1 \right\rangle \left\langle i'_1 \right| \ldots \left| i_N \right\rangle \left\langle i'_N \right|$$

i'_n

$M^{i_n i'_n}_{\beta_{n-1}\beta_n} = \beta_n$  β_{n-1}

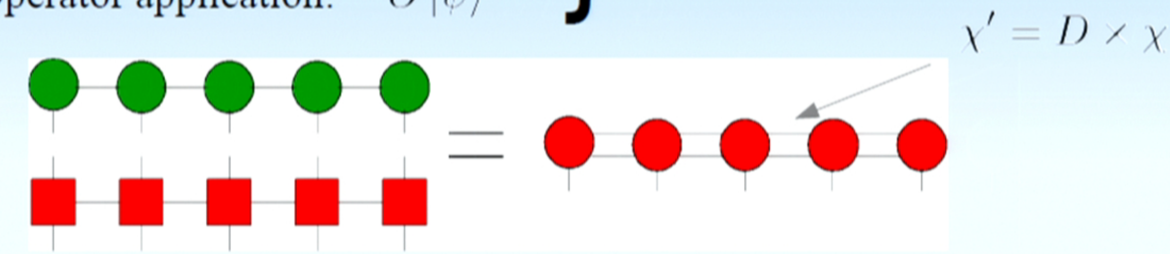
i_n



Operations on MPS

- Addition: $a\,|\psi\rangle + b\,|\phi\rangle$
- Operator application: $\hat{O}\,|\psi\rangle$

} **Increase of matrix dimension χ!**



- Compress MPS to original bond dimension χ by minimizing distance

$$||\,|\tilde{\phi}\rangle - |\phi\rangle\,||$$

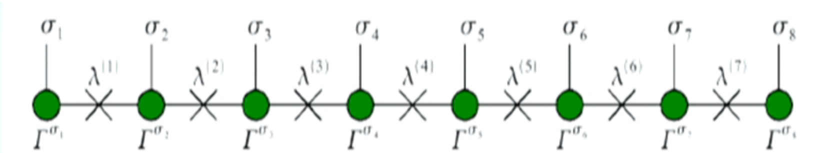
- **Applications:** Krylov-based methods for solving large sparse eigenvalue problems:
  - Lanczos (Dargel et. al. 2011, 2012)
  - Chebyshev expansion (Holzner et. al. 2011) → this talk

Dynamics I: time evolution

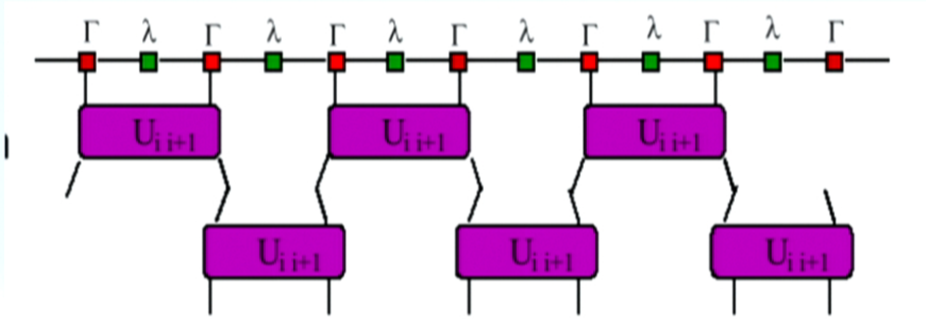
- Full Diagonalization for small systems

- TEBD, tDMRG for large systems:
  - Express states as **Canonical Matrix Product State**

$$|\psi\rangle = \sum_{\{\sigma\}} \Gamma^{\sigma_1}\lambda^{(1)}\Gamma^{\sigma_2}\lambda^{(2)}\Gamma^{\sigma_3}\ldots\Gamma^{\sigma_{L-2}}\lambda^{(L-2)}\Gamma^{\sigma_{L-1}}\lambda^{(L-1)}\Gamma^{\sigma_L}\,|\sigma_1\ldots\sigma_L\rangle$$



  - Very good approximation in 1d (basis for DMRG). Exact for sufficiently large matrices
  - Time evolution by Trotter expansion of U = exp(-it H)



Quenches in the XXZ Heisenberg spin ½ chain

- XXZ Heisenberg chain = hardcore bosons (~ spinless fermions)

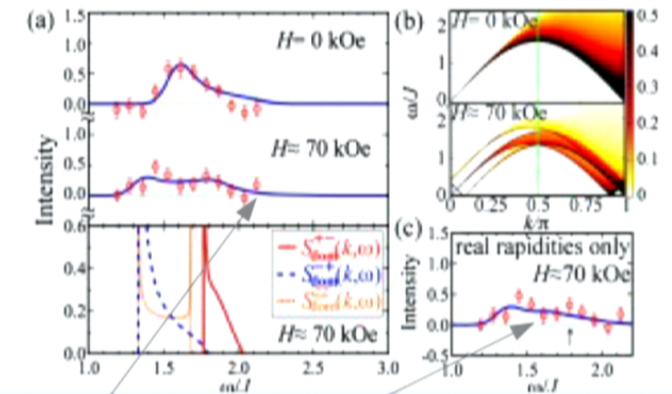
$$H = \sum_i \frac{J_{xy}}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right) + J_z S_i^z S_{i+1}^z , \quad \Delta = \frac{J_z}{J_{xy}}$$

- Integrable, solved by Bethe ansatz
- Spectrum contains Bound States ("M-strings")

Difficult to see in standard condensed matter experiments (few %)

- Quenches?

Kohno PRL 2009



Spectra with and without bound state contributions

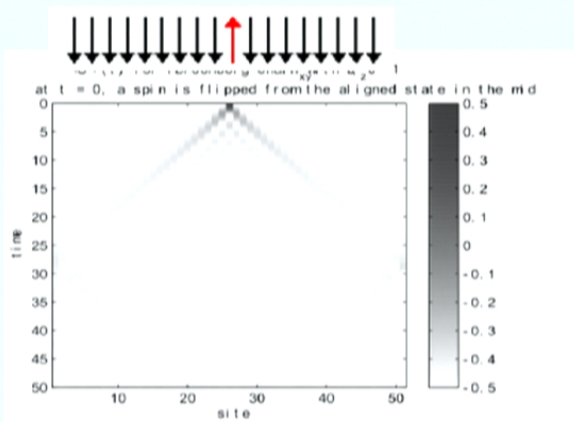
Caux et al J Stat.Mech 2005
Pereira, White, Affleck PRL 2008, PRB 2009
Sashi et al, PRB 2011

Quantum quenches: non-equilibrium time evolution

- Global Quenches:
  - Thermalization? Steady Steate? Generalized Gibbs Ensemble?

- Local quenches: Prepare system in ground state, at t=0, change H or act with S_i^+
  - investigate time evolution
  - Has almost exclusively been studied with *single site* quenches

- Example: single spin flip in FM



$\langle S^z \rangle(\mathbf{t}),\ J_z = 1$

⇒ "linear" propagation

↔ Lieb Robinson bound

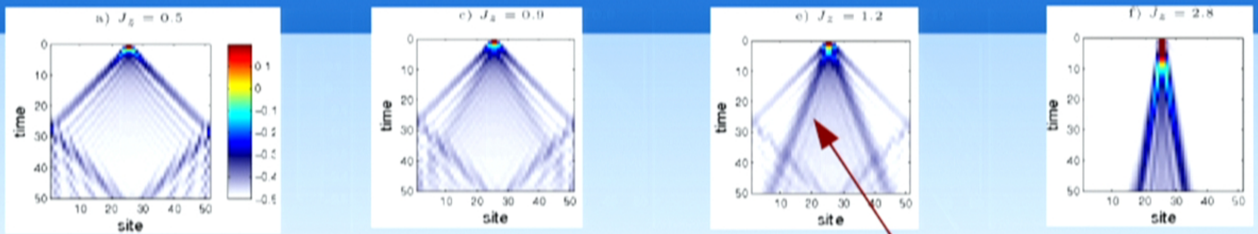
Lieb,Robinson Comm.Math.Phys 1972

Sims,Nachtergaele arXiv:1102.0835

Gobert et al. PRE 2005; Langer et al. PRB 2009; Ren, Zhu PRA 2010; Santos,Mitra PRE 2011; Langer et al 1107.4136; Santos, Dykman PRB 2003; Petrosyan et al PRA 2007; Boness et al. PRE 2010; Steinigeweg PRL 2011; Pereira et al. PRL 2008; Calabrese, Cardy J Stat Mech 2007; Stephan,Dubail 1105.4846.

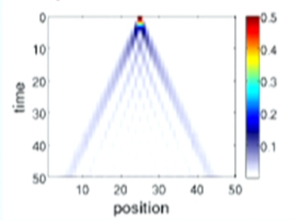
Two-spin excitation in FM

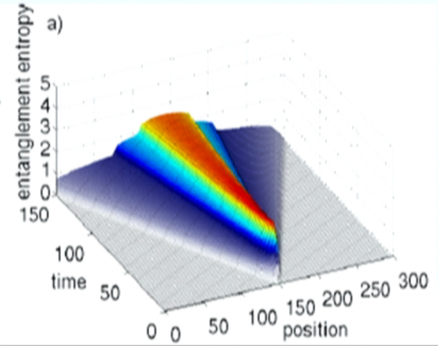
S_z

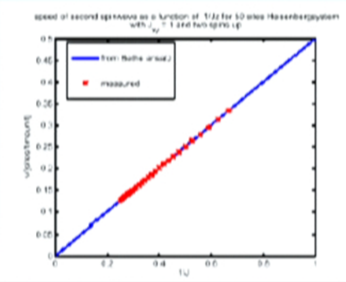


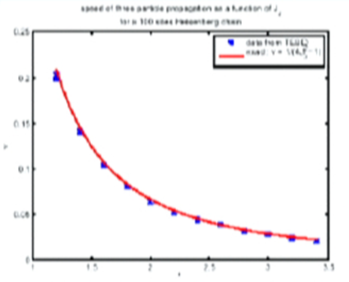
- Two distinct propagation branches beyond $J_z = 0.7$
- New lower branch is *bound state*
- It dominates at large J_z, with decreasing velocity
- Low entanglement entropy, step-like structure

P(↑ ↑)



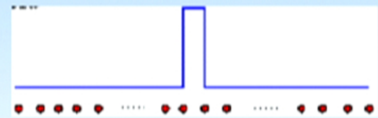






Local quench in the AF groundstate at non-zero magnetization

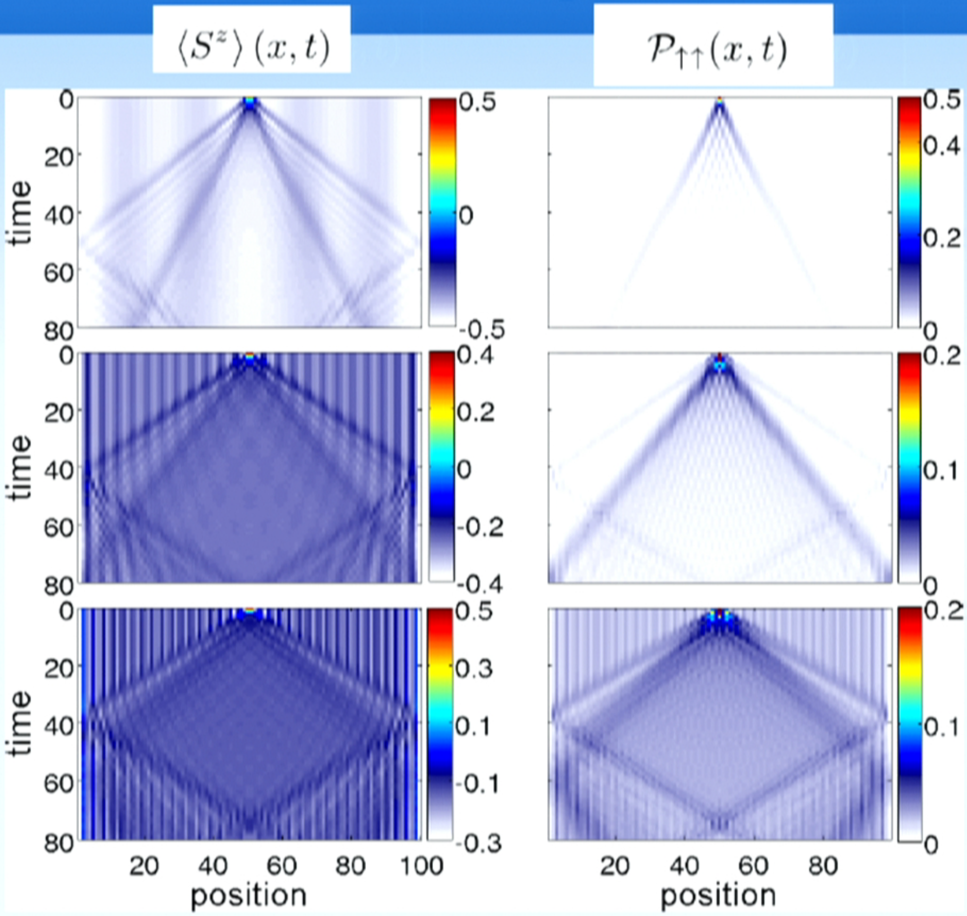
- Prepare ground state with a local infinite magnetic field, then switch field off



- AF at nonzero magnetization is in the Luttinger liquid phase *for any J_z*
- Highly entangled state, “spinon” excitations
- Do bound “string-states” remain visible ?
- Accessible in cold atom experiments (Fukuhara et al. Nature 502, 76 (2013))
- Related to “x-ray edge” problem

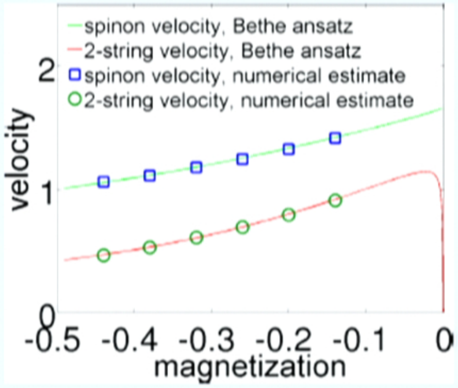
Evolution from AF groundstate at J_z=1.2, finite magnetization, 2 spins fixed up

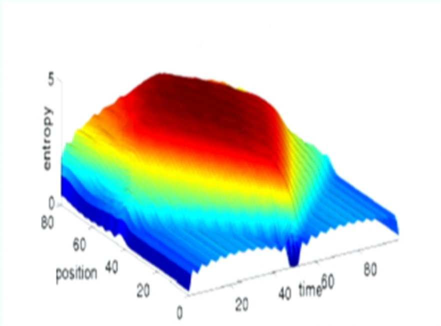
- Low filling 6% (=large magnetization): like magnons and bound magnons
- Larger filling 24% Larger velocity
- Filling 36%: fewer momenta contribute to bound state → washed out

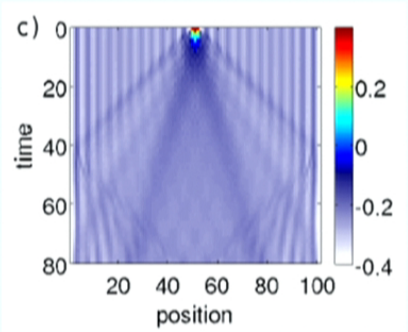


Bound states in the AF

- Bound states remain clearly visible
- Velocities agree precisely with Bethe ansatz:
- At zero magnetization no bound states
- Different entanglement structure,still steplike







- Three-strings: agree with Bethe ansatz:

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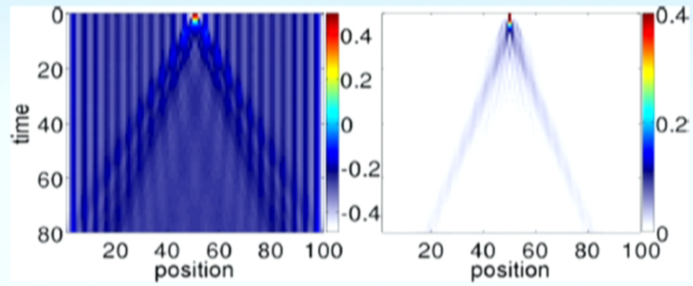
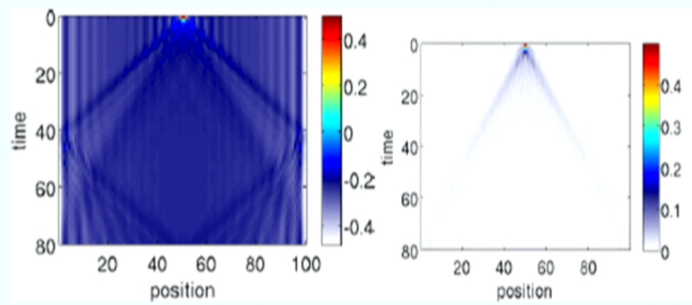
Non-integrable models

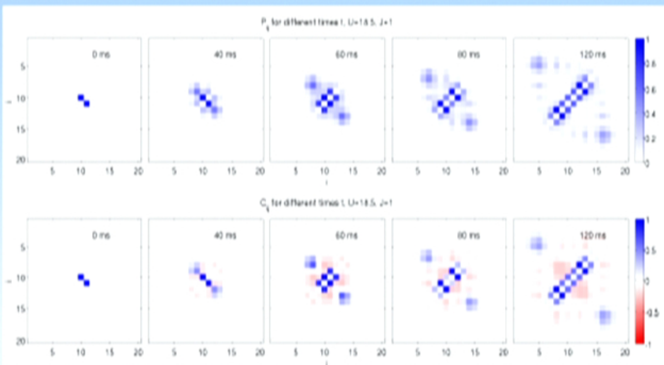
- Experiments (e.g. cold atoms) may not precisely reproduce the XXZ model
- Bound states remain visible in nonintegrable models !
- Next-nearest neighbor coupling J/10

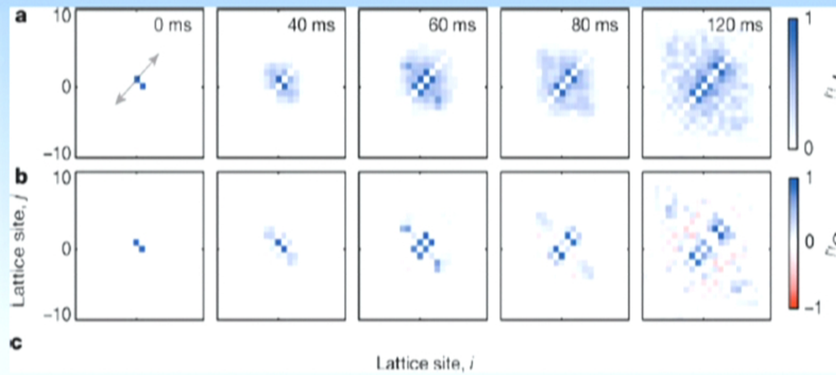


- Chain in parabolic field ("optical trap")



Realization with cold atoms





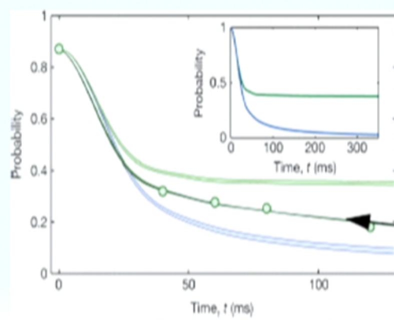
TEBD

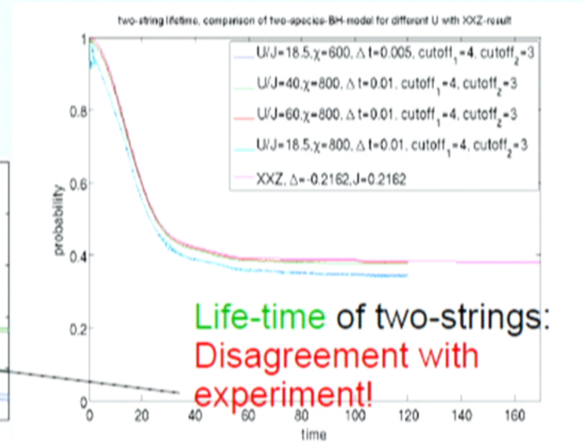
Experiment Fukuhara et al. Nature 502, 76

Experiment: two species bose hubbard model (two hyperfine states of Rb)

P_{ij}: probability of finding two spins simultaneously at sites i,j

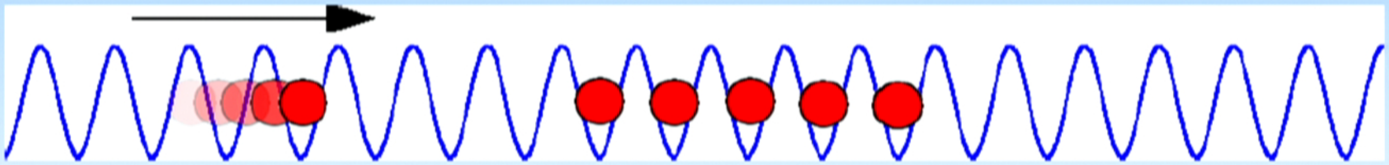
C_{ij}: P_{ij}-$P_i P_j$



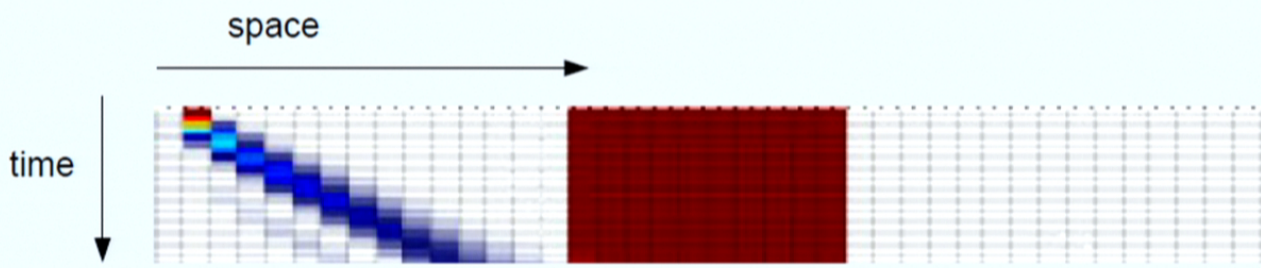


Life-time of two-strings:
Disagreement with experiment!

Solitonic excitations in lattice models



- "Stable" cluster hit by a single particle:
- Spinless fermions, integrabel and non-integrabel version
- Bose-Hubbard model
- Fermi Hubbard model



Stable clusters for spinless fermions and bose hubbard

Spinless fermions:

$$H_{tV} = t\sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right) + V\sum_i (n_i - \frac{1}{2})(n_{i+1} - \frac{1}{2})$$

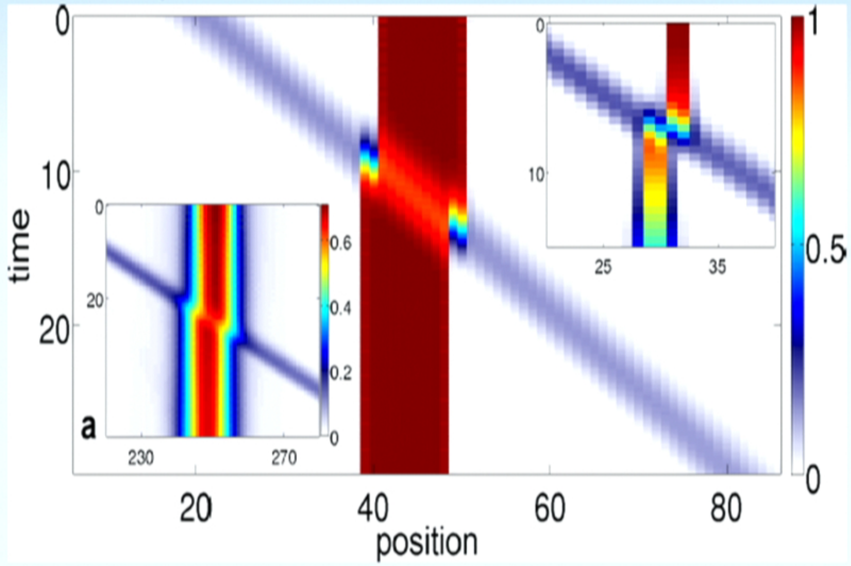
Localized particle hits a "stable" wall of bound particles

No backward scattering

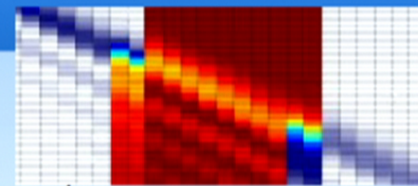
A *hole* moves through the wall!: *Particle-hole transmutation*

Wall moves against the direction of motion by *two* lattice sites

Resembles a fermionic *Quantum Newtons Cradle*. Also like *Klein tunneling:* particle-hole creation

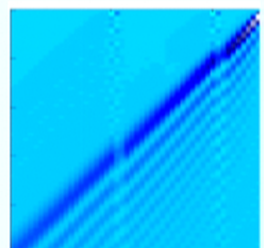


Conservation laws

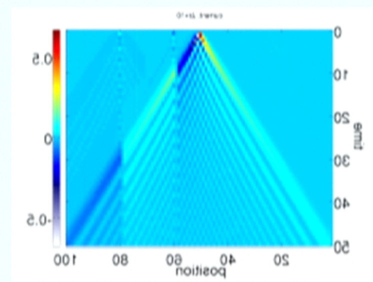


- *Local* interaction: cannot reach through thick wall

- Conserved quantities: *energy current, energy, particle number, …*
- Energy current conservation:
  need movement through wall: only a *hole* possible;
  carries same energy current as particle. Magnetic current is not conserved
- Energy conservation:
  Hole already carries same *energy* as particle
  => *no reflected particle*
- Particle number conservation:
  => *Two* particles must stick to the wall when a particle-hole pair is created
- ***Open question:*** *is full integrability needed, or just energy current conservation ?*



energy current



magnetic current

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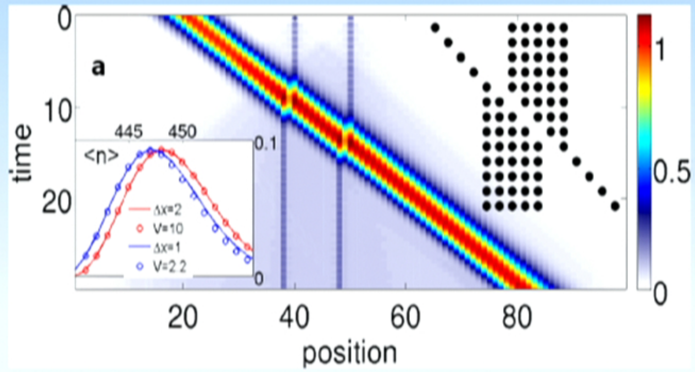
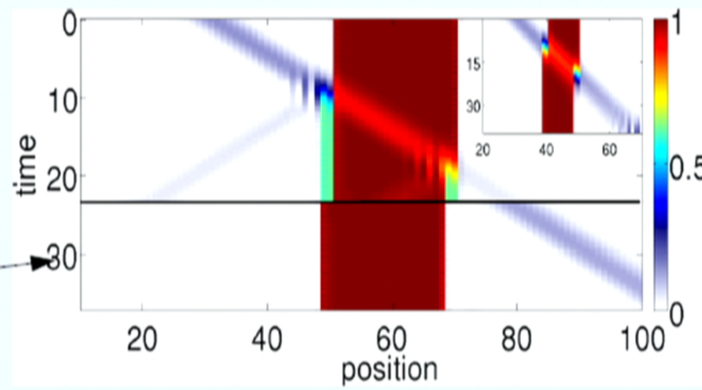
Breaking Integrability

- Bipartite entanglement: classical picture!
- Jump of the signal by two sites!
- Integrability breaking perturbation $V_2 \sum_i n_i n_{i+2}$
- Partial backscattering
- Simple final state:

$$|\Psi\rangle = |T\rangle + |R\rangle$$

- Projection onto probability of having transmission
- Inset: integrabel model with next nearest neighbor hopping: full transmisson





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Bose and Fermi Hubbard model

Fermi Hubbard model:

Cluster: doubly occupied sites

clusters do not bind → large interaction U/t=50

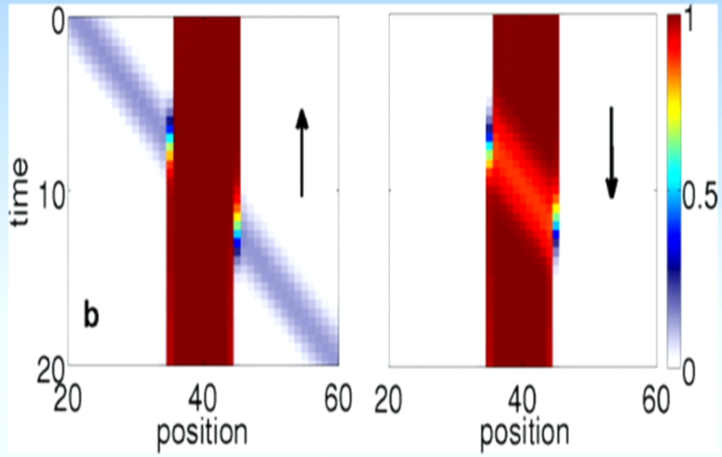
Shift by one site = two particles

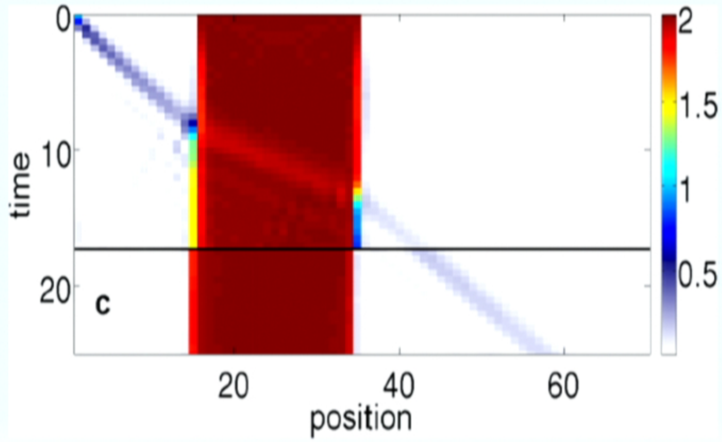
Spin flip of the signal

Bose Hubbard: non-integrable

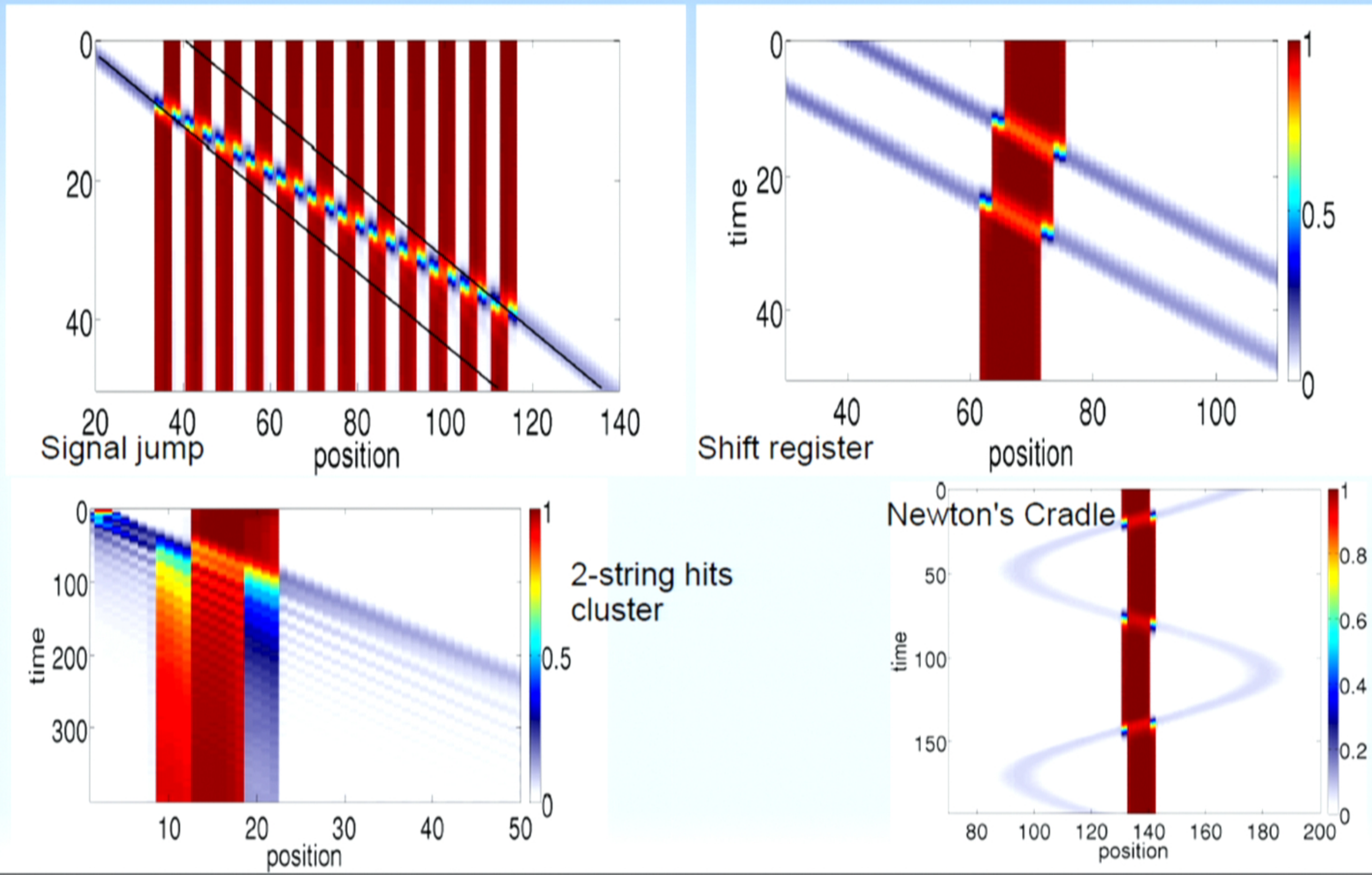
Cluster of doubly occupied sites

Hole travels faster by factor of 2





Toy application



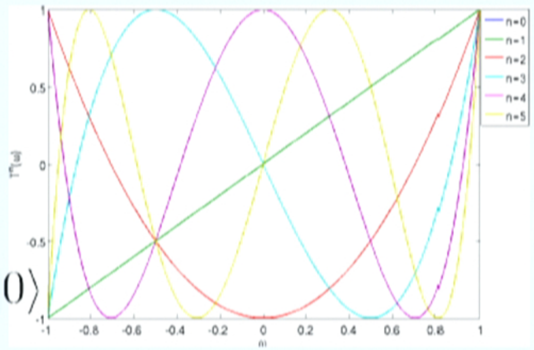
Dynamics II: Spectral functions with the Chebyshev technique

- Spectral function $A(\omega) = \langle 0| c\, \delta(\omega - H)\, c^\dagger |0\rangle$
- Chebyshev orthogonal polynomials: $T_n(\omega) = \cos(n\, \mathrm{acos}(\omega))$
- Use $\delta(\hat{H} - \omega) = \frac{1}{\sqrt{1-\omega}} \left(1 + \sum_{n=1}^{\infty} T_n(\hat{H}) T_n(\omega) \right)$

$$\rightarrow A(\omega) = \frac{1}{\sqrt{1-\omega}} \left(\langle 0| c c^\dagger |0\rangle + \sum_{n=1}^{\infty} \underbrace{\langle 0| c T_n(\hat{H}) c^\dagger |0\rangle}_{\mu_n} T_n(\omega) \right)$$

- Recursion:

$$T_0(\hat{H}) = \mathbb{1},$$
$$T_1(\hat{H}) = \hat{H}$$
$$T_{n+1}(\hat{H}) = 2\hat{H} T_n(\hat{H}) - T_{n-1}(\hat{H})$$



- Use MPS to compute $\mu_n = \langle 0| c T_n(\hat{H}) c^\dagger |0\rangle$
- $|0\rangle$ from DMRG run

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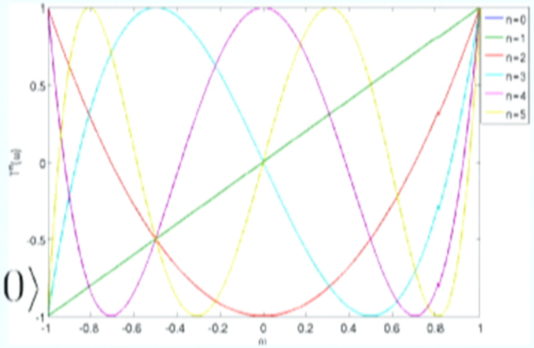

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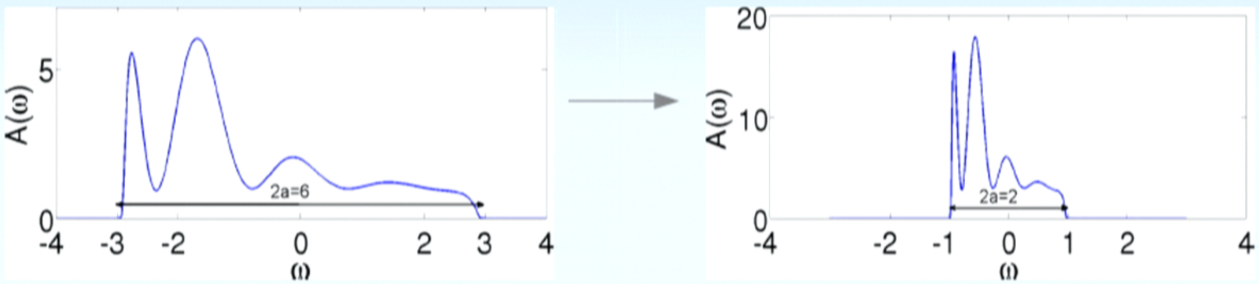
Chebyshev expansion of spectral fuctions

- Chebyshev expansion diverges outside of [-1,1] :

  Need to rescale Hamiltonian:

  $$H \to \tilde{H} = \frac{H - E_0}{a}$$

  single particle excitation spectrum is then contained in [-1,1]



- Calculation of Chebyshev moments μ_n from recursion:

$$\left.\begin{array}{l} |t_0\rangle = c^\dagger |0\rangle \quad |t_1\rangle = \tilde{H}|t_0\rangle \\ |t_n\rangle = 2\tilde{H}|t_{n-1}\rangle - |t_{n-2}\rangle \end{array}\right\} \mu_n = \langle t_0 | t_n \rangle$$

- Groundstate $|0\rangle$ from DMRG run
- *All steps can be done using MPS*

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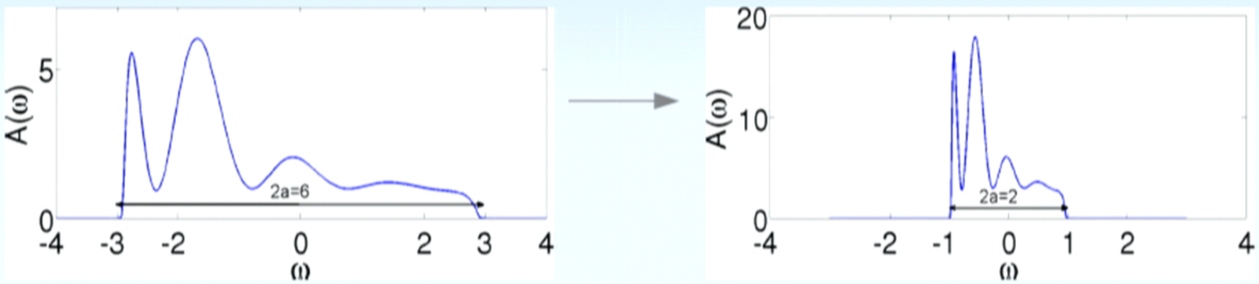

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Goals

- **Calculate spectral functions of 1-d systems at T=0**
- **Impurity solver for DMFT**
  - Existing techniques:
    - *ED:* only small systems
    - *NRG*: fast, high resolution at $\omega \approx 0$, bad resolution at high ω; hard for multiorbital
    - *DDMRG*: very accurate, very expensive
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Chebyshev expansion of spectral functions

Difficulties:

- With finite expansion order N
  - Get finite resolution $\propto 1/N$
  - Gibbs oscillations from hard cutoff (similar to Fourier series):
    - Usually: use damping: $\mu_n \to \tilde{\mu}_n = g_n \mu_n$
    - e.g. Lorentz damping $g_n^L = \dfrac{\sinh(\lambda(1 - n/N))}{\sinh(\lambda)}$
- Energy truncation:
  - Numerical inaccuracies/compression of matrix dimension $\to$ diverging recursion series
  - Existing approach: At every site, build Krylov-subspace of effective DMRG-hamiltonian, diagonalize it and cut off high energies: Slow; can introduce systematic error

Example with damping: exactly solvable Resonating Level Model

- Non-interacting orbital, coupled to non-interacting (finite) bath:

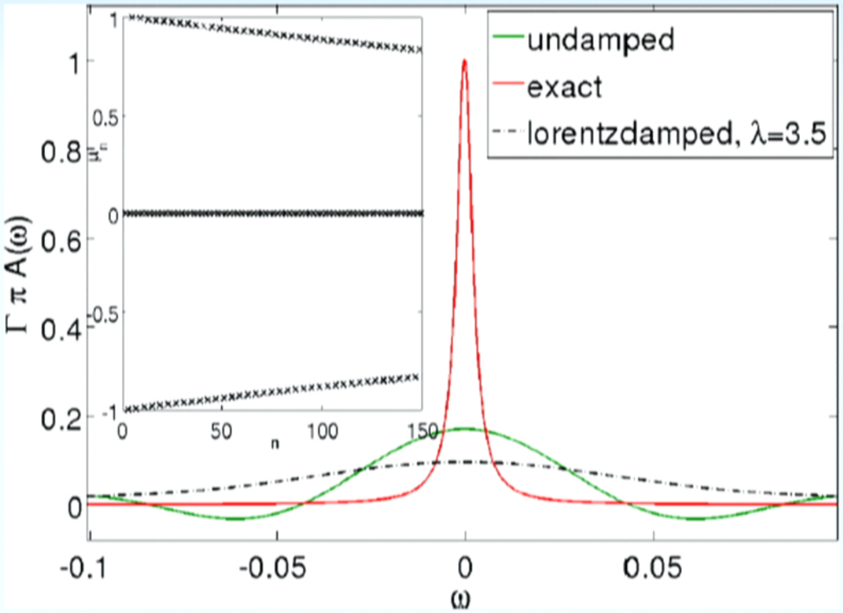
$$H = \epsilon_f n_0 + \sum_k \epsilon_k n_k + V \sum_k (c_0^\dagger c_k + h.c.)$$

- Rectangular hybridization

$$\Gamma = \pi V^2 \rho_0(0) = 0.005$$

→ spectrum has narrow peak

- Lorentz damping ($\lambda = 3.5$) removes oscillations, but **resolution** !



Improving resolution: linear prediction

- For analytic functions $A(\omega)$, moments μ_n *decay exponentially fast,* usually with damped oscillations

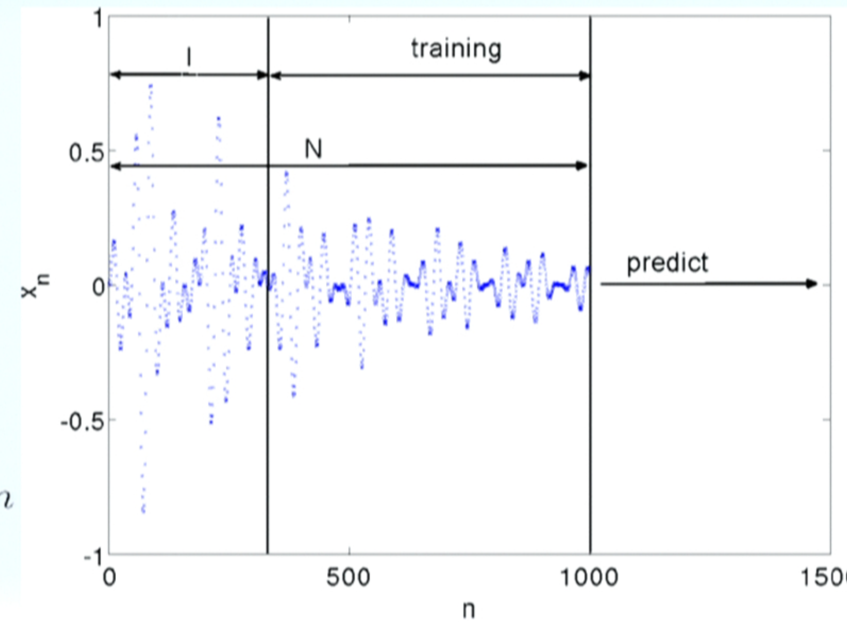
Idea: **Use linear prediction method to estimate additional moments**

- Given time series $\{x_n\}, n = \{1, 2, \ldots, N\}$ make ansatz for x_{N+1} using l previous data points:

$$x_{N+1} = -\sum_{n=0}^{l-1} a_n x_{N-n}$$

- Optimize ansatz on training given data points:

$$\left.\begin{aligned} &\min_{a_n} \sum_{n=l}^{N} (\tilde{x}_n - x_n)^2 \\ &\tilde{x}_n = -\sum_{i=0}^{l-1} a_i x_{n-i} \end{aligned}\right\} \rightarrow a_n$$



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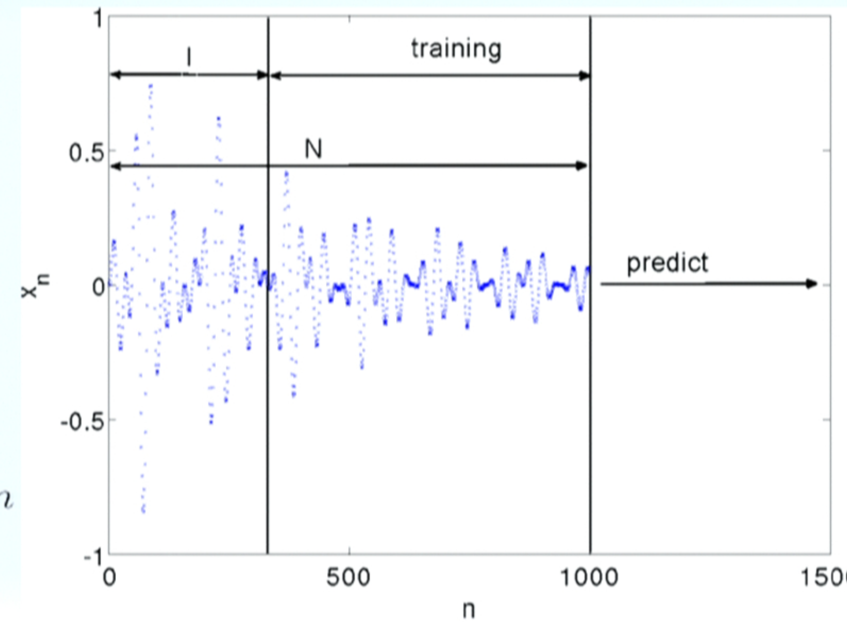
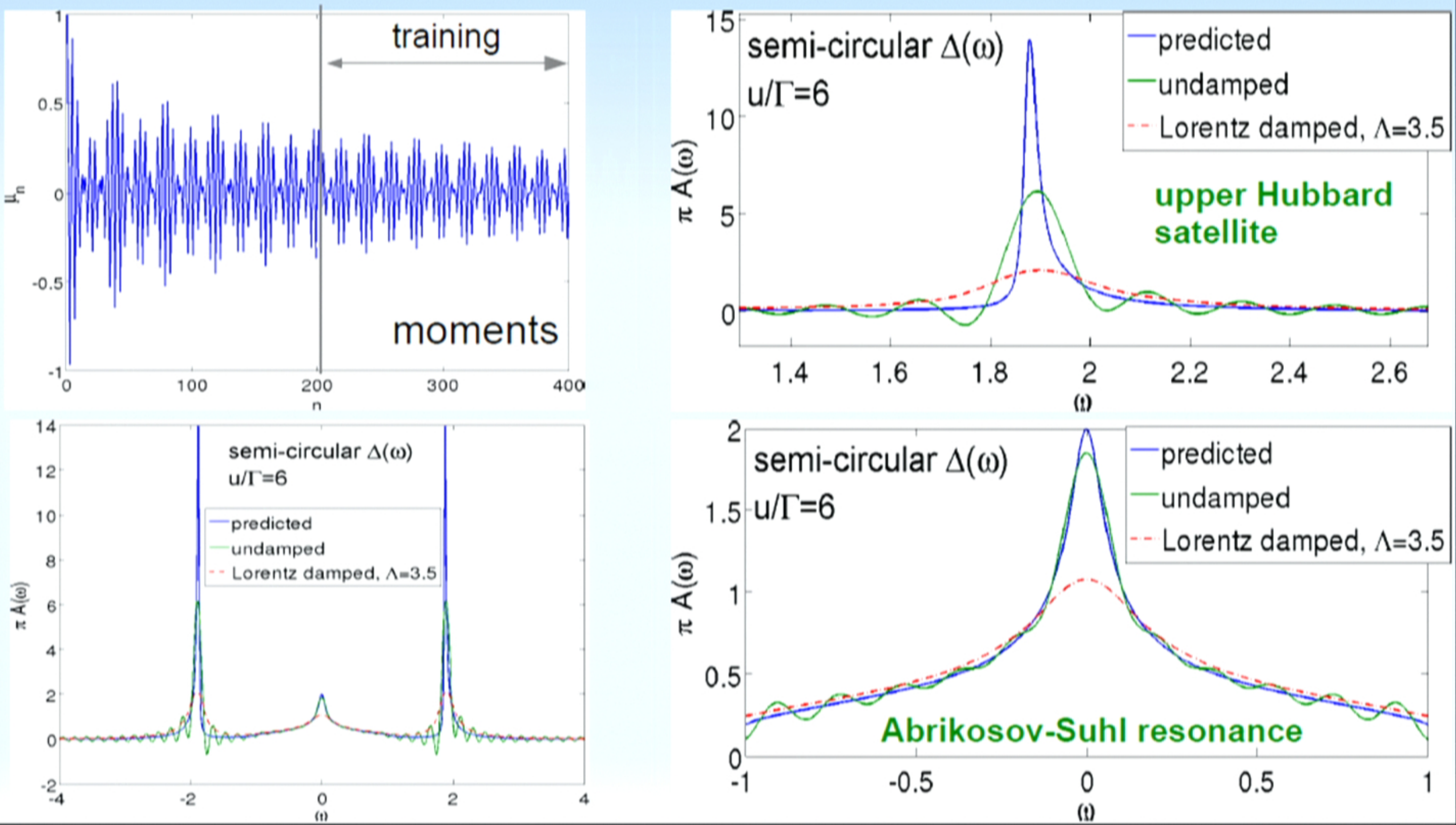


Results for the interacting model: SIAM

$\Gamma = \pi V^2 \rho_0(0) = 0.5$, $U = 3$, Chainlength=120 sites, $\lambda = 200$,
$a = 12$, N_{train} =200, 8000 predicted moments, semicircular $\Delta(\omega)$



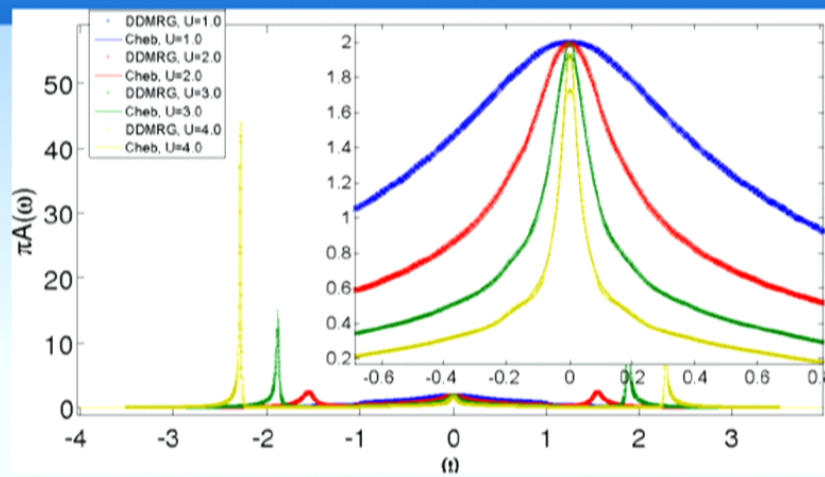
Test of precision for interacting model: Chebyshev-MPS vs DDMRG

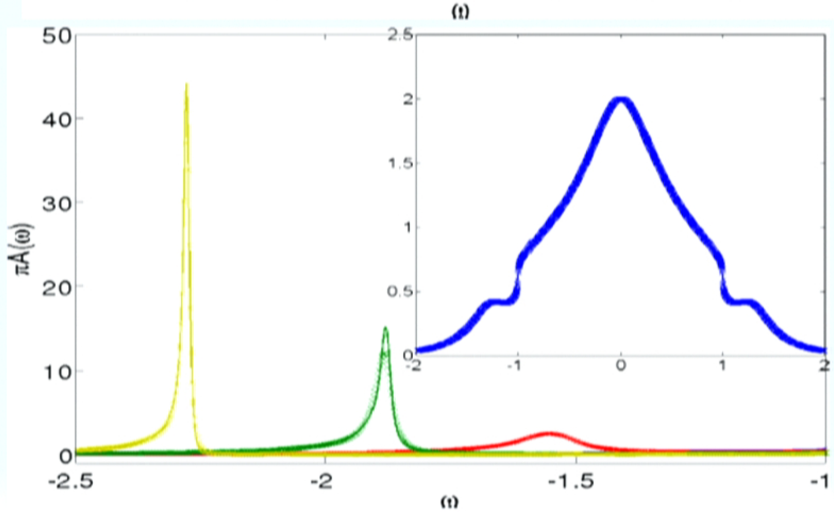
$$\Gamma = \pi V^2 \rho_0(0) = 0.5$$

$$U/\Gamma = 2, 4, 6, 8$$

Friedel sum rule better than in DDMRG

Raas, Uhrig, Anders, PRB 69, 041102(R), ('04),
Raas, Uhrig, EPJ B 45 (3), 293 ('05)

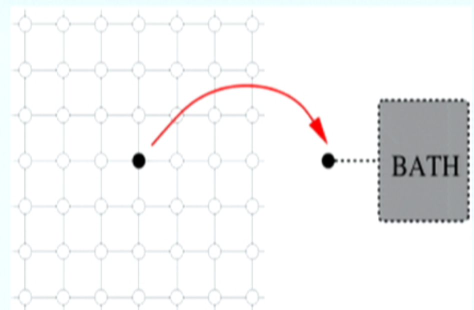




Dynamical Mean-Field theory

- **Goal:** local spectral density $A(\omega)$ of interacting, d-dimensional lattice model
- How? Emulate interacting lattice-influence by suitable, free lattice → map to an **impurity problem**

$$\Delta(\omega) = \sum_{\nu} \frac{|V_\nu|^2}{\omega + i\eta - \epsilon_\nu}$$



Variational parameters:
hybridization and bath-dispersion

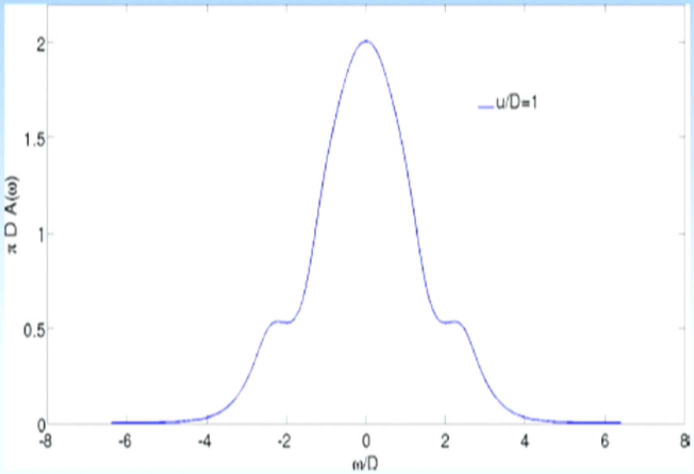
Self-consistency equation

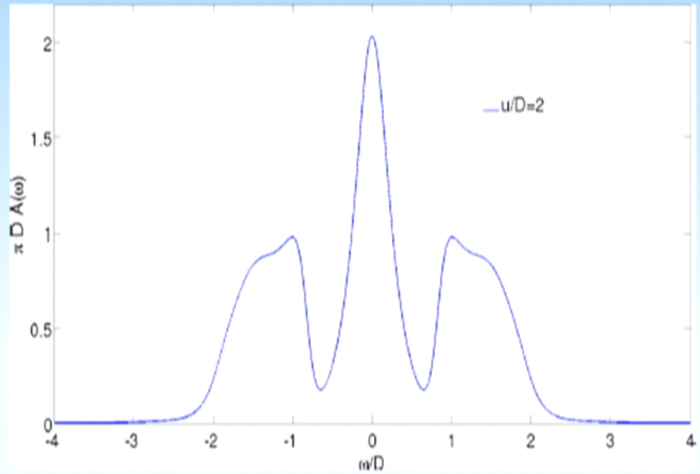
$$G^{lat}(\omega) = \int d\epsilon \frac{\rho(\epsilon)}{\Delta(\omega) + [G^{imp}(\omega)]^{-1} - \epsilon} \stackrel{!}{=} G^{imp}(\omega)$$

DOS of the original, non-interacting lattice

Impurity Greens function

DMFT for Hubbard model on Bethe lattice





$\rho(\epsilon)$: semic-circular with bandwidth D

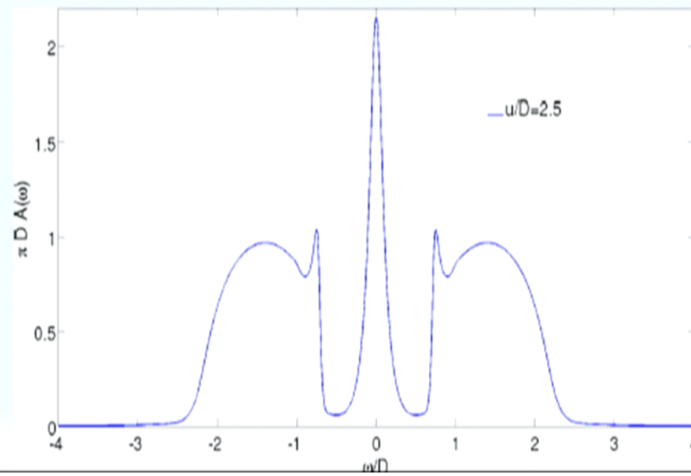
Exact results!

Formation of **quasiparticle peak**

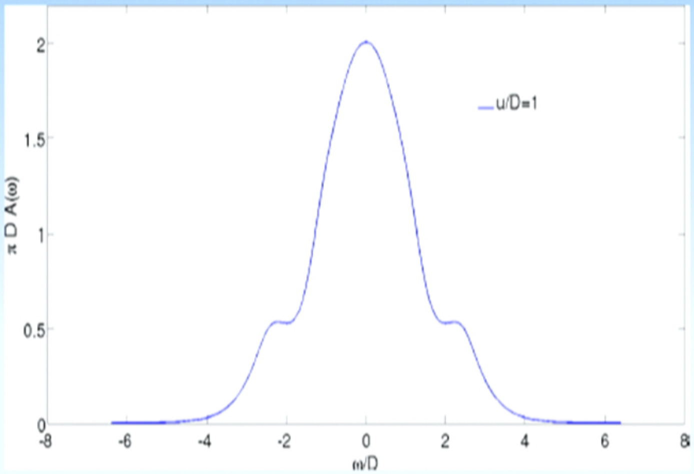
Hubbard satellites

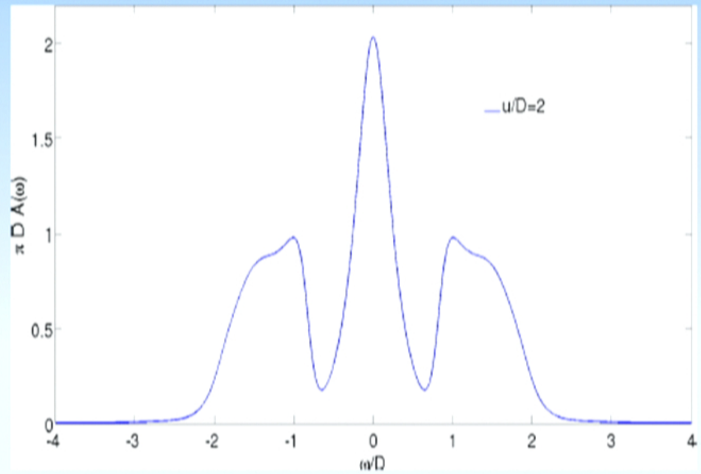
Special feature at inner edges of Hubbard satellites

U/D=2.8 hard to stabilize



DMFT for Hubbard model on Bethe lattice





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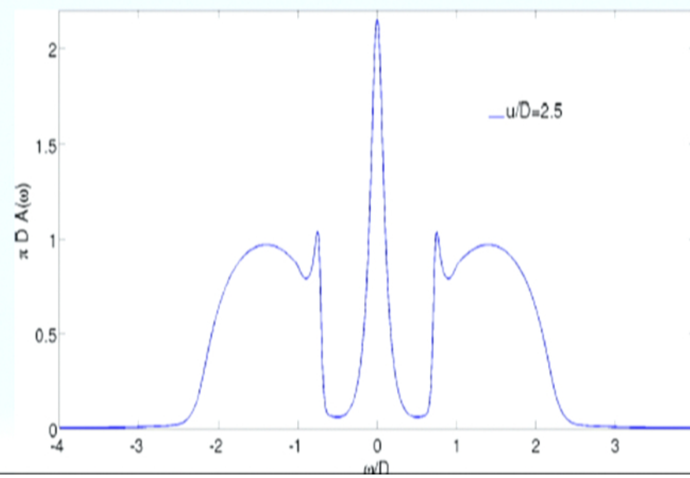


Chebyshev expansion without energy truncation

- **Idea: Use better rescaling function**

$$\frac{H}{a} \quad \rightarrow \quad \mathbb{1} - \exp(-\tau H)$$

- **Spectrum of** $\mathbb{1} - \exp(-\tau H)$ **is contained in [0,1]**

  $\rightarrow$ **No energy truncation needed**

- $\exp(-\tau H)$ can be trotterized

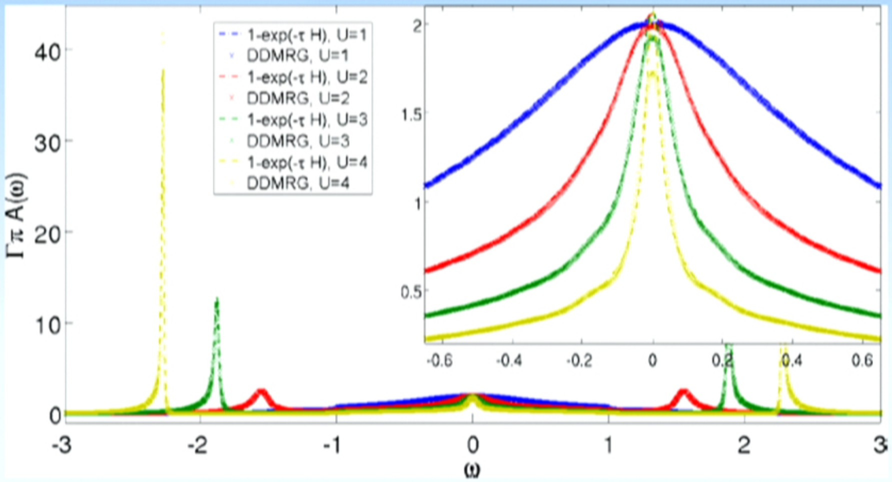
  $\rightarrow$ efficient algorithms available (tDMRG,TEBD,tMPS)

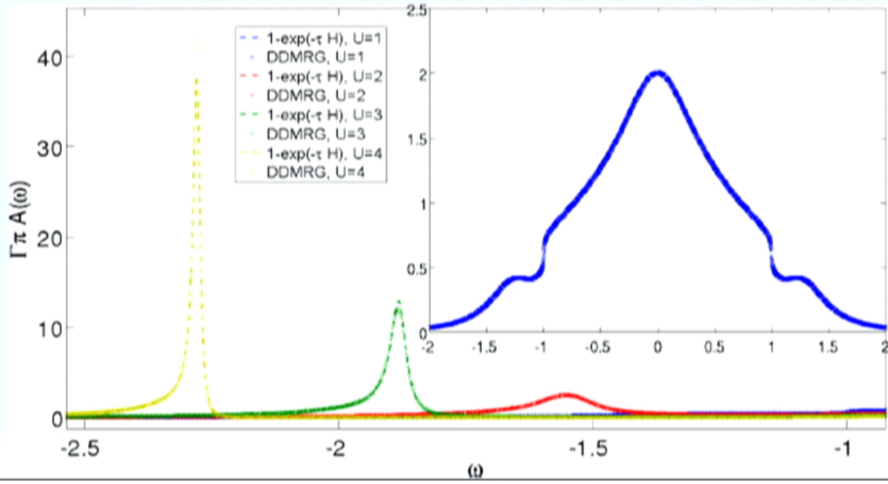
- Similar resolution

$\mathbb{1} - \exp(-\tau H)$ Chebyshev vs. DDMRG

$\Gamma = \pi V^2 \rho_0(0) = 0.5$

$U/\Gamma = 2, 4, 6, 8$





TEBD as DMFT solver

- Spectral function in real time:

$$A(t) = \frac{1}{2\pi}(G^{>}(t) + G^{<}(t))$$

compute $G^{<}(t) \equiv \langle 0| c^{\dagger} e^{iHt} c |0\rangle \quad G^{>}(t) \equiv \langle 0| c e^{-iHt} c^{\dagger} |0\rangle$

$$G^{>}(t) = (G^{<}(t))^{*} = G^{<}(-t)$$

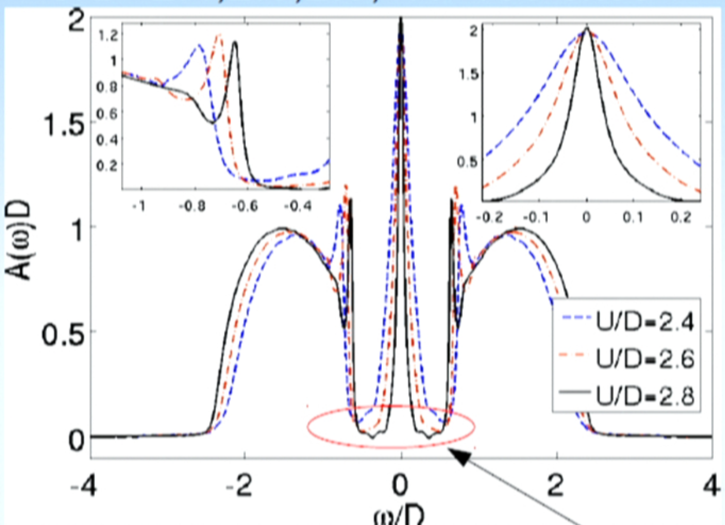
particle-hole symmetry: hermiticity

Fourier-transform $\rightarrow A(\omega)$

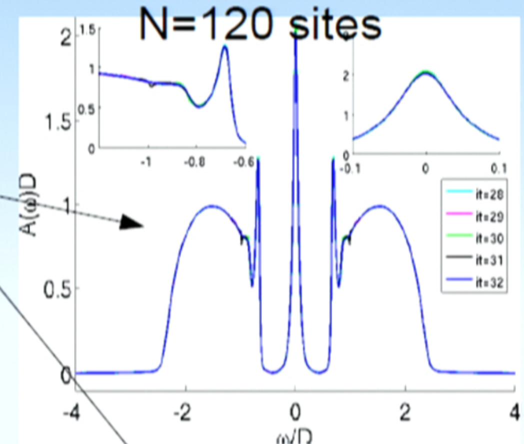
Use linear prediction to improve resolution

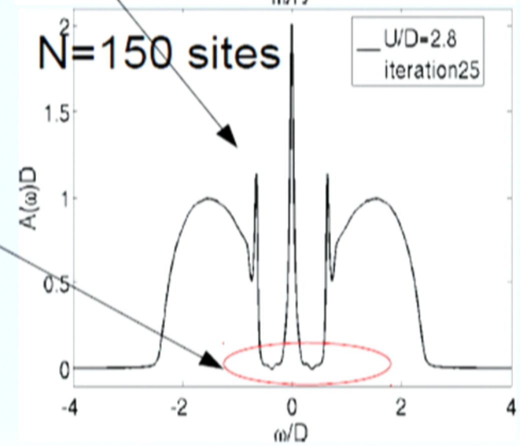
TEBD as DMFT solver

U/D=2.4,2.6,2.8, N=150 sites



U/D=2.8





Very fast! Single spectrum ~ ½ h

Wiggles: artifacts!

Conclusions

- Dynamics of many-body quantum systems with Matrix Product States
- Quenches in the XXZ model:
  - Spinon propagation, 2 and 3 string propagation
  - Robust against perturbations
  - Realized in experiment (Nature 502, 76-79 (2013))
- Solitonic excitations in lattice models:
  - New, unexpected physics
  - Role of integrability
  - Cold atoms?
- Greens functions using Chebyshev expansions:
  - Promising alternative to DDMRG
  - Extensions: linear prediction
  - Alternative expansion using exponentials
  - Real time methods are promising impurity solvers!
- Quantum transport through interacting quantum dot