Matrix product state formulation of frequency-space dynamics at finite temperatures

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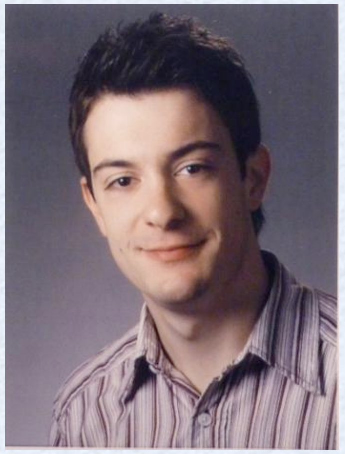
A.C. Tiegel, S.R. Manmana, T. Pruschke, and A. Honecker,
Phys. Rev. B (rapid comm.) **90**, 060406(R) (2014).

Frequency space approach to spectral functions at finite T



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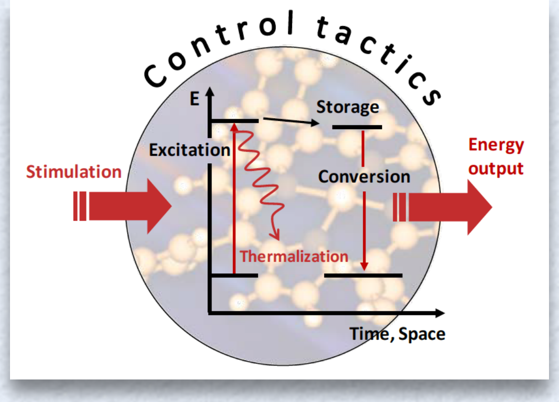


SFB / CRC 1073
“Atomic Scale Controll of Energy Conversion”

Dynamical correlation functions: DMRG approach for T>0?

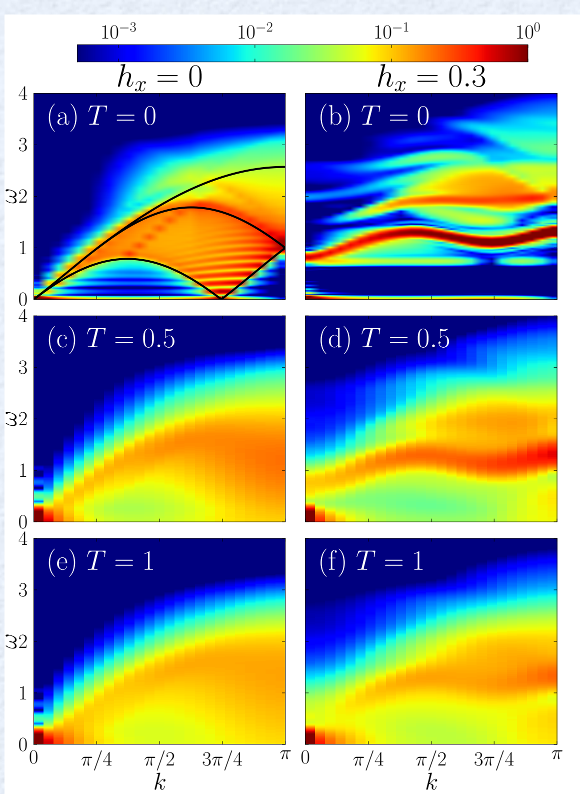
[A.C. Tiegel, S.R. Manmana, T. Pruschke, and A. Honecker, PRB **90**, 060406(R) (2014)]

Main question of this talk:
Unbiased computation of dynamical spectral functions via DMRG at T>0?

➠ Use Liouvillian formulation:

$$G_A(k,\omega) = -\frac{1}{\pi}\mathrm{Im}\left\langle \Psi_T \left| A^\dagger \frac{1}{z-\mathcal{L}} A \right| \Psi_T \right\rangle$$

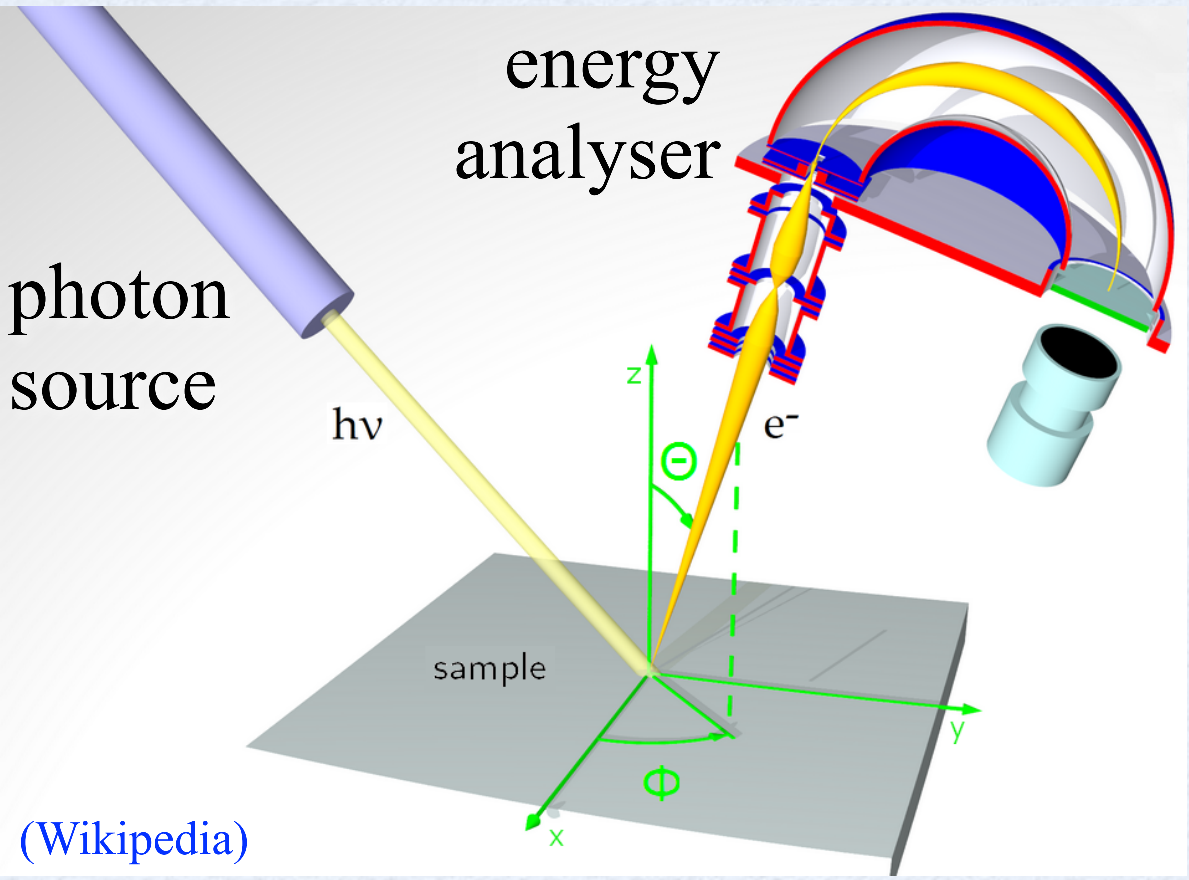
$$\mathcal{L} = \mathcal{H}_P \otimes I_Q - I_P \otimes H_Q$$



- here: proof of principle results (no optimized code)
- flexibility of approaches to resolvent
- *high* resolution, small errors
- works at all frequencies
- no further approximations (e.g. linear prediction)

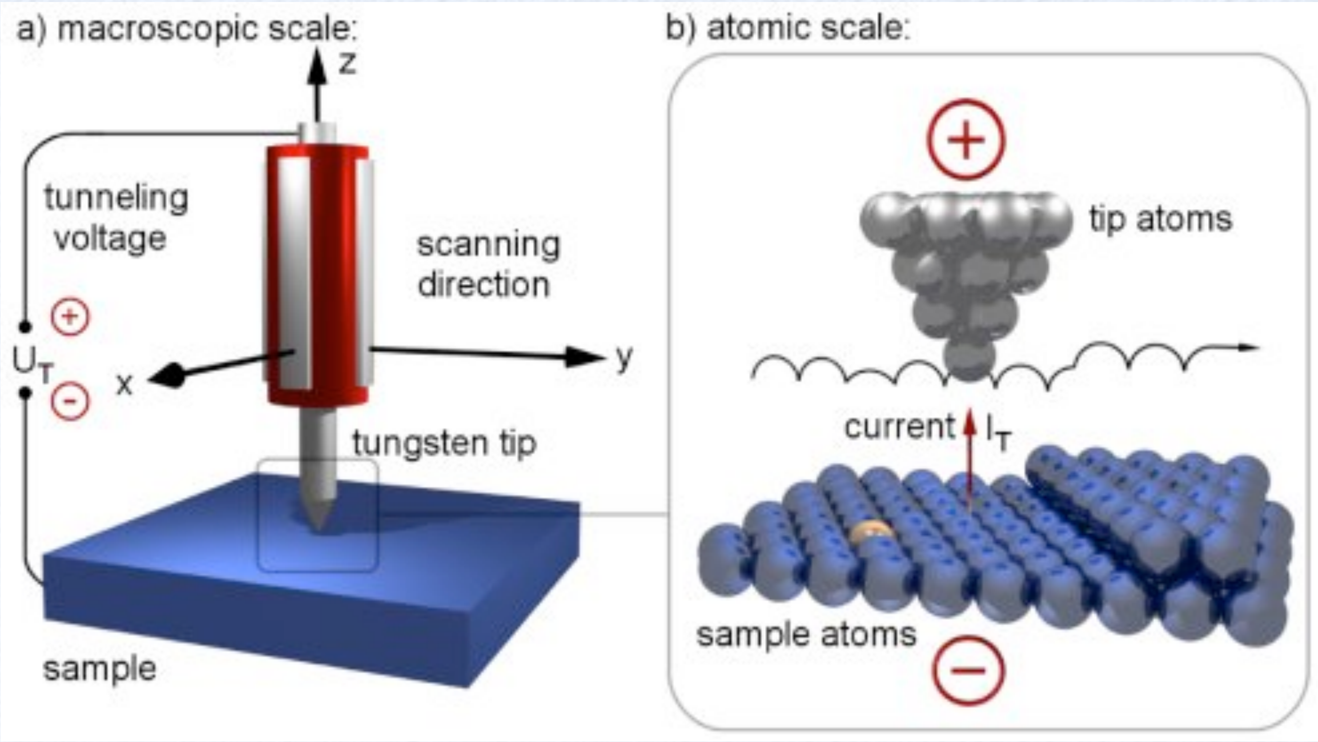
Quantum Many-Body Systems: Spectral Functions

angle-resolved photoemission (ARPES)



(Wikipedia)

scanning-tunneling spectroscopy



(www.physics.rutgers.edu/bartgroup/)

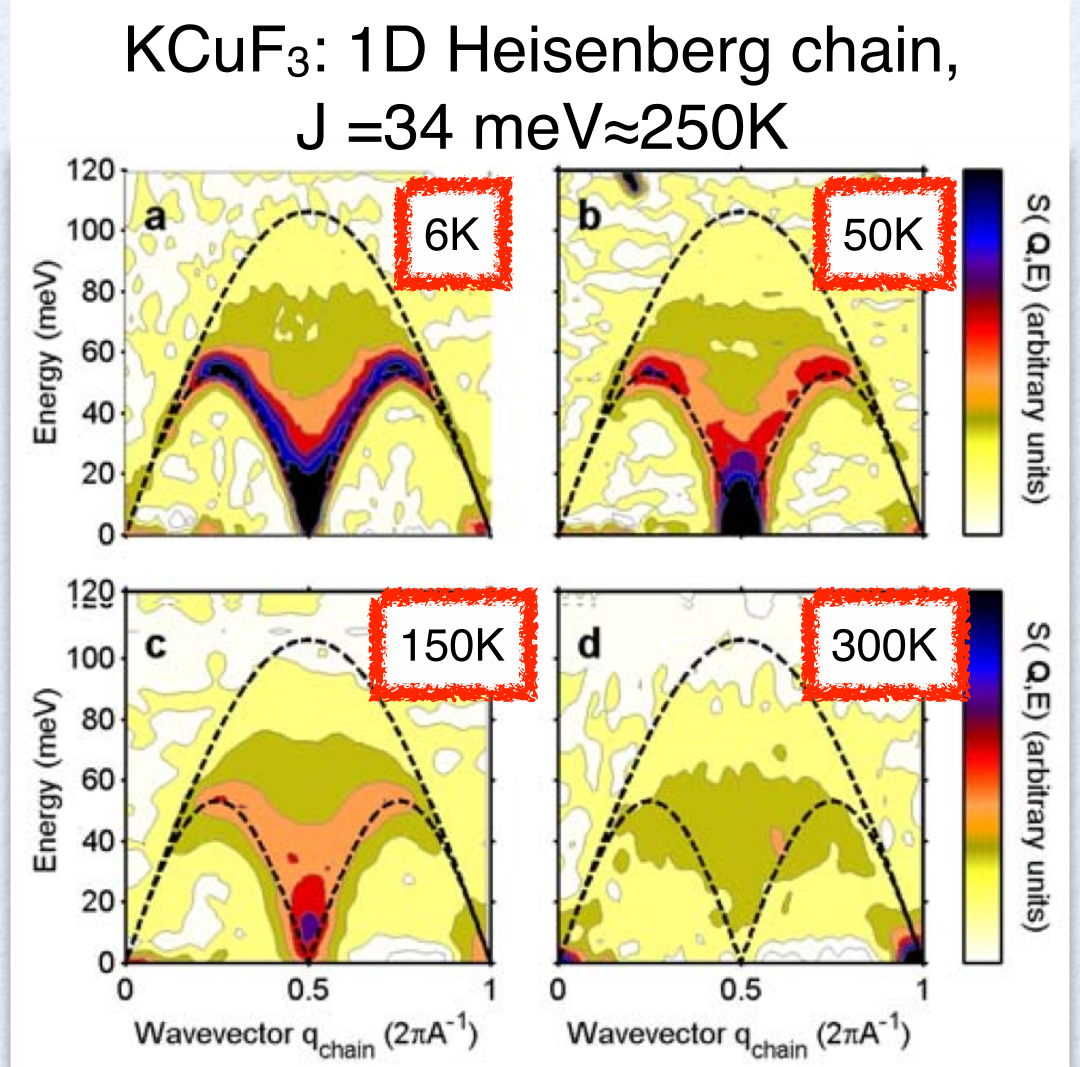
Linear response: measure quantities of type:

$$C_{B^\dagger,A}(\omega) \equiv \sum_n \langle \Psi_0 | B | n \rangle \langle n | A | \Psi_0 \rangle \, \delta(\omega - (E_n - E_0))$$

➟ insights into (local) density of states, excitations of the system, structure factors

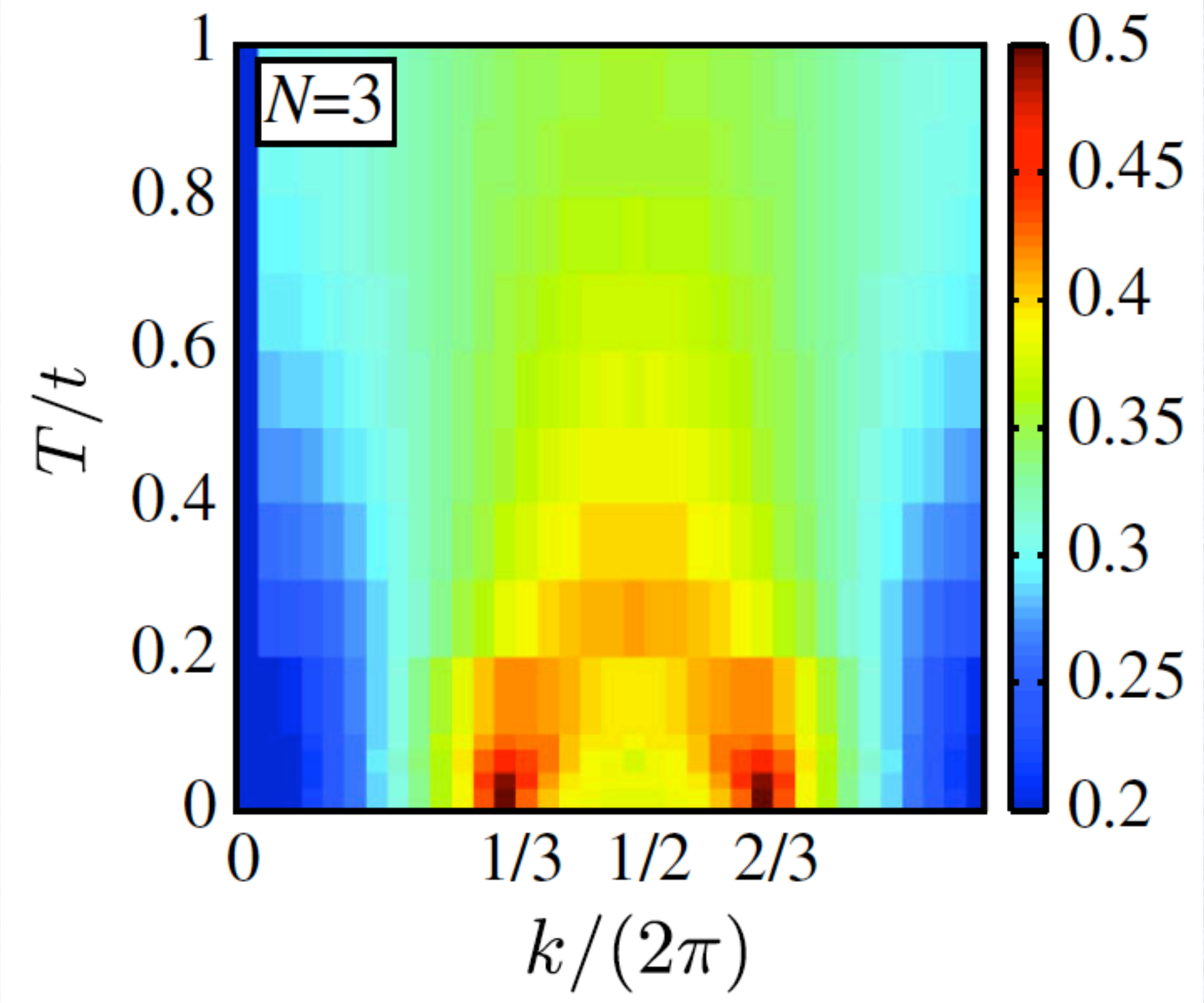
Dynamical correlation functions: finite temperatures

Materials (neutron scattering):



[B. Lake *et al.*, Nat. Mat. 4 (2005) 329]

Optical lattices (QMC prediction) :
SU(N) Hubbard systems



[L. Bonnes *et al.*, PRL **109**, 205305 (2012)]

Dynamical correlation functions

Dynamical correlation functions at T = 0:

$$G_A(\omega) = -\frac{1}{\pi}\mathrm{Im}\left\langle \psi_0 \left| A^\dagger \frac{1}{\omega+E_0+i\varepsilon-H} A \right| \psi_0 \right\rangle = \sum_n |\langle n\,|A|\,\psi_0\rangle|^2\,\delta\left(\omega-(E_n-E_0)\right)$$

$$\mathcal{H}_0\,|n\rangle = E_n\,|n\rangle$$

Dynamical correlation functions at T > 0:

$$G_A(\omega,T) = \frac{1}{Z}\sum_{n,m} e^{-\beta E_m}\langle m|A|n\rangle\langle n|A|m\rangle\delta(\omega-(E_n-E_m))$$

➠ Need the full spectrum...difficult ☹

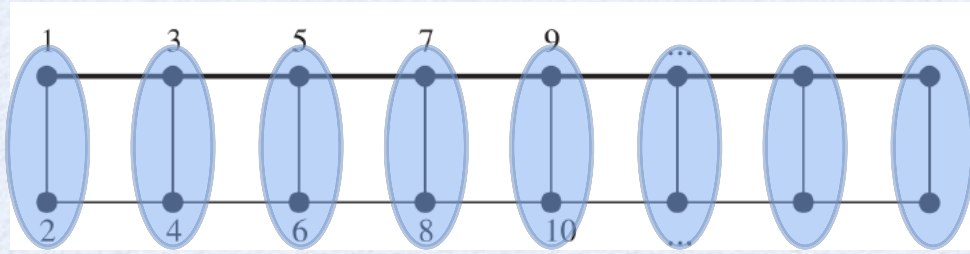
Ways out: continued fraction expansion, (D)DMRG, QMC,...

Here: DMRG+continued fraction/Chebyshev expansions

Finite temperature methods: purification with matrix product states

☞ Compute thermal density matrix via a pure state in an extended system:

[U. Schollwöck, Annals of Physics (2011)]



$$|\Psi_T\rangle \sim e^{-(H_P \otimes I_Q)/(2T)} \left[\otimes_{j=1}^{L} |\mathrm{rung-singlet}\rangle_j \right]$$

$$\Rightarrow \varrho_T = e^{-H/T} = \mathrm{Tr_Q} |\Psi_T\rangle \langle \Psi_T|$$

☞ Real time evolution at finite temperature:

$$|\Psi_T\rangle (t) = e^{-i(H_P \otimes U_Q)t} |\Psi_T\rangle \Rightarrow G_A(T,t) \overset{\text{Fourier}}{\Rightarrow} G_A(T,\omega)$$

- Problem: reach long times for large systems
- Ways out: linear prediction, backward time evolution in Q

[T. Barthel, U. Schollwöck & S.R. White, PRB (2009); C. Karrasch, J.H. Bardarson & J.E. Moore, PRL (2012)]

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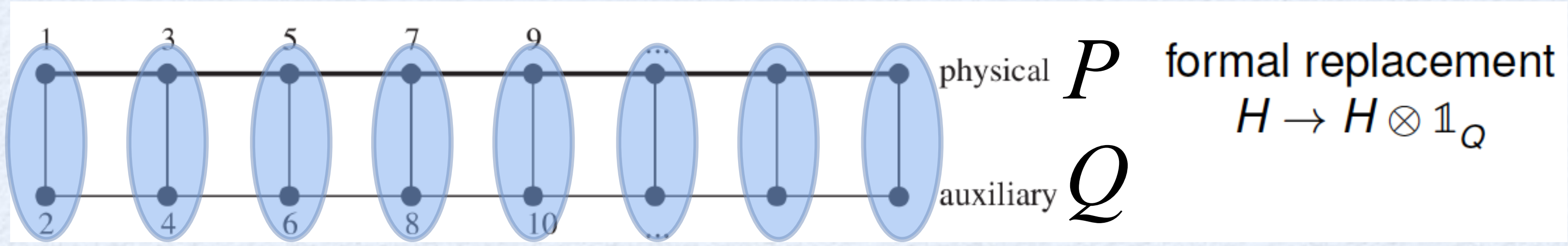

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[T. Barthel, U. Schollwöck & S.R. White, PRB (2009); C. Karrasch, J.H. Bardarson & J.E. Moore, PRL (2012)]

Dynamical correlation functions at finite T: Liouvillian formulation

$$G_A(\omega, T) = \frac{1}{Z} \sum_{n,m} e^{-\beta E_m} \langle m|A|n\rangle \langle n|A|m\rangle \delta(\omega - (E_n - E_m))$$

Note: 1) *Difference* of *all* energies

2) MPS approach: $|\Psi_T\rangle$ vector in the Liouville space spanned by $\mathcal{H}_P \otimes \mathcal{H}_Q$

➠ Dynamics is actually governed by Liouville equation [Barnett, Dalton (1987)]

$$\frac{\partial}{\partial t}|\Psi_T\rangle = -i\mathcal{L}|\Psi_T\rangle, \qquad \mathcal{L} = \mathcal{H}_P \otimes I_Q - I_P \otimes H_Q$$

(backward evolution in Q by Karrasch et al.)

$$G_A(k, \omega) = -\tfrac{1}{\pi} \mathrm{Im} \left\langle \Psi_T \left| A^\dagger \tfrac{1}{z - \mathcal{L}} A \right| \Psi_T \right\rangle$$

[A.C. Tiegel et al., arXiv:1312.6044 : proof of principle calculations]

Earlier: Superoperator approach to mixed-state dynamics [Zwolak & Vidal (2004)]

Liouville space formalism: "Thermofields"

J. Phys. A: Math. Gen. **20** (1987) 411–418. Printed in the UK

Liouville space description of thermofields and their generalisations

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† Optics Section, Blackett Laboratory, Imperial College of Science and Technology, London SW7 2BZ, UK
‡ Physics Department, University of Queensland, St Lucia, Queensland, Australia 4067

Received 14 January 1986, in final form 13 May 1986

Abstract. The thermofield representation of a thermal state by a pure-state wavefunction in a doubled Hilbert space is generalised to arbitrary mixed and pure states. We employ a Liouville space formalism to investigate the connection between these generalised thermofield wavefunctions and a generalised thermofield state vector in Liouville space which is valid for all cases of the quantum density operator. The system dynamics in the Schrödinger and Heisenberg pictures are discussed.

+ references therein

$$i\frac{d\varrho}{dt} = \left[\hat{H}, \varrho\right] \Rightarrow i\frac{d}{dt}|\varrho\rangle\rangle = \mathcal{L}|\varrho\rangle\rangle$$

von Neumann equation

Liouville equation

Dynamical correlation functions: Lanczos recursion

[E. Dagotto, RMP (1994)]

☞ use continued fraction expansion (CFE)

$$G_A(z) = -\frac{1}{\pi}\mathrm{Im}\left\langle \psi_0 \left| A^\dagger \frac{1}{z-\mathcal{L}} A \right| \psi_0 \right\rangle = -\frac{1}{\pi}\mathrm{Im}\frac{\langle\Psi_0|\, A^\dagger\, A\,|\Psi_0\rangle}{z-a_0-\frac{b_1^2}{z-a_1-\frac{b_2^2}{z-..}}}$$

via Lanczos recursion

$$|f_0\rangle \;=\; A\,|\Psi_0\rangle\,, \qquad |f_{n+1}\rangle = \mathcal{L}\,|f_n\rangle - a_n\,|f_n\rangle - b_n^2\,|f_{n-1}\rangle$$

$$a_n \;=\; \frac{\langle f_n|\,\mathcal{L}\,|f_n\rangle}{\langle f_n|f_n\rangle}\,, \qquad b_{n+1}^2 = \frac{\langle f_{n+1}|f_{n+1}\rangle}{\langle f_n|f_n\rangle}\,, \qquad b_0 = 0$$

Dynamical correlation functions: Chebyshev recursion

[MPS: A. Holzner *et al.*, PRB **83**, 195115 (2011); A. Weiße *et al.*, RMP **78**, 275 (2006)]

☞ Representation via Chebyshev polynomials:

$$G_A(\omega) = \frac{2}{\pi W\sqrt{1-\omega'^2}}\left[g_0\,\mu_0 + 2\sum_{n=1}^{N-1} g_n\,\mu_n T_n(\omega')\right]$$

with

$$\mu_n = \langle t_0|t_n\rangle = \left\langle \Psi_T \left| A^\dagger T_n(\mathcal{L}')A\right| \Psi_T\right\rangle$$

$$|t_0\rangle = A|\Psi_T\rangle, \quad |t_1\rangle = \mathcal{L}'|t_0\rangle, \quad |t_n\rangle = 2\mathcal{L}'|t_{n-1}\rangle - |t_{n-2}\rangle$$

W : bandwidth of $\mathcal{L}$

$\mathcal{L}'$: rescaled Liouvillian, so that $W \to [-1,1]$

$\omega' \in [-1,1]$, $T_n(\omega') = \cos\left[n\left(\arccos\omega'\right)\right]$

g_n : damping factors $\rightarrow$ Gaussian broadening $\eta \sim 1/N$

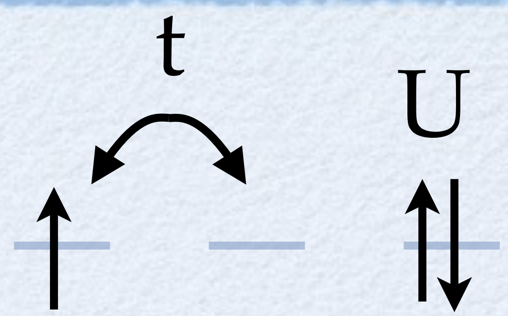
$$g_n^J = \frac{(N-n+1)\cos\frac{\pi n}{N+1} + \sin\frac{\pi n}{N+1}\cot\frac{\pi}{N+1}}{N+1}$$

"Jackson damping"

Effective Models for Quantum Magnets

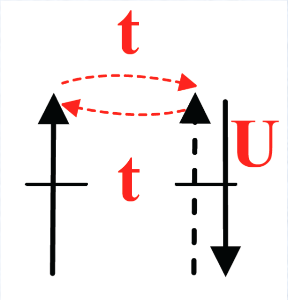
Starting point : Hubbard model

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} \left[c^{\dagger}_{i+1,\sigma} c_{i,\sigma} + h.c. \right] + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$



Heisenberg exchange: 2nd order perturbation theory for U >> t

$$J\, \vec{S}_1 \cdot \vec{S}_2 \qquad\qquad J = \frac{4t^2}{U}$$



Real materials: additional spin-orbit coupling

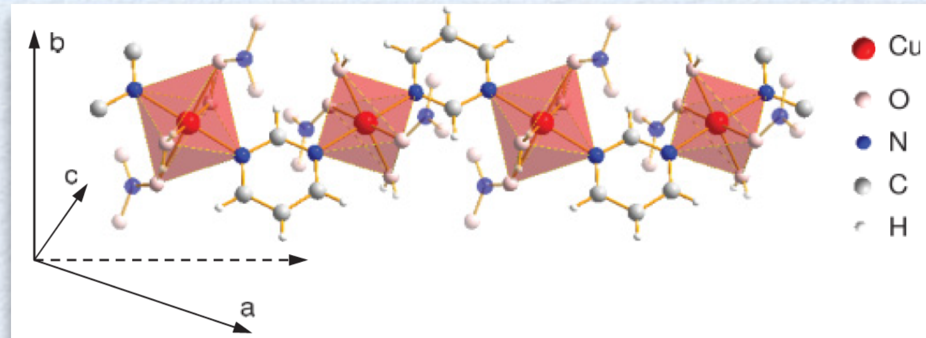
$$\sim \lambda\, \vec{L} \cdot \vec{S} \quad \lambda \ll 1 \qquad \vec{D} \cdot \left(\vec{S}_1 \times \vec{S}_2 \right) \qquad |\vec{D}| \sim \lambda$$

- Heisenbergterm symmetric under permutations, SU(2) invariant
- Dzialoshinskii-Moriya-Term antisymmetric, breaks SU(2) invariance
- Typically D ~ 1 - 10% J

Here: interplay of D, J and T in dynamical quantities

Dynamical properties of quantum magnets: ESR on Cu-PM in magnetic fields

Copper pyrimidine dinatrate:



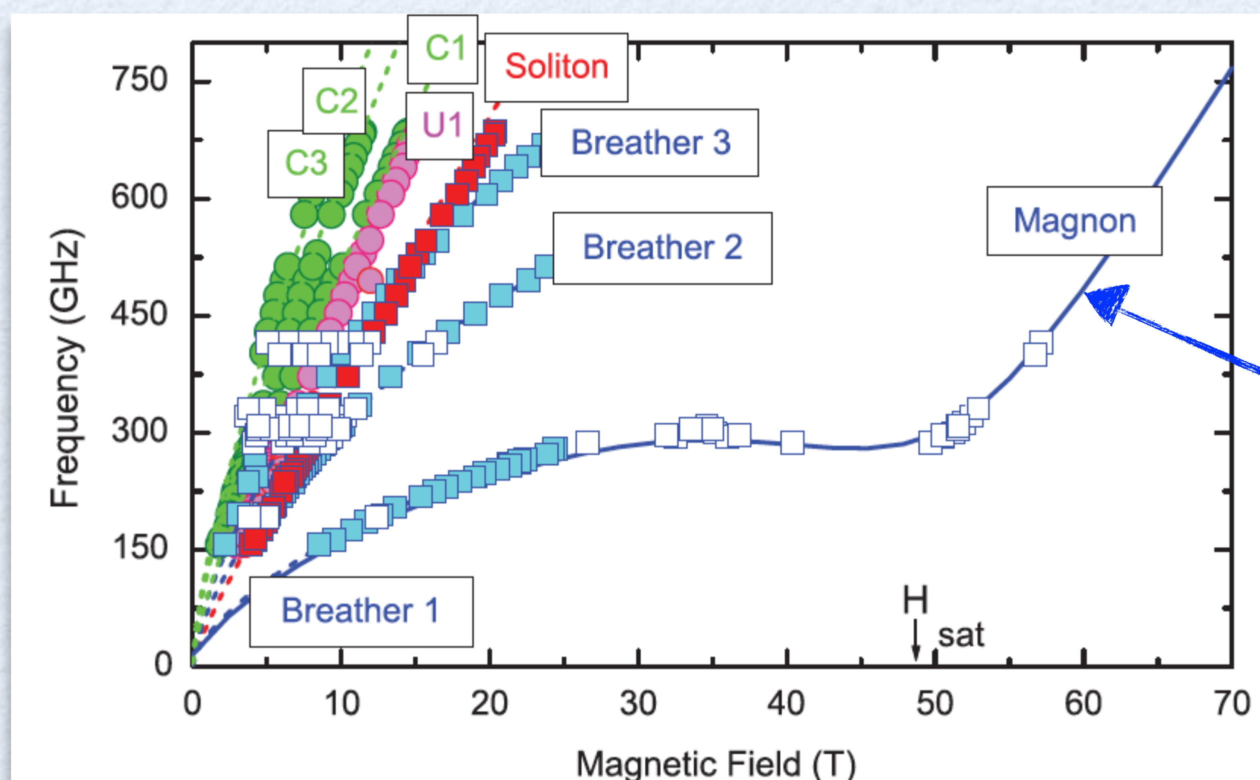
[S. Zvyagin et al., PRB(R) (2011)]

(Quasi-)1D Heisenberg AFM, described by

$$\mathcal{H} = \sum_j \left[J \mathbf{S}_j \cdot \mathbf{S}_{j+1} - H S_j^z - h\,(-1)^j\, S_j^x \right]$$

effect of staggered g-tensor + DM interaction

ESR spectrum in magnetic field:

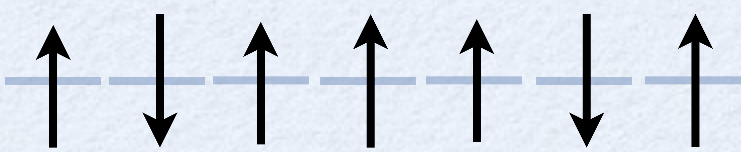


DMRG results

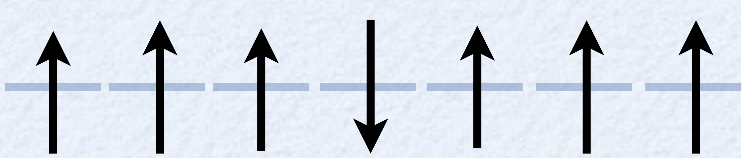
Spectral functions at finite field

Finite-T dynamics
in strong magnetic fields:

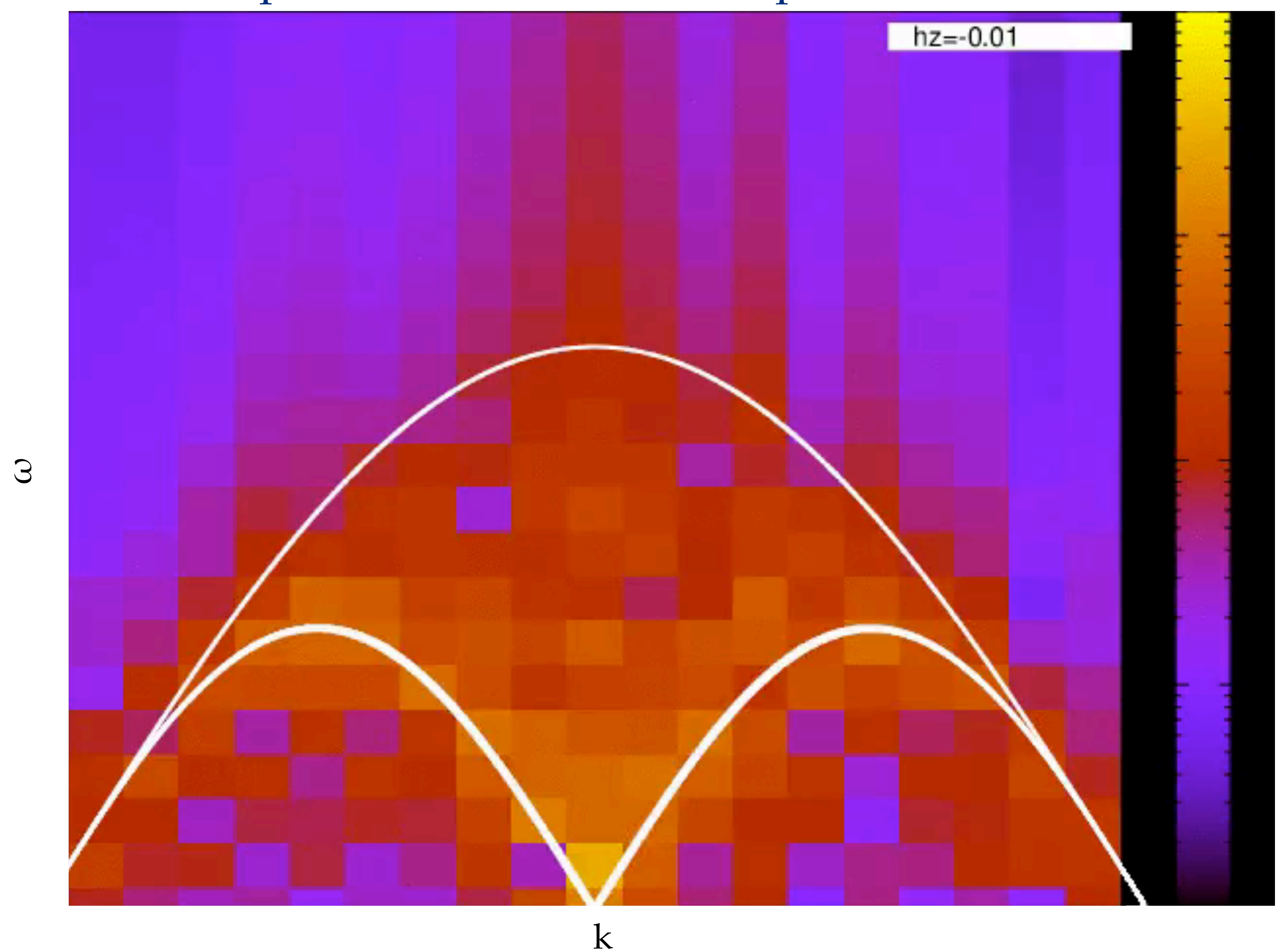
small H: spinons



large H: magnons



Time evolution at T=0.2 + Fourier transform
(non-optimized code, no linear prediction)

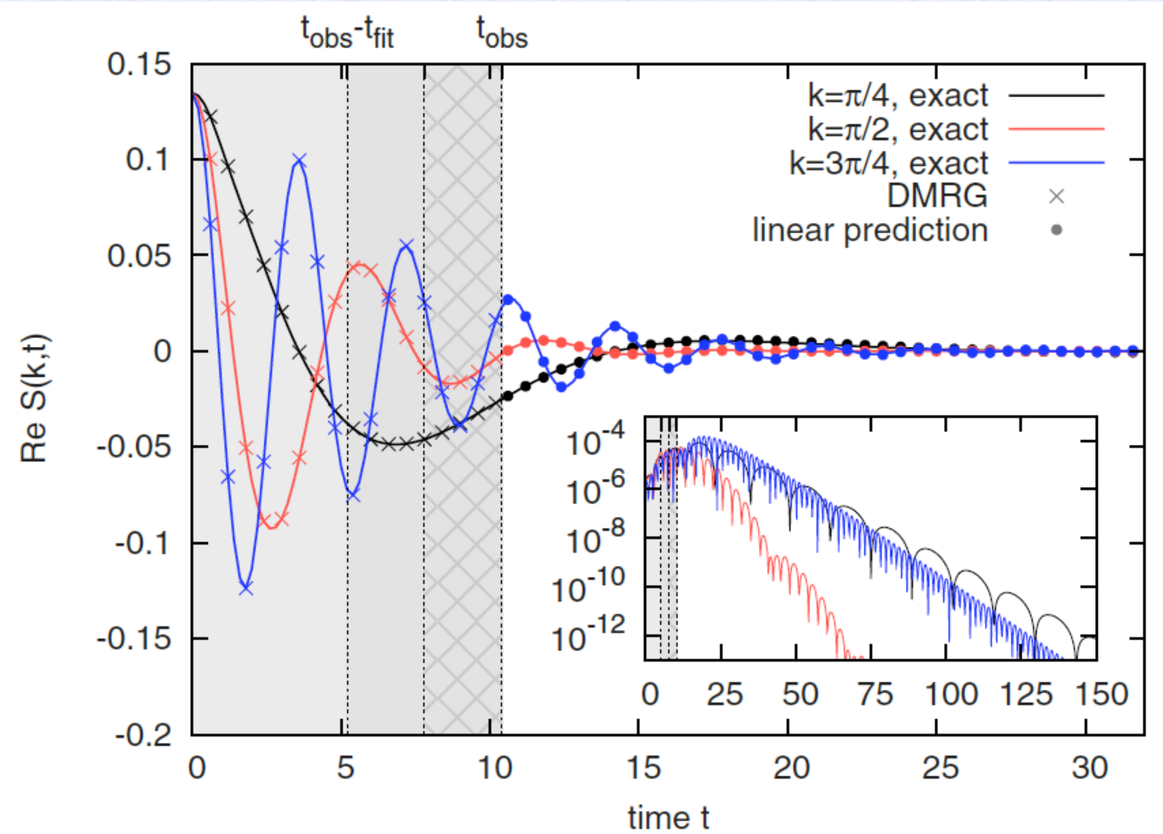


[T. Köhler, Master thesis, Univ. Göttingen 2013]

Time evolution approaches:
linear prediction

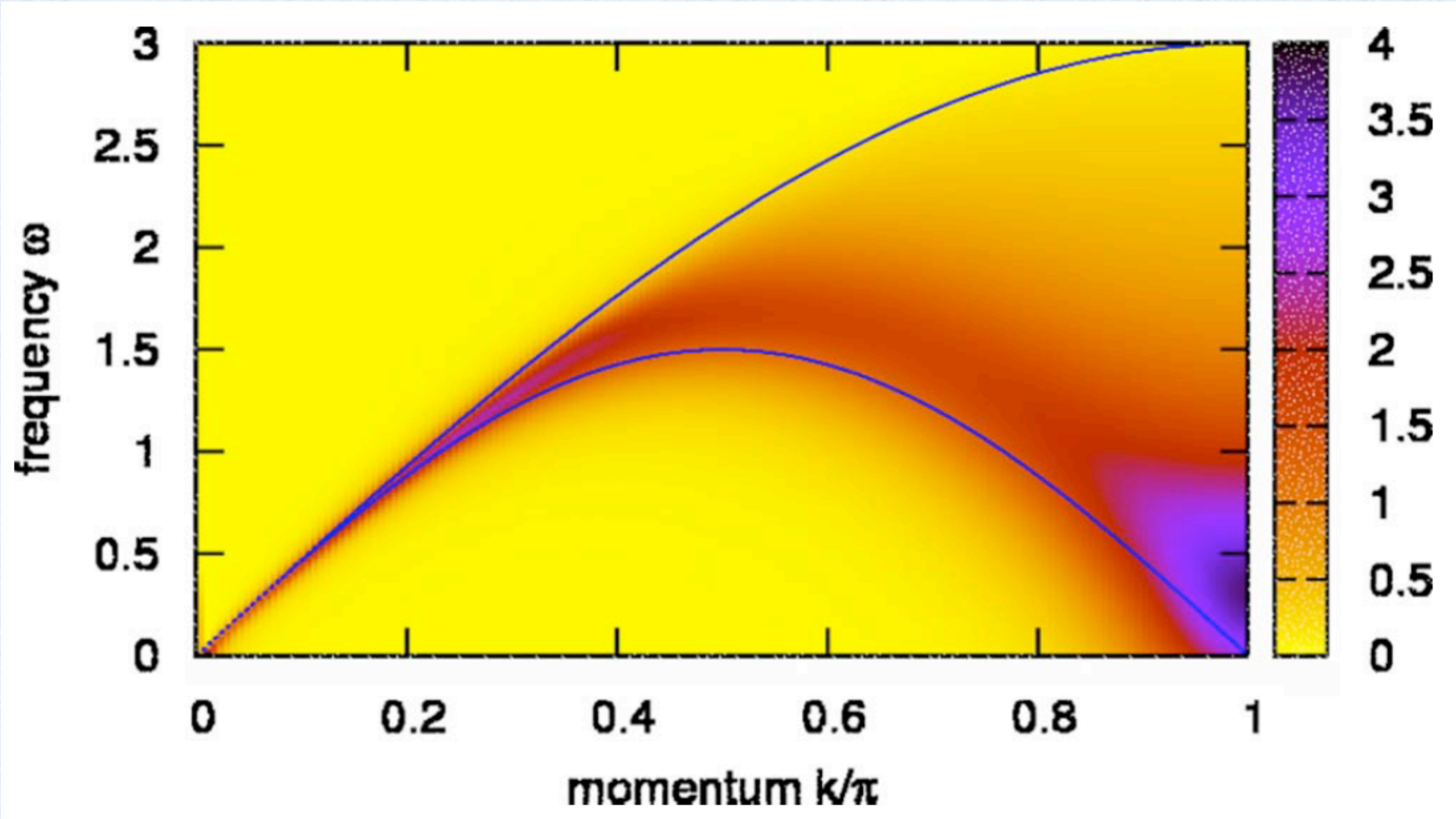
[T. Barthel, U. Schollwöck & S.R. White, PRB (2009)]

real time behavior: linear prediction



→ increase useable time scale
by factor of 3

Fourier space:



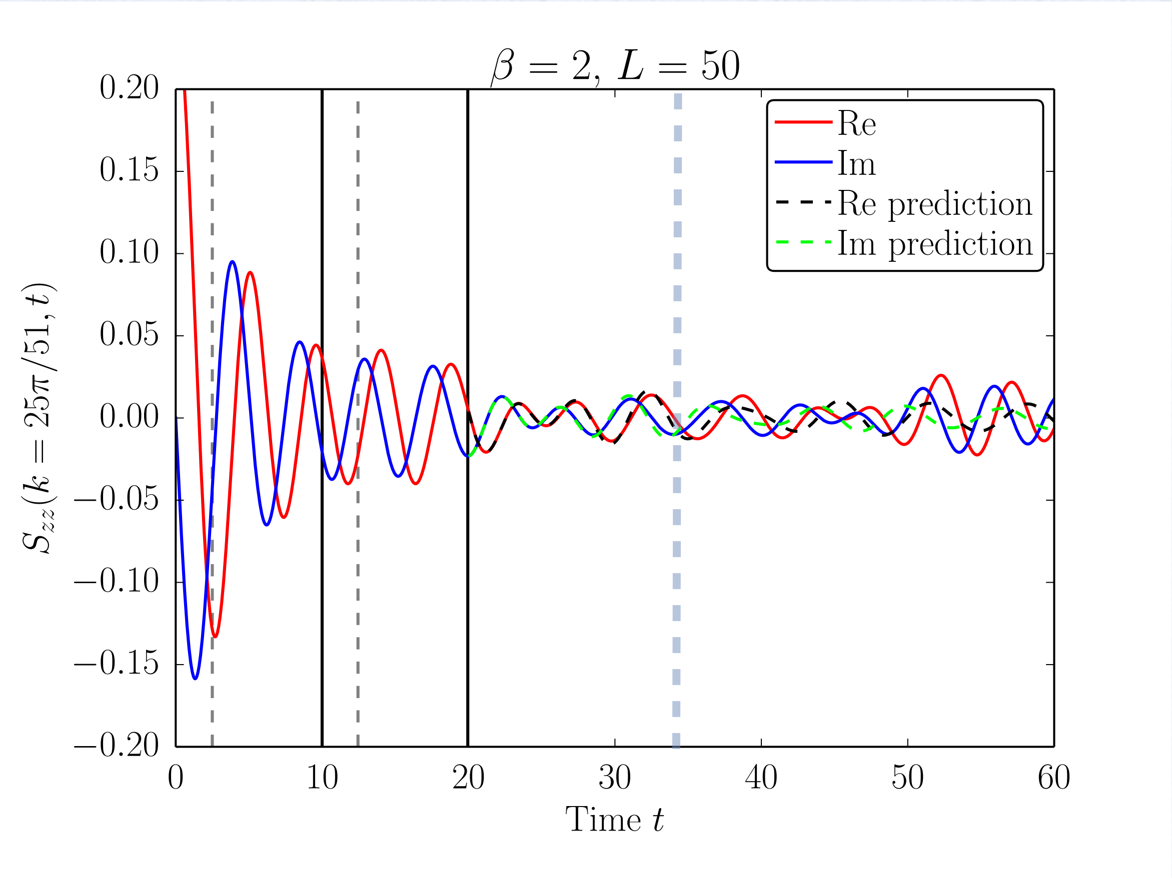
Can work well, but wish for better control.

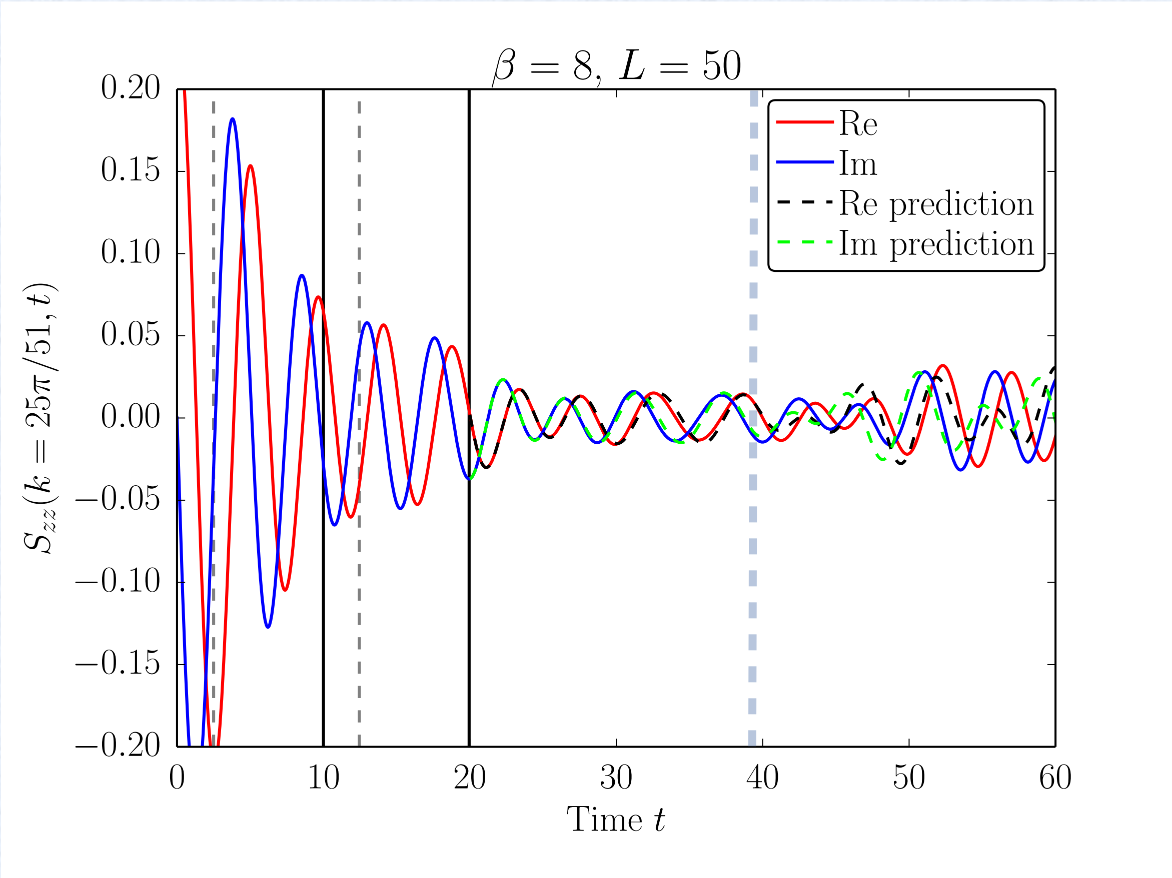
Time evolution approaches: linear prediction for XX model

[T. Köhler, A. Tiegel, A. Honecker, SRM, work in progress]

Exactly solvable XX-model:

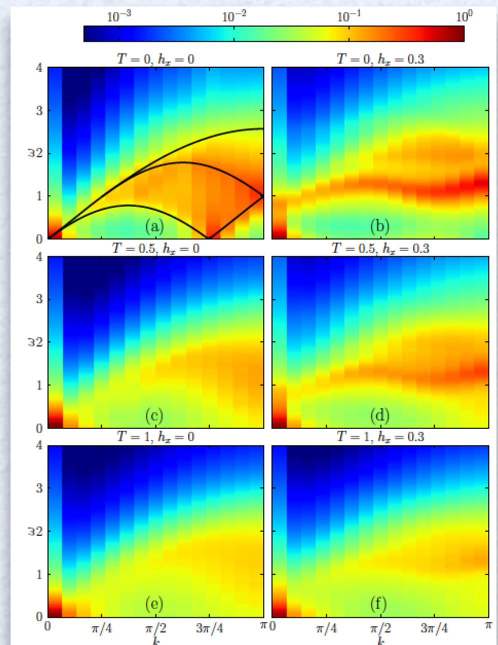
$$H_{XX} = J \sum_{i}^{L-1} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right)$$



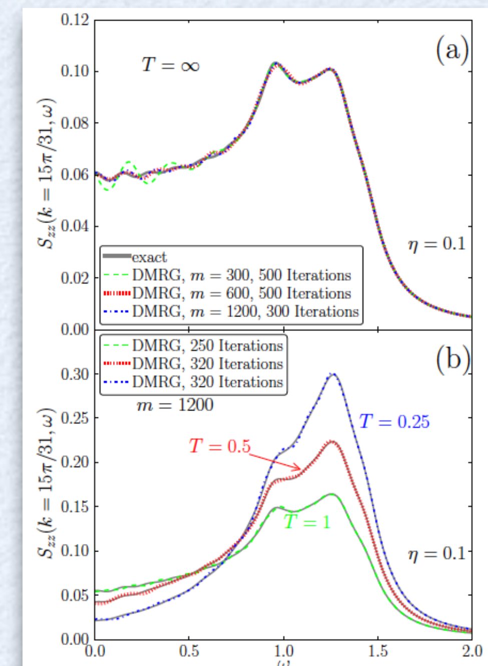


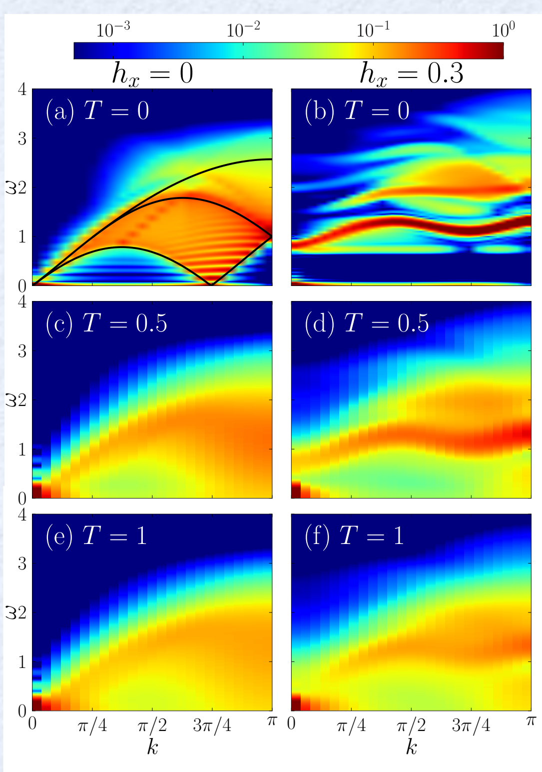
"Useable time scale" varies with temperature and details (which observable? Etc.), hard to reach a factor of 2.

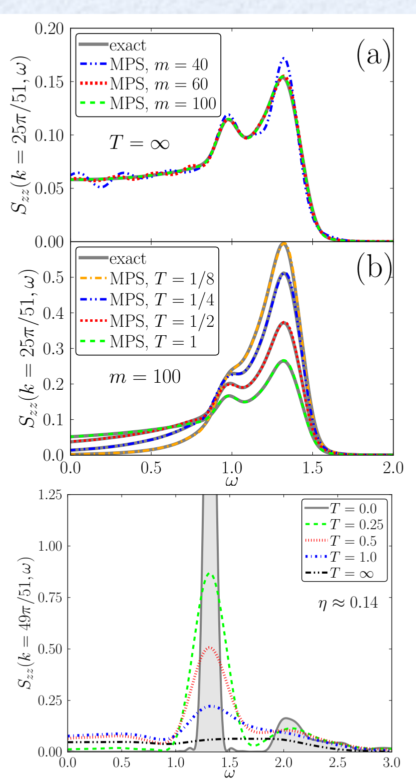
Liouvillian finite-T approach

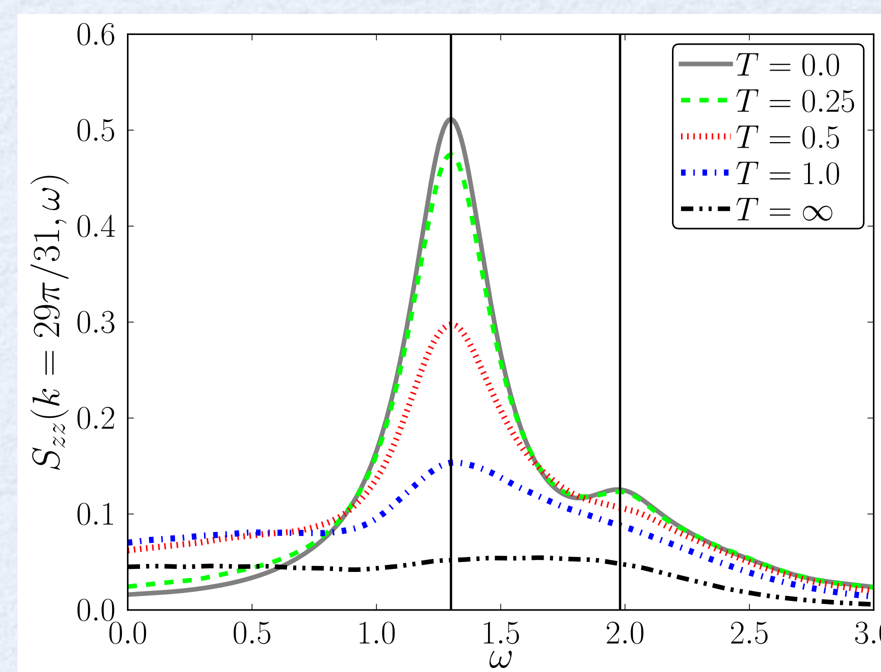


Proof of Principle Calculations!









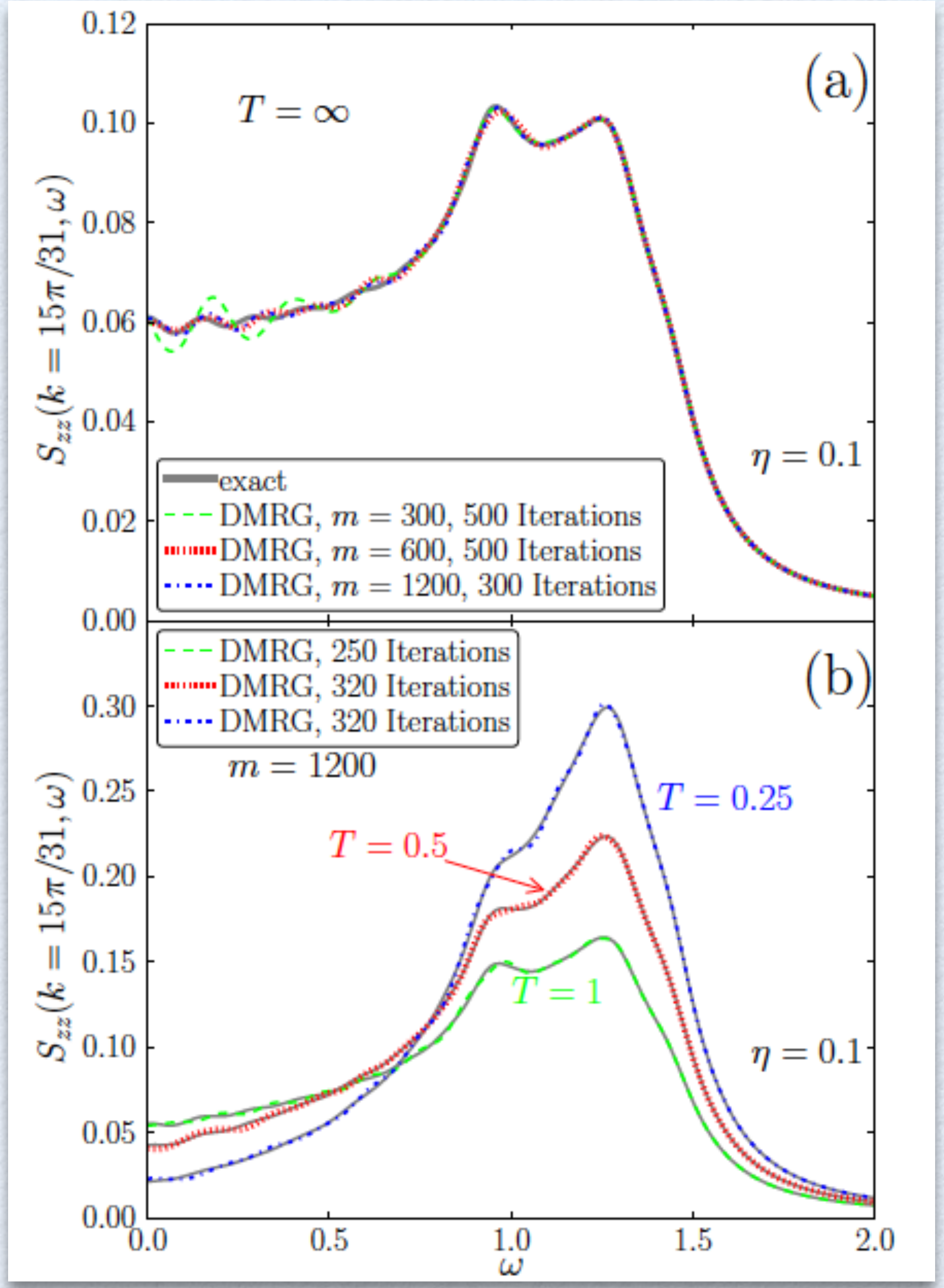
Liouvillian finite-T approach: comparison to exact results

Continued fraction expansion:

$$H_{XX} = J \sum_{i}^{L-1} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right)$$

$$S_k^\alpha = \sqrt{\frac{2}{L+1}} \sum_{i=1}^{L} \sin(ki)\, S_i^\alpha$$

Excellent agreement with exact results!

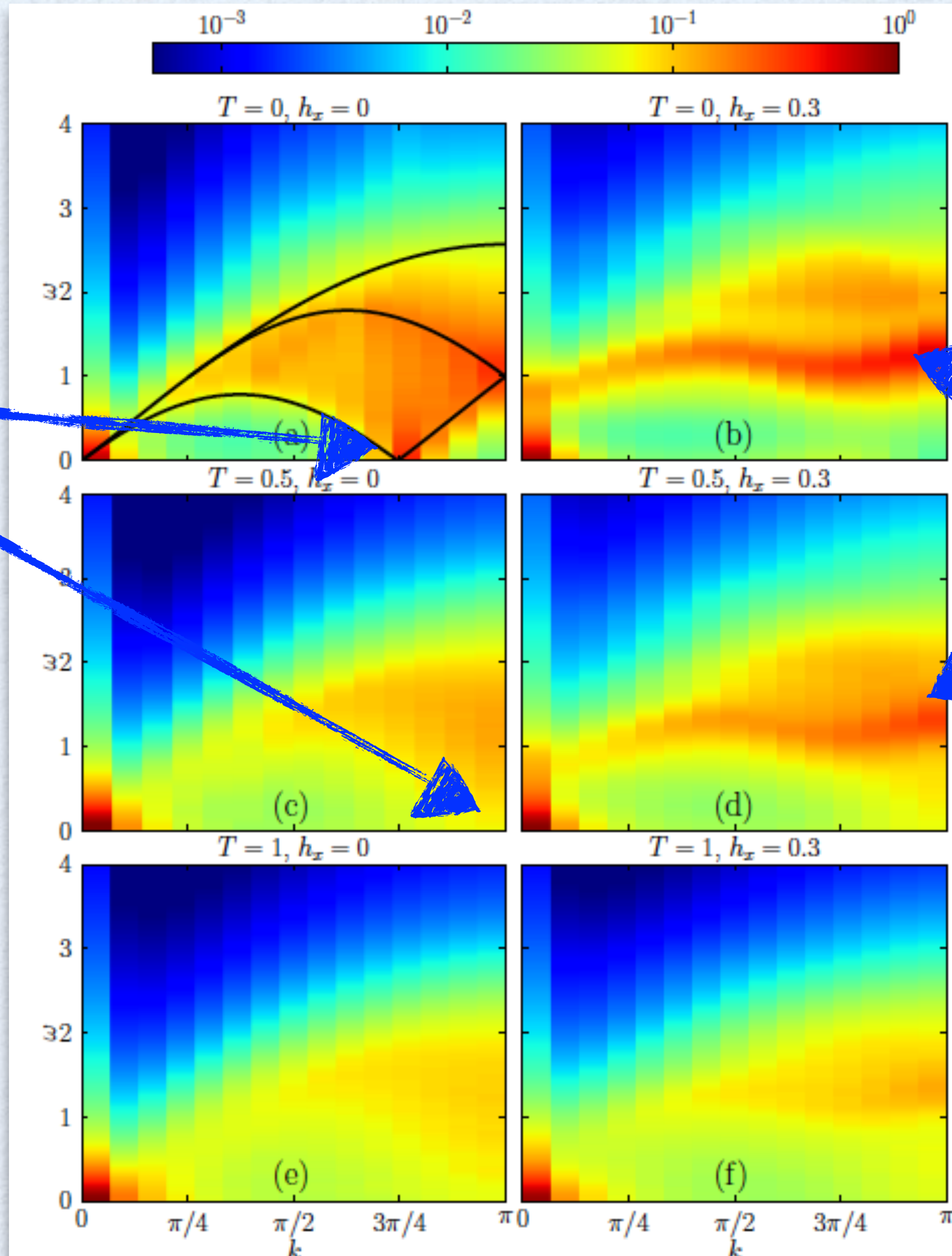


Liouvillian finite-T approach: Heisenberg antiferromagnet in magnetic field

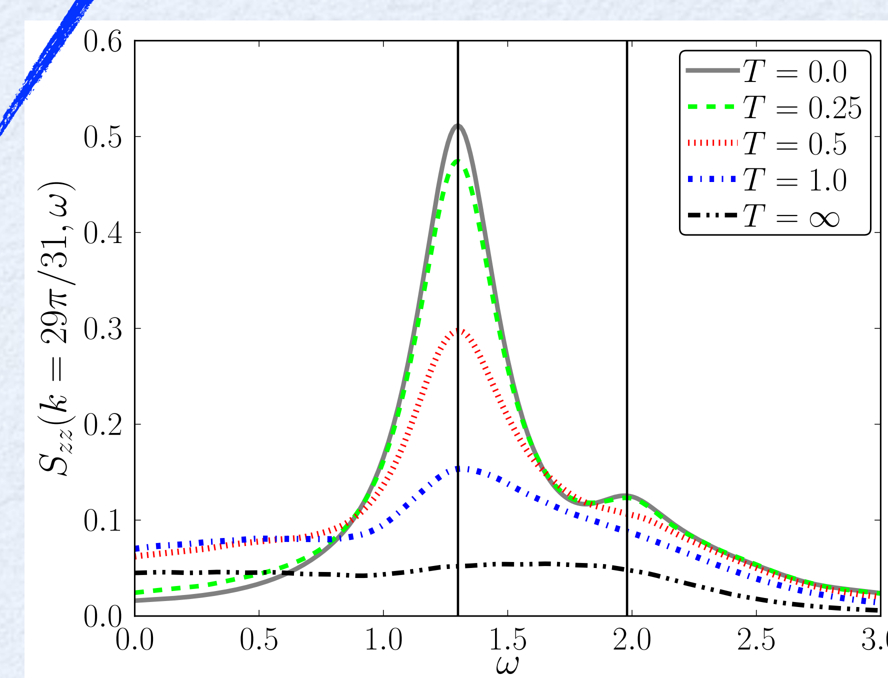
no DM

with DM

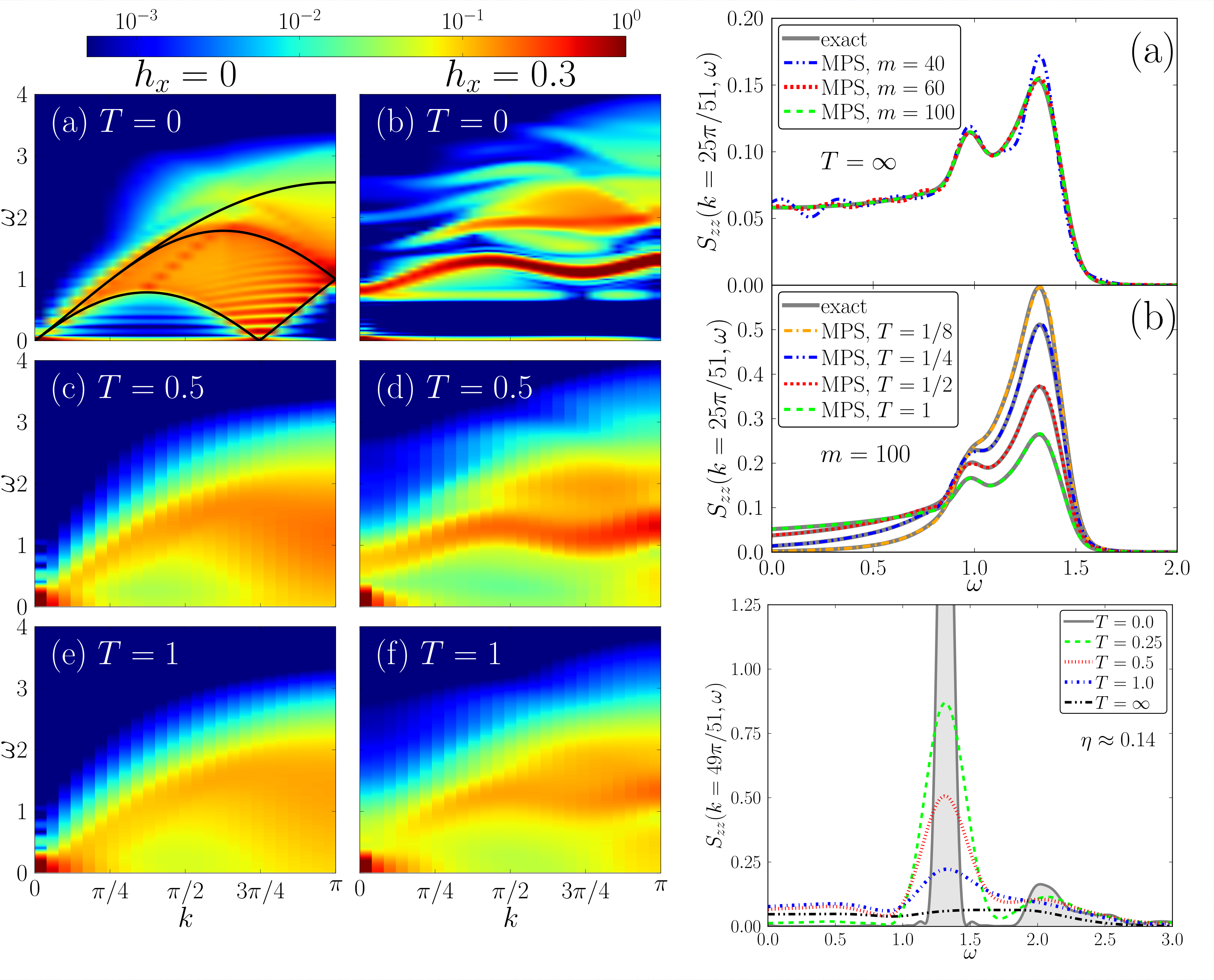
Melting of a Luttinger liquid



Formation of bands, thermal broadening



Liouvillian finite-T approach: using the Chebyshev expansion



- Better resolution with smaller m
- further optimization: expect 10x higher resolution

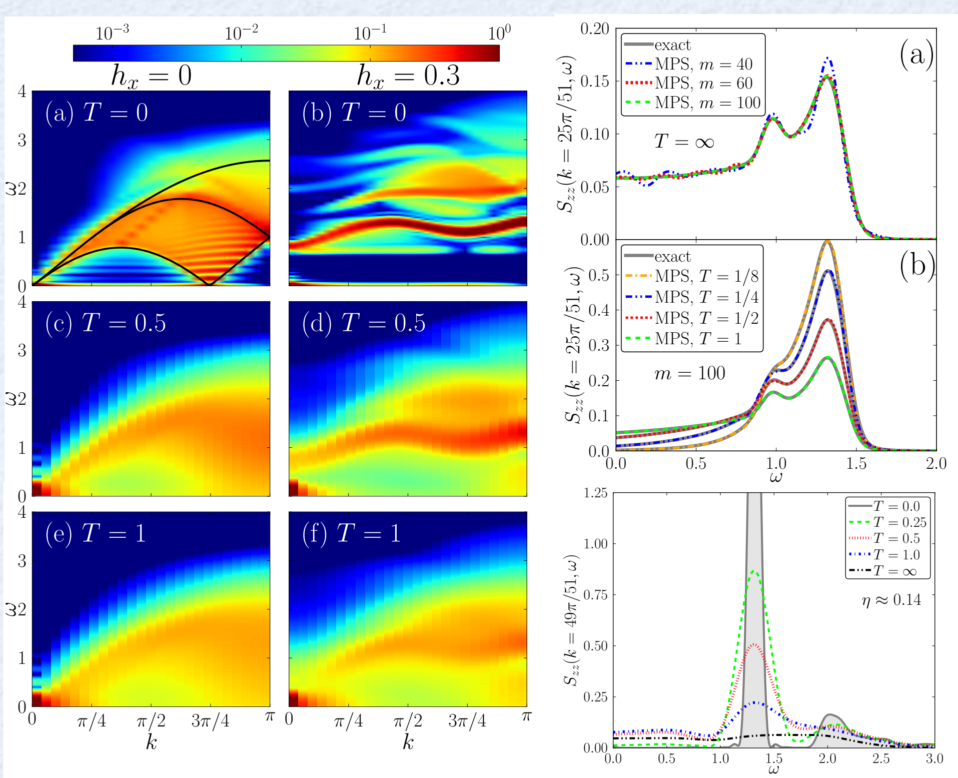
Conclusions

Instead of real-time evolution, go to Liouville space and work directly in frequency space:

$$G_A(k,\omega) = -\frac{1}{\pi}\mathrm{Im}\left\langle \Psi_T \left| A^\dagger \frac{1}{z-\mathcal{L}} A \right| \Psi_T \right\rangle \quad \mathcal{L} = H_P \otimes I_Q - I_P \otimes H_Q$$

Independent of method: also possible to use PEPS, further tensor networks, other numerical approaches (ED, QMC?)

Heisenberg chain with Dzyaloshinskii-Moriya interaction:



very accurate
observe "melting" of LL,
formation of bands via DM interaction

Next steps: optimize code,
ESR lines,
other systems (S>1/2, fermions, bosons)