Spectral functions from the time dependent density matrix renormalization group

- DMRG
  - Low entanglement approach
  - Curent capabilities
  - tDMRG
- How to use tDMRG for spectral functions
- S=1 Heisenberg chain, S=1/2 XXZ chain

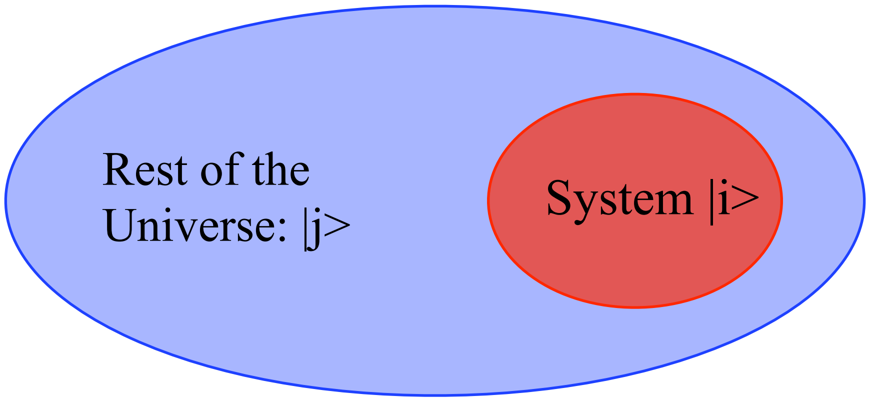
collaborators:

UCIrvine
University of California, Irvine

Adrian Feiguin, Ian Affleck, Rodrigo Pereira, Sasha Chernyshev

Origins of DMRG--RG, Stat Mech

- RG: throw away unimportant states, effective H in truncated basis (Ken Wilson, "NRG")
- Statistical Mechanics Viewpoint (Feynman SM lectures)



$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle$$

$$\rho_{ii'} = \sum_{j} \psi^*_{ij} \psi_{i'j}$$

$$\langle A \rangle = \sum_{\alpha=1}^{m} w_\alpha \langle \alpha | A | \alpha \rangle$$

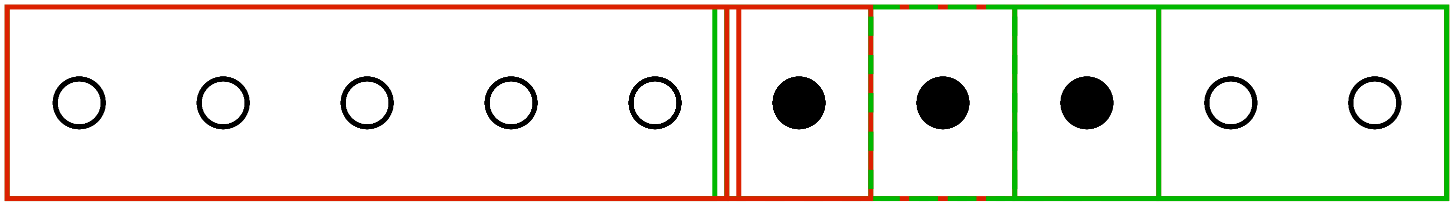
- Key idea: throw away eigenstates with small probability
- Algorithm based on this: density matrix renormalization group (DMRG, srw(1992))

DMRG as a low entanglement approximation

- Vidal, Verstraete, Cirac: DMRG and QI **entangled**.
- Entanglement: Which is more entangled?
  - 1) $|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$ or
  - 2) $|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$??
- Answer: 1) is perfectly entangled. 2) is unentangled:
  - $(|\uparrow\rangle + |\downarrow\rangle)\ (|\uparrow\rangle + |\downarrow\rangle)$
- To measure entanglement, must change to the Schmidt basis where the Ψ is diagonal: $\Psi = U\,D\,V$
- Density matrix eigenvalues are square of D !
  - $\rho = U\,D^2\,U^\dagger$
- Now QI is supplying many ideas to DMRG!

DMRG Algorithm

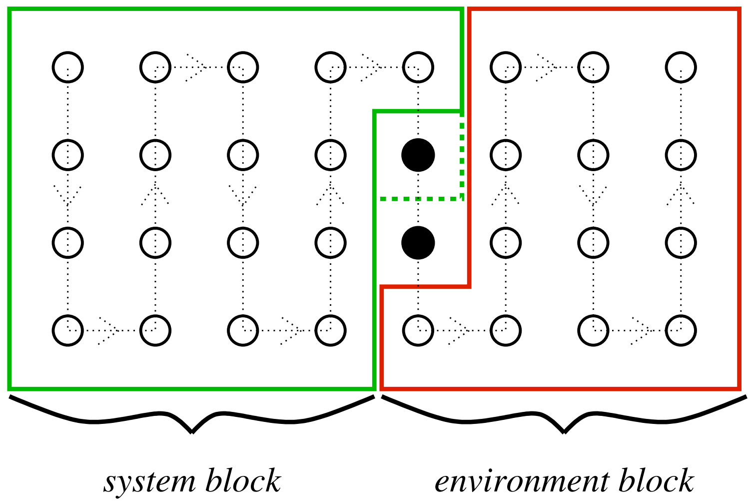
- Finite system method:



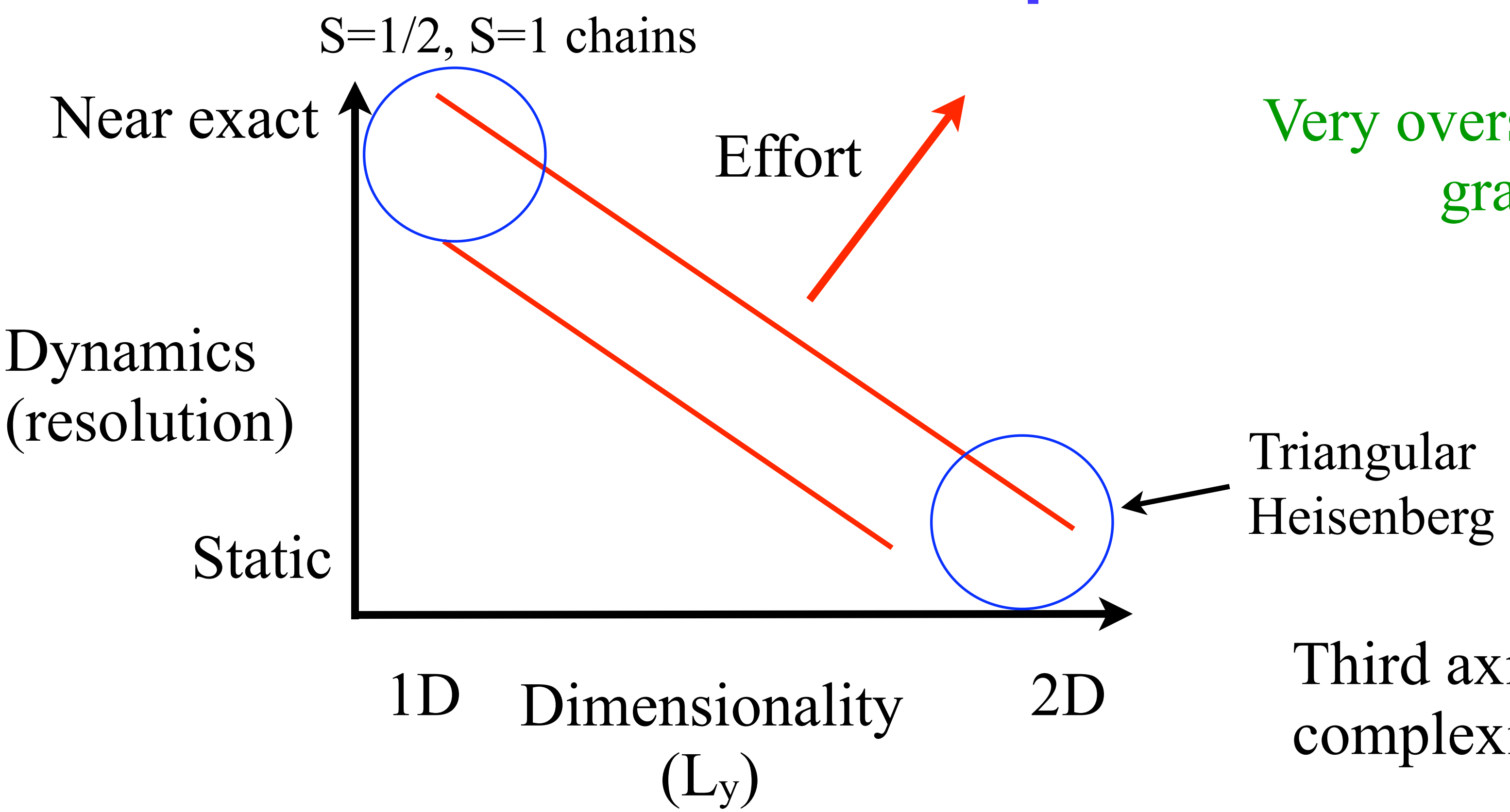
- Wavefunction = matrix product state(Ostlund & Rommer, 1995)

$$\psi(s_1, s_2, \ldots) = \mathrm{Tr}\{A_1^{s_1} A_2^{s_2} \ldots\}$$

- 2D: map onto chain
  - Accuracy falls of exp'ly in width



Current capabilities

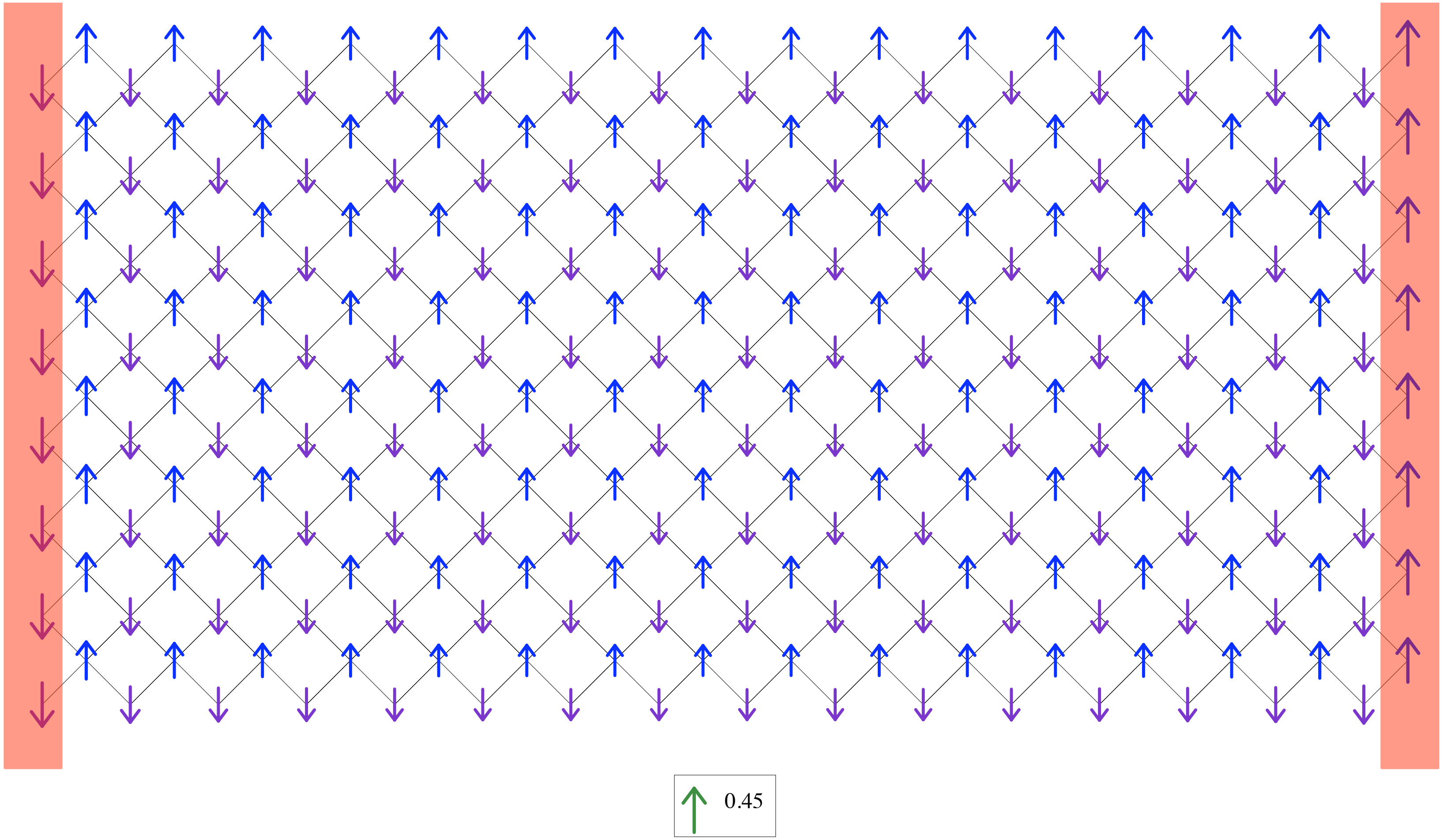


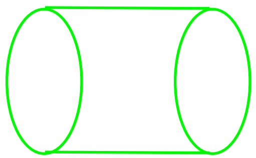
Very oversimplified graph

Third axis (not shown): complexity of model

- Computational scaling to 2D
  - TV-scan 1D DMRG cpu ~ $L_x\, L_y\, m^3$, $m \sim \exp(a\, L_y)$
  - Projected entangled pair states (PEPS, tensor prod states):
    - cpu ~ $L_x\, L_y\, m^{10}$, $m \sim$ constant ~ 10 (x 1000's of iterations)

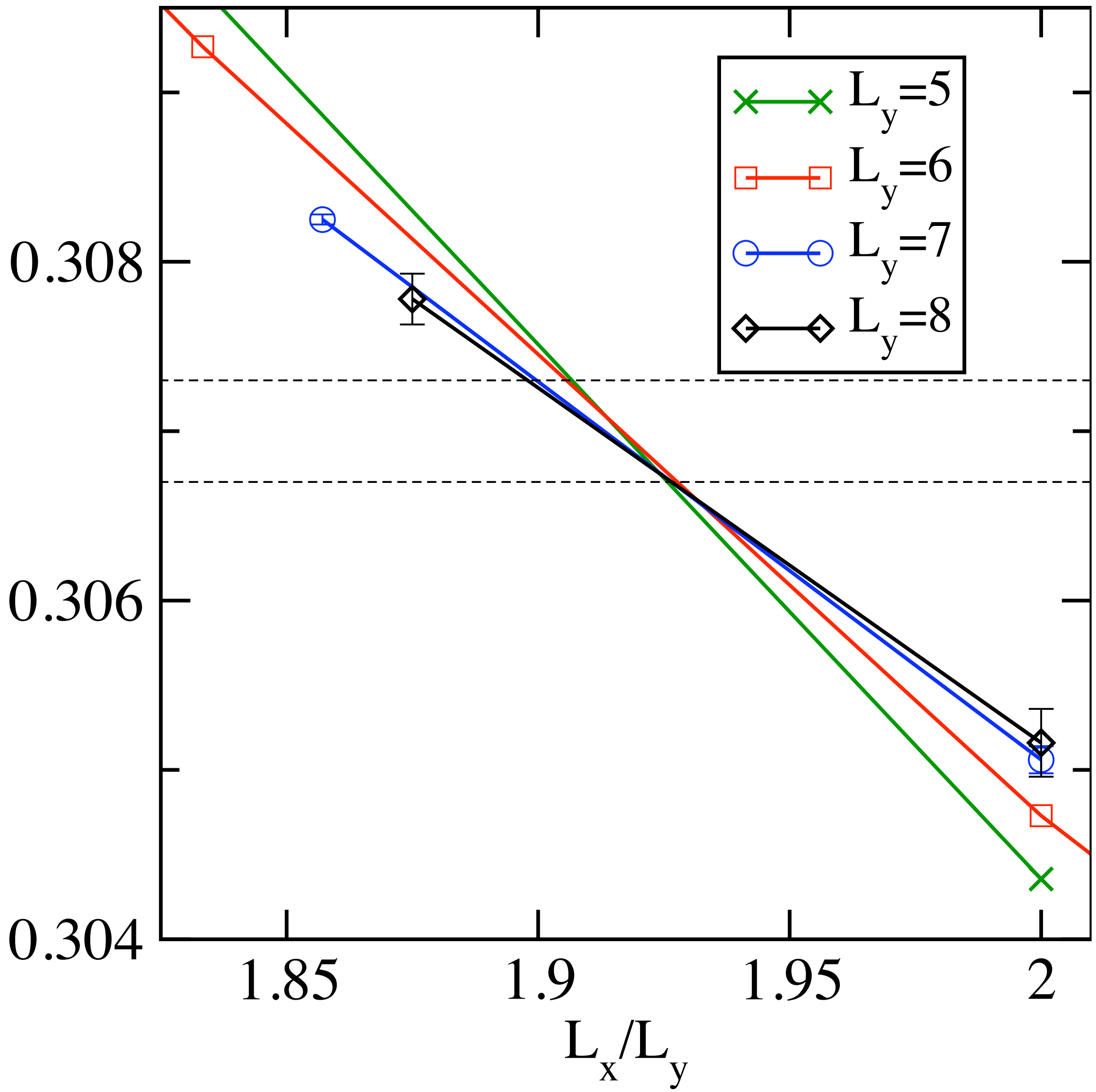
Heisenberg square lattice





- Tilted lattice has smaller DMRG errors for its width
- For this cluster obtain M = 0.3052(4) in center
- “Exact” 2D M = 0.307 (Sandvik, QMC)
- Standard PBC cluster, this size, M = 0.34

Heisenberg square lattice

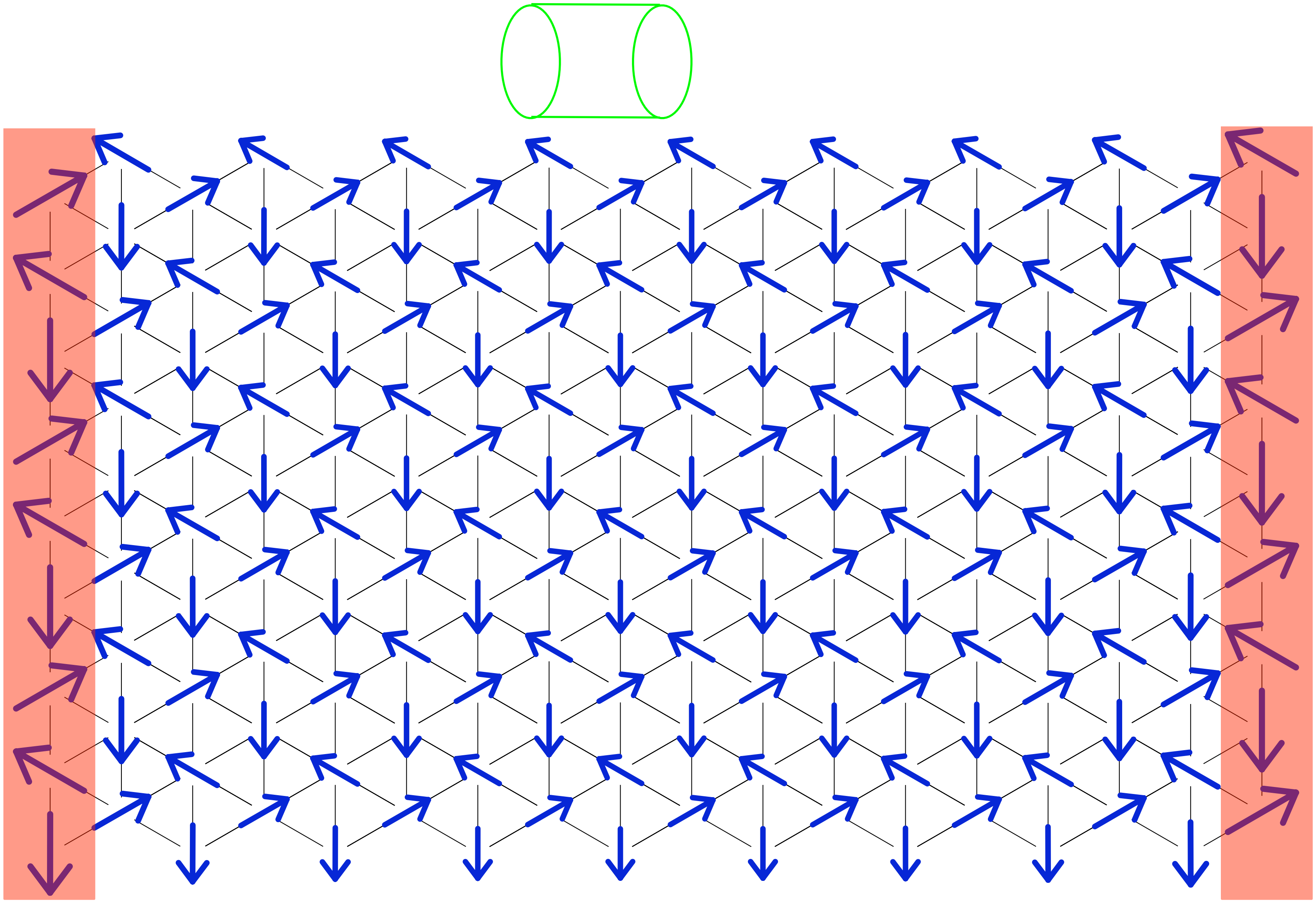


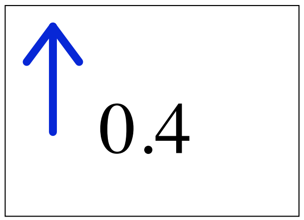
Sandvik QMC (error bars)

New finite size scaling approach using cylindrical BCs

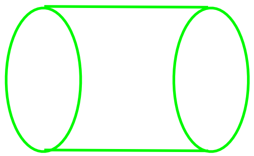
See White and Chernyshev, PRL 99, 127004 (2007).

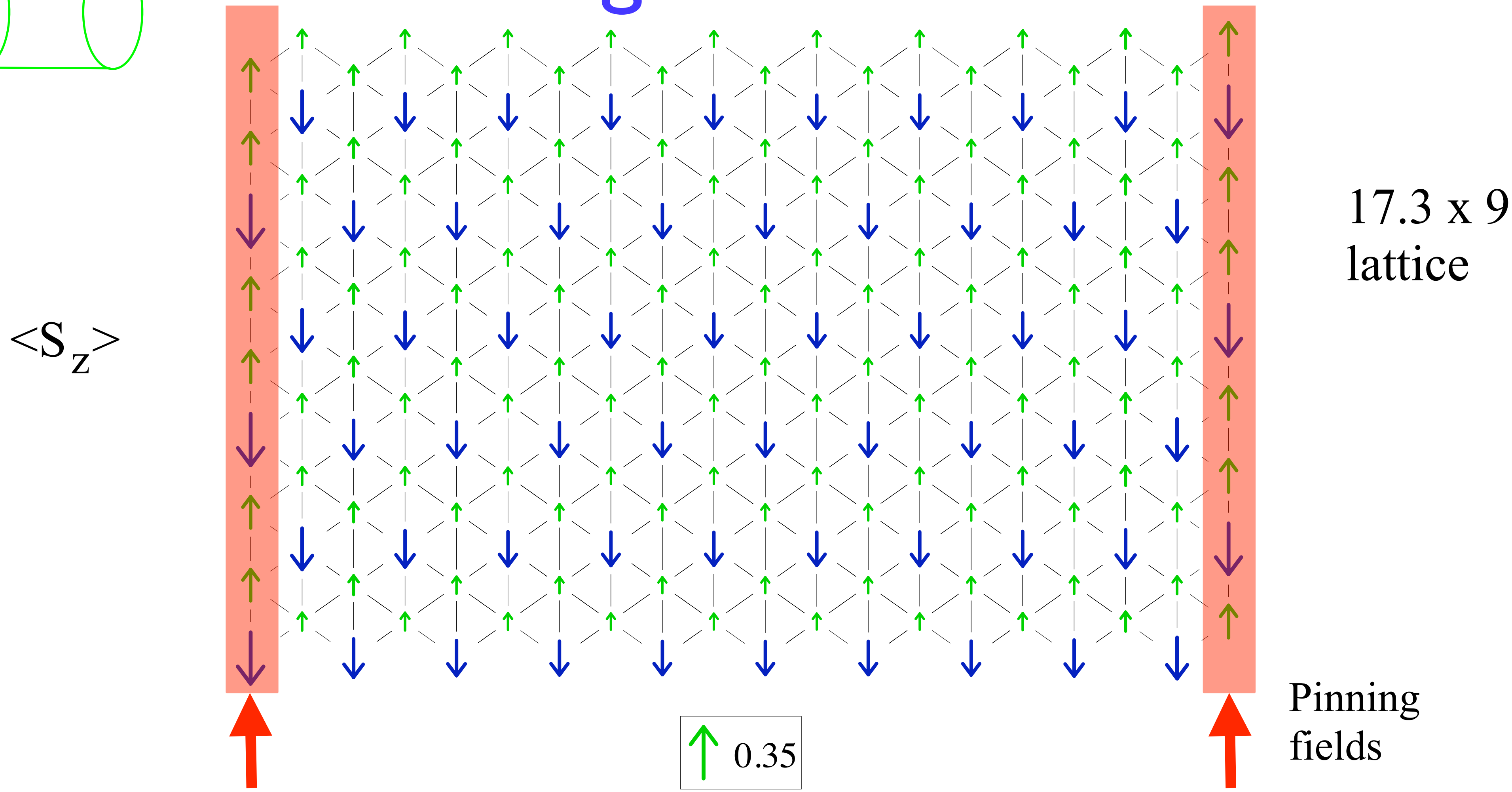
Triangular Heisenberg, pinned cylindrial BCs





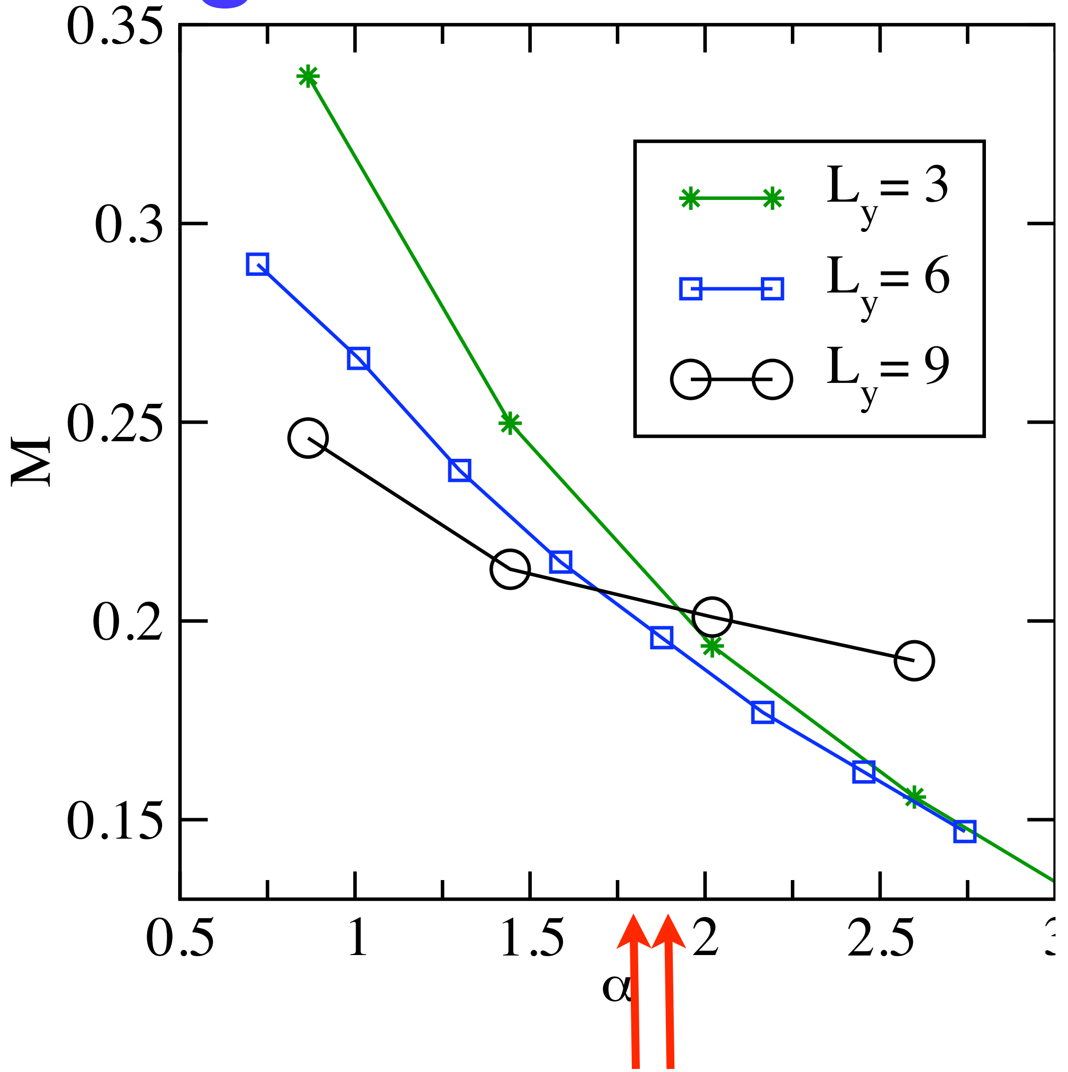
Triangular Lattice





- Only one sublattice pinned, other two rotate in a cone
- Other two have z component -M/2
- Here only have L_y= 3, 6, 9, ...

Triangular lattice, Scaled Data



Results are consistent with, and as good as best GFMC and series expansions.

See White and Chernyshev, PRL 99, 127004 (2007).

Back to 1D: Time Evolution (Vidal,...)

Suzuki Trotter decomposition:

$$\exp(-iH\tau) \approx \exp(-iH_{12}\tau)\ \exp(-iH_{34}\tau)\ \ldots\ \exp(-iH_{23}\tau)\ \ldots$$

Key idea: adapt basis to each instant of time

Each sweep = one time step

Fourth order breakup--negligible time step errors

Growth of entanglement with t: stop after moderate time

Calculation of Spectral functions

- Start with standard ground state DMRG, get φ
- Apply operator to center site

$$|\psi(t=0)\rangle = S_0^+|\phi_0\rangle$$

- Time evolve:

$$|\psi(t)\rangle = e^{-i(H-E_0)t}|\psi(0)\rangle$$

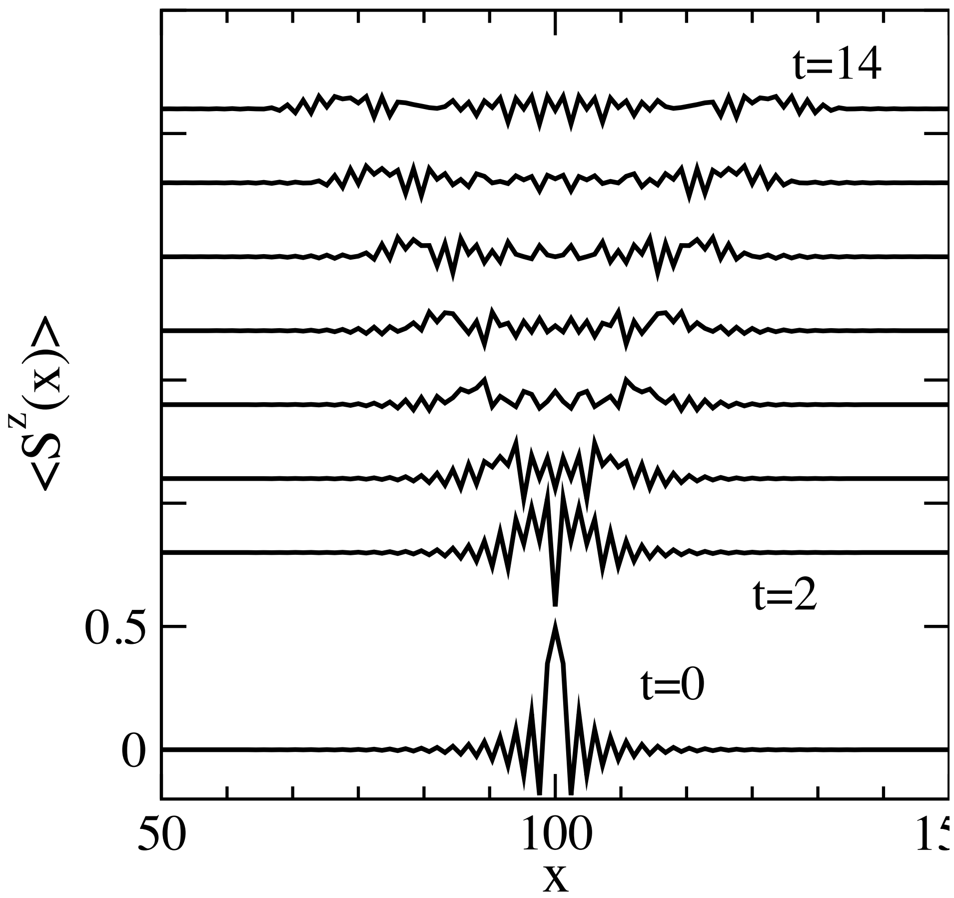
- Measure time dependent correlation function

$$G(x,t) = \langle\phi_0|S_x^-|\psi(t)\rangle = \langle\phi_0|S_x^-(t)S_0^+(0)|\phi_0\rangle$$

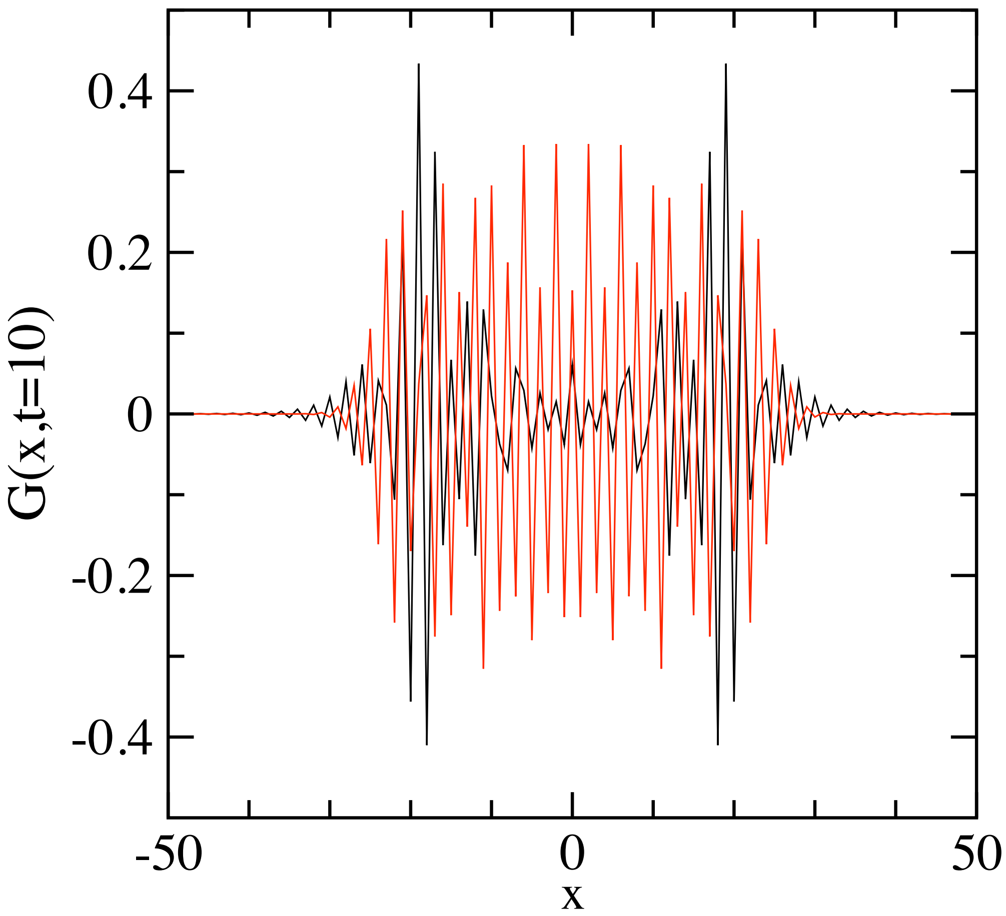
- Fourier transform with x=0 to get N(ω) or in x and t to get S(k,ω)
  - But what about finite size effects, finite time, broadening, etc??

Finite size effects: gapped systems

S=1 Heis chain

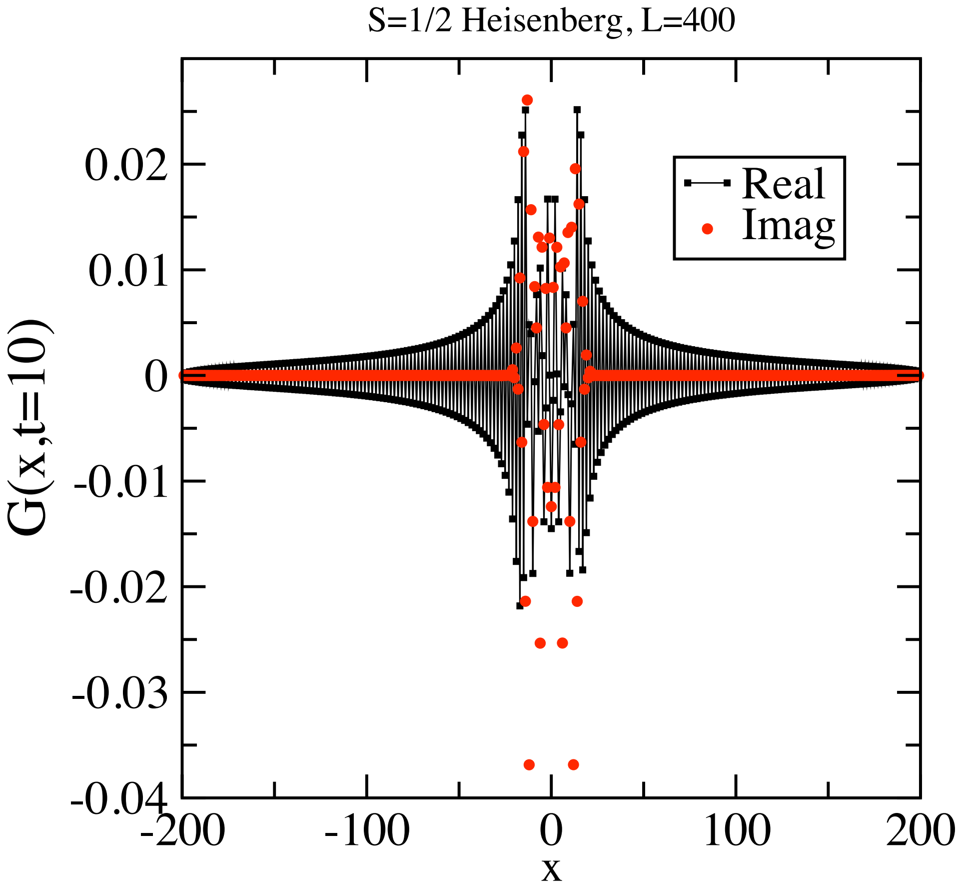


Real and Imag parts

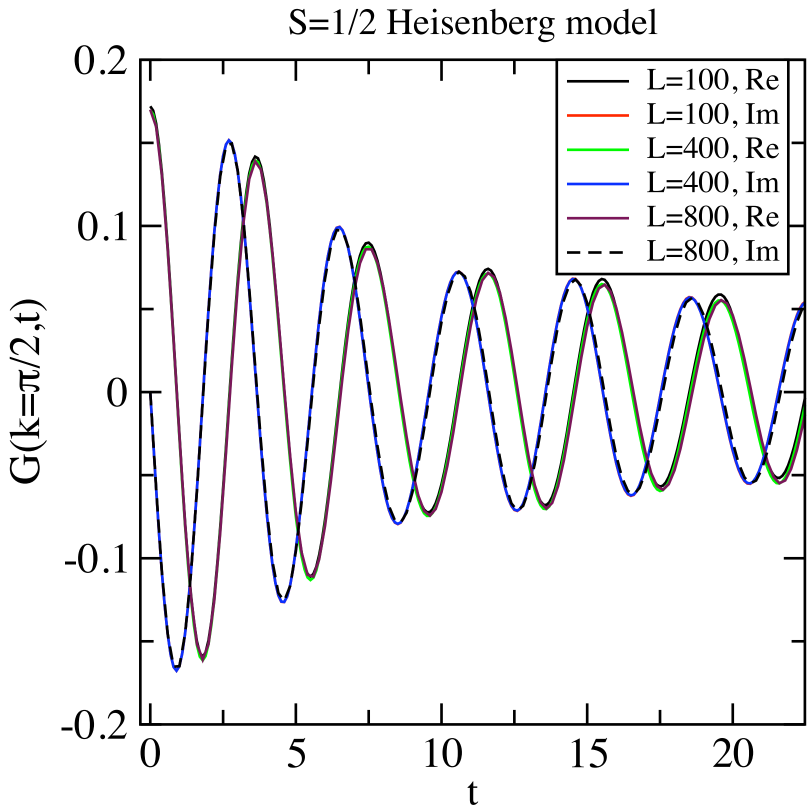


For $t < L/(2\,v)$, finite size effects are negligible.

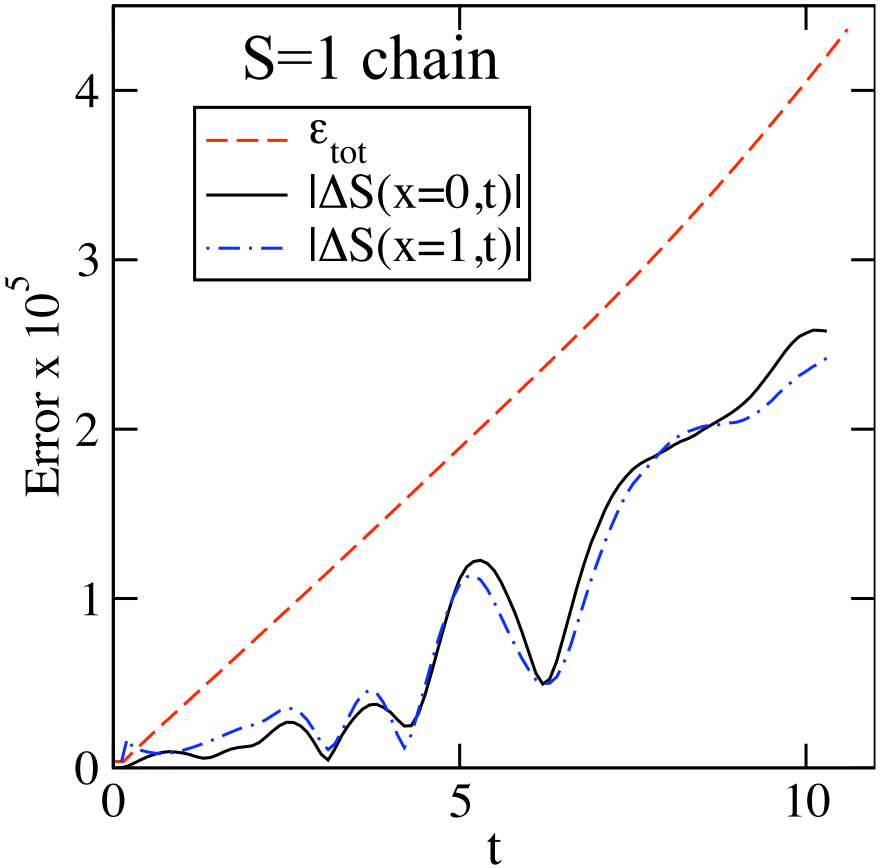
Finite size effects: gapless systems



For $t < L/(2\ v)$, finite size effects are negligible in the imaginary part. Fourier transform can be done just on the imaginary part (then throw away negative freq part).



Errors in time evolution



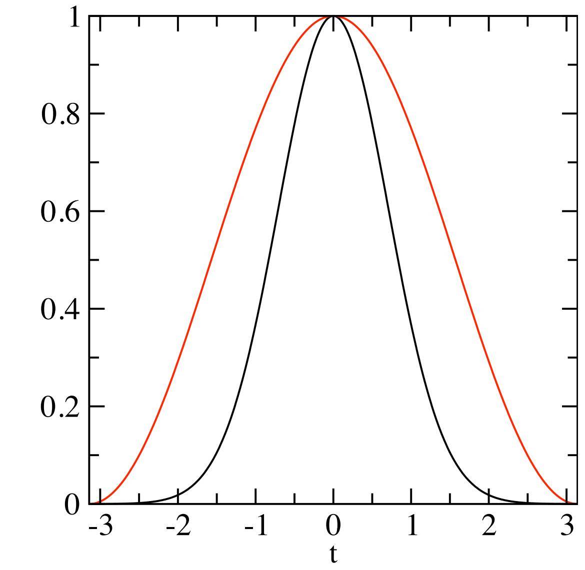
Errors vary as total summed truncation error. Here a specified truncation error was specified and m slowly grew.

Conclusion: We can obtain very accurate data representing the thermodynamic limit up to t=20-40. Beyond that the numerical work grows rapidly.

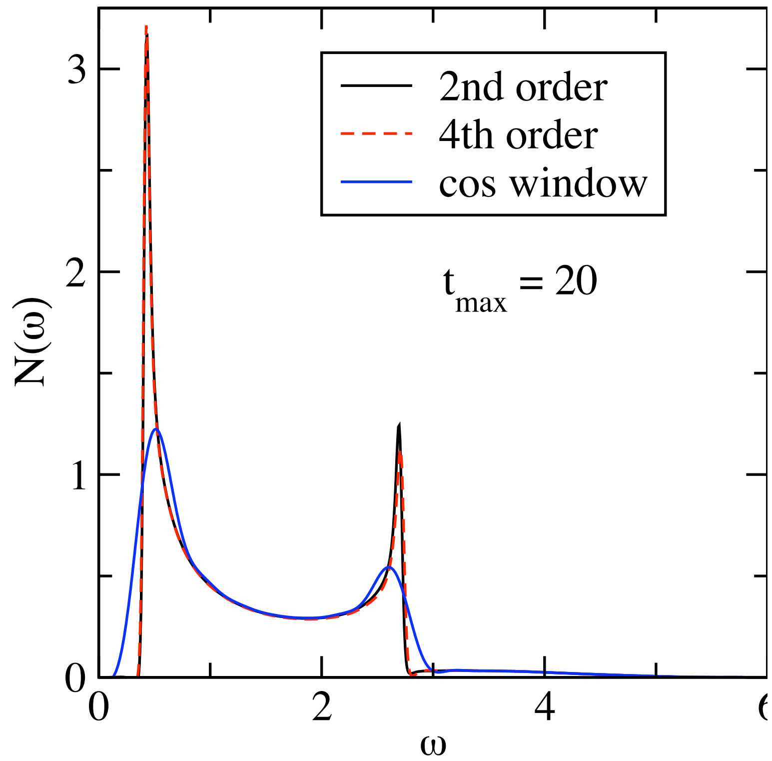
Note: one run gives all k and ω (but need to worry about broadening in ω).

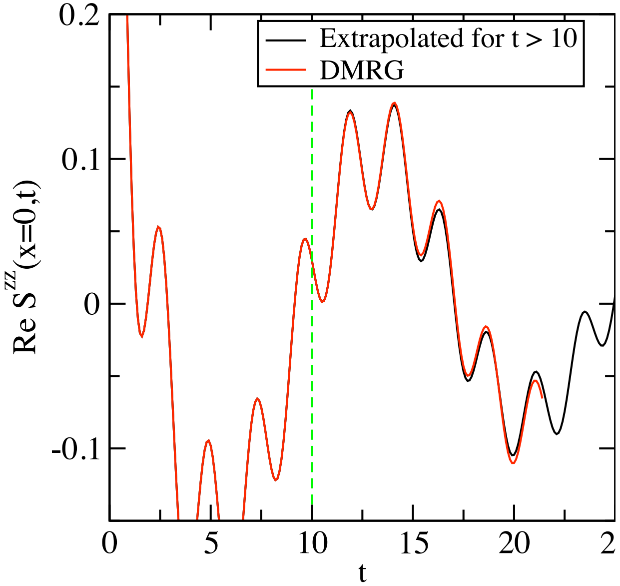
Extrapolation to large time: linear prediction

S=1 chain



Windows
for time
FT





$$y_i = \sum_{j=1}^{n} d_j y_{i-j}$$

See *Numerical Recipes*

Parameters d_j determined from correlation functions of available data.

Extrapolation in time: fitting singularities

- The large time behavior is usually very simple, determined by a few singularities in the spectrum often giving oscillating power law decay.
- We can fit the larger time data to asymptotic forms and extend the data to very large times.
- Example: $N(\omega)$ for S=1 chain: inverse square root singularities come from top and bottom of magnon band

Fitting edge singularities

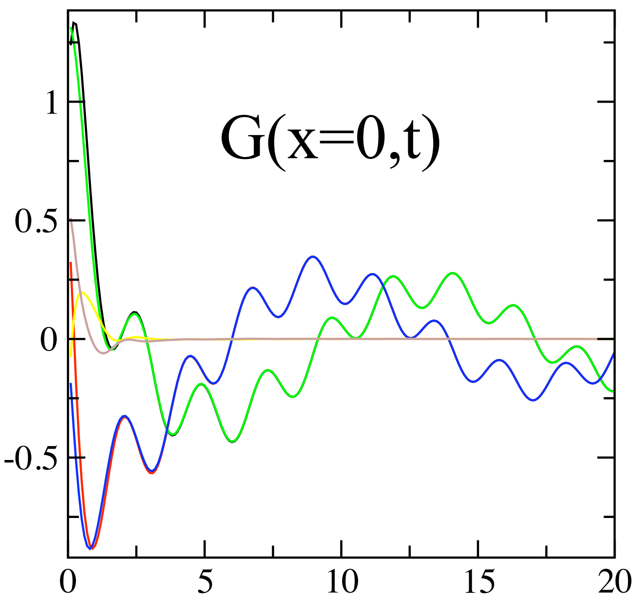
The following identity fits lower edge singularities:

$$\int_{-\infty}^{\infty} d\omega e^{-i\omega t}\theta(\omega - b)e^{-a(\omega-b)}(\omega - b)^g = \Gamma(1+g)e^{-ibt}(a+it)^{-1-g}$$

Only the r.h.s. is used: the fit is used to extend the data, then we FT

Simulated annealing fit:

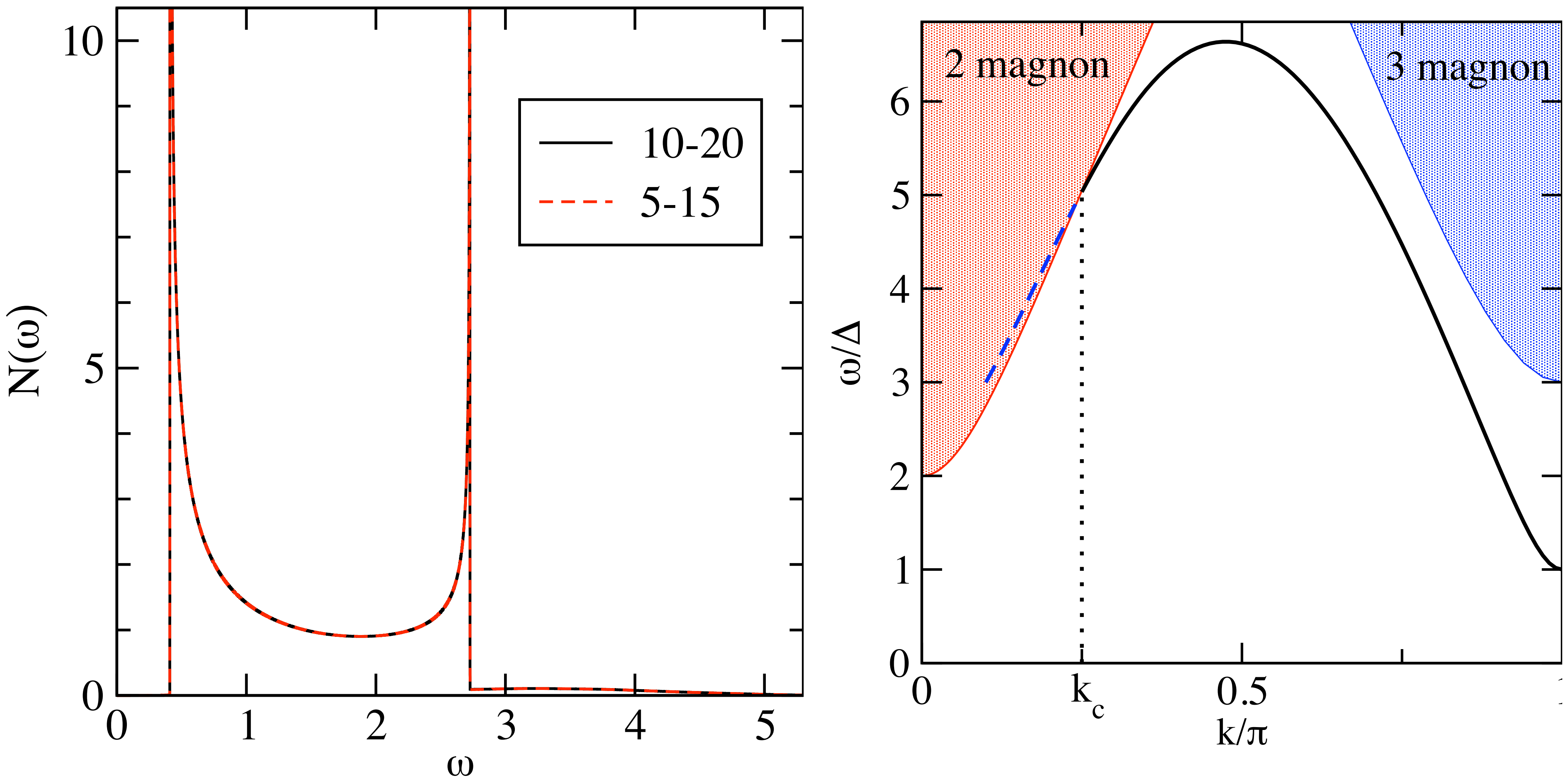
$$0.77848e^{-0.41043it}(0.5513+it)^{-1/2} +$$
$$0.29358e^{-2.7249it}(-3.2282-it)^{-1/2}$$



S=1, Re, Im, fit

Deviations are $\sim 10^{-4}$
Value for Haldane gap is correct to 4 places!

N(ω) for S=1 chain, asymptotic fit



Detailed results for S=1: see White & Affleck, PRB, 2008

S=1/2 XXZ model (Pereira, White, Affleck, Nov. PRL)

- Physics very nicely described by Alex Kamenev yesterday.
- Singularities in spectrum: look at p-h excitations in spinless fermion model from the Jordan Wigner transfromation
  - p, h both near k_F: low energy, LL description. In $N(\omega)$, describes lower edge singularity at $\omega=0$
  - p and/or h away from k_F: need to go beyond usual treatment
- New treatment: p/h away from k_F have few decay modes: treat as mobile impurities in LL (Balents, Pustilnik, Khodas, Kamenev, Glazman)
  - Bethe ansatz to exactly determine the key couplings
  - Similar approach to Cheianov and Pustilnik, small disagreement

- Result: exact exponents for all singularities in N(ω) and S(k,ω)

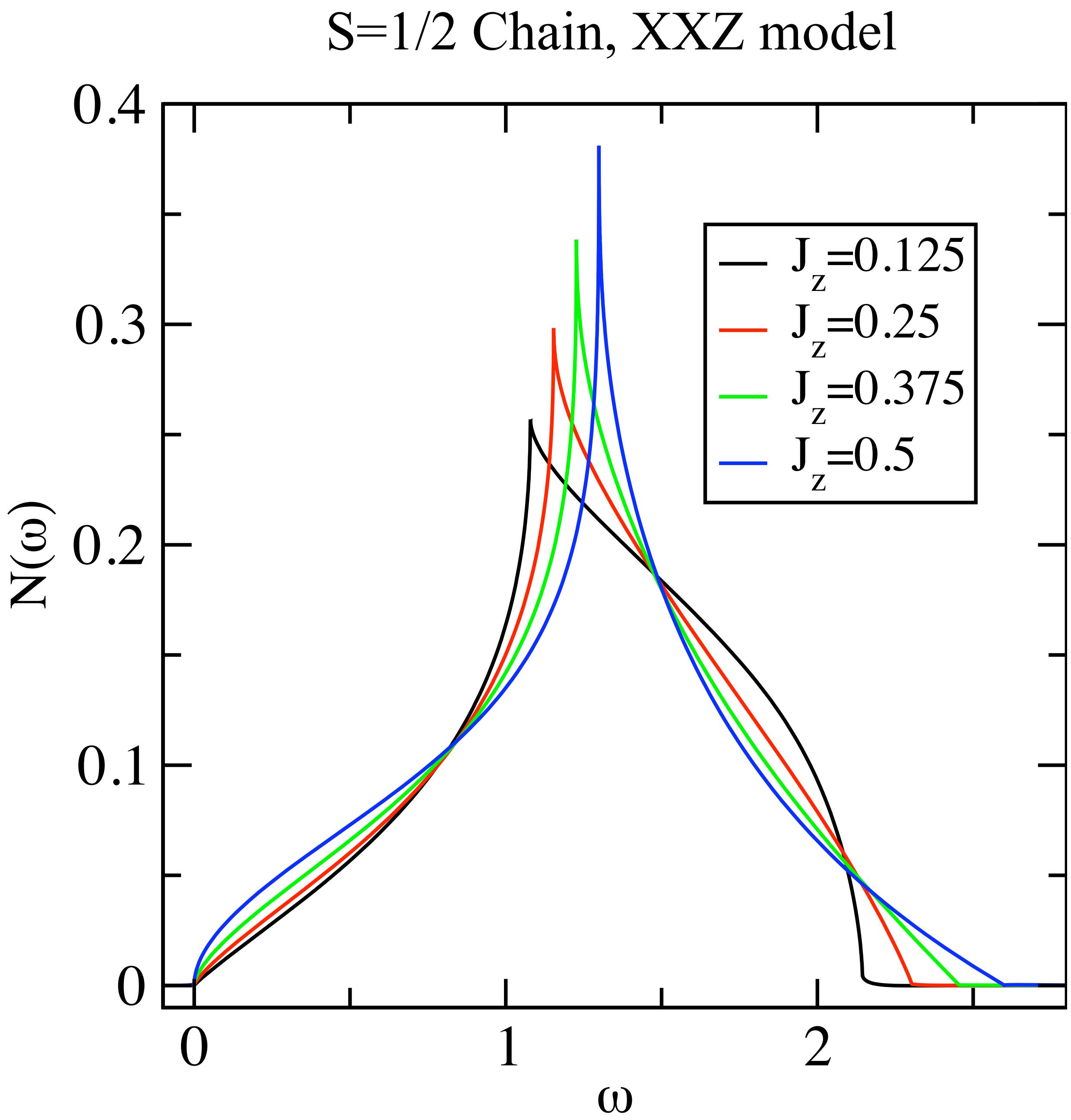
TABLE I: Exponents for the spin self-correlation function $G(t)$ for $h = 0$. The parameters W, η, η_2 and σ were obtained numerically by fitting the DMRG data according to Eq. (15). These are compared with the corresponding FT predictions (with v and K taken from the Bethe ansatz).

Δ	W	v	η	$\frac{1}{2}+K$	σ	$2K$	η_2	
0	1	1	1.5	1.5	2	2	1	1
0.125	1.078	1.078	1.451	1.426	1.954	1.852	1.761	2
0.25	1.153	1.154	1.366	1.361	1.811	1.723	2.034	2
0.375	1.226	1.227	1.313	1.303	1.694	1.607	2.000	2
0.5	1.299	1.299	1.287	1.25	1.491	1.5	2.120	2
0.75	1.439	1.438	1.102	1.149	1.324	1.299	2.226	2

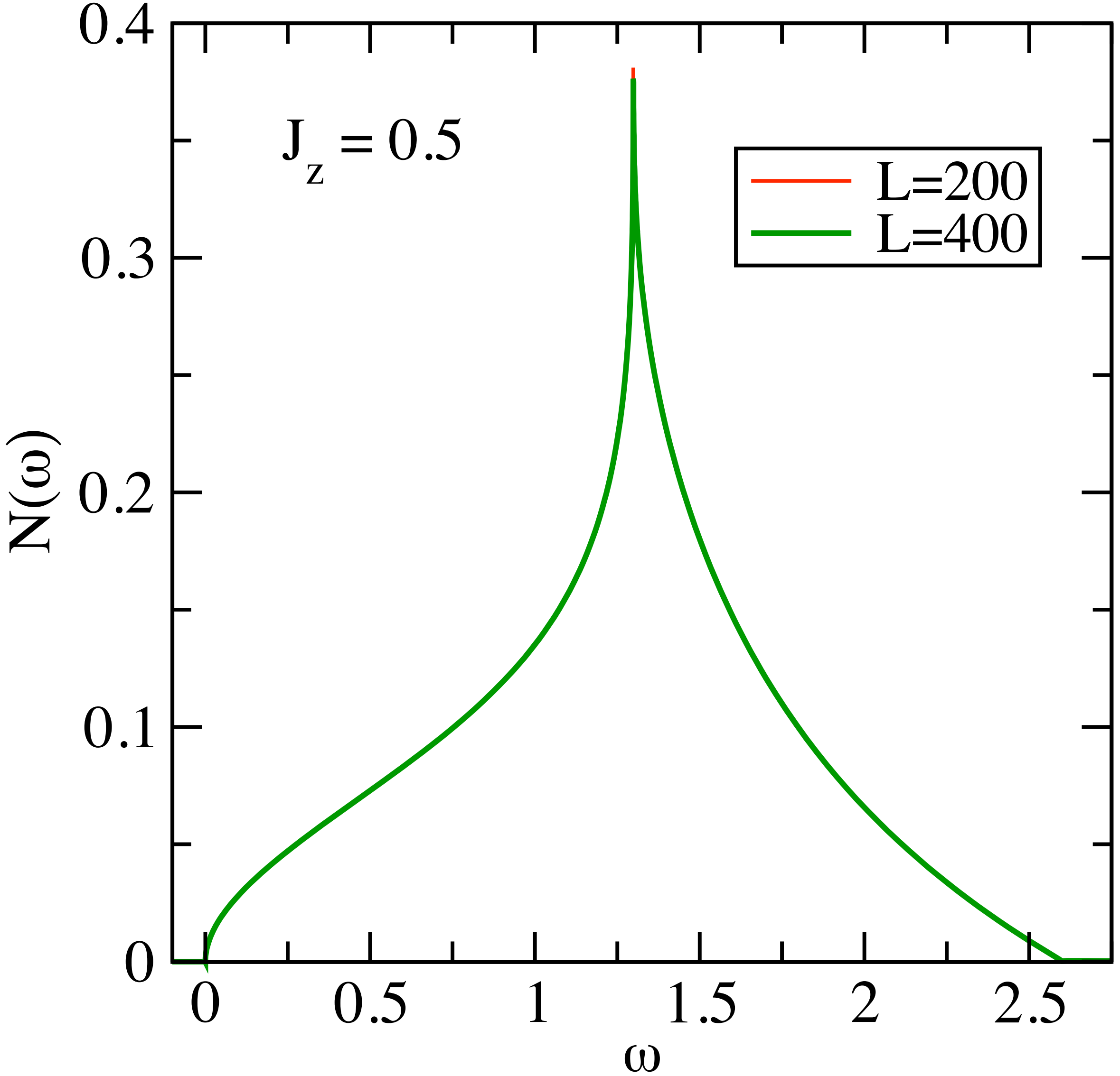
D
M
R
G

$$G(t) \sim B_1 \frac{e^{-iWt}}{t^{\eta}} + B_2 \frac{e^{-i2Wt}}{t^{\eta_2}} + \frac{B_3}{t^{\sigma}} + \frac{B_4}{t^2}$$

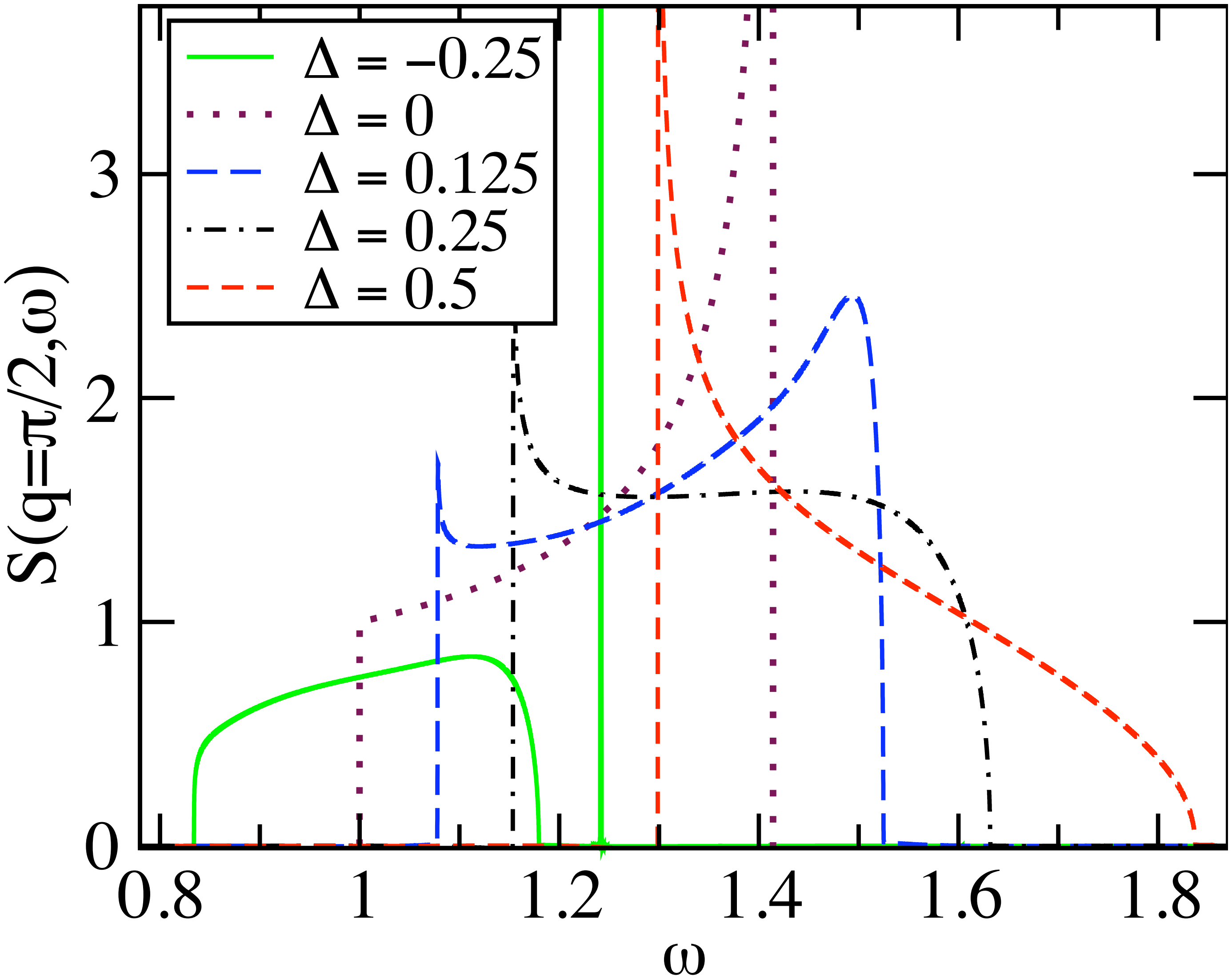
x=0


S=1/2 Chain, XXZ model
0.4
0.3
0.2
0.1
0
N(ω)
0
1
2
ω
J_z=0.125
J_z=0.25
J_z=0.375
J_z=0.5

How accurate are the spectra?



S(k,ω)



Conclusions

- DMRG can do big enough systems for some models to extrapolate order parameters to the thermodynamic limit
- tDMRG allows precise determination of spectral functions for 1D systems
- New results for singularity exponents in the XXZ model

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