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

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Alexander C. Tiegel, Salvatore R. Manmana, Thomas Pruschke, and Andreas Honecker,
Phys. Rev. B (rapid comm.) **90**, 060406(R) (2014).

Frequency space approach to spectral functions at finite T

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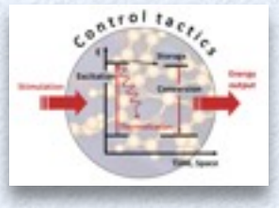
Funding:

Helmholtz Virtual Institute
"New states of matter and their excitations"



SFB/CRC 1073
"Atomic Scale Controll of Energy Conversion"

Dynamical correlation functions: DMRG approach for T>0?

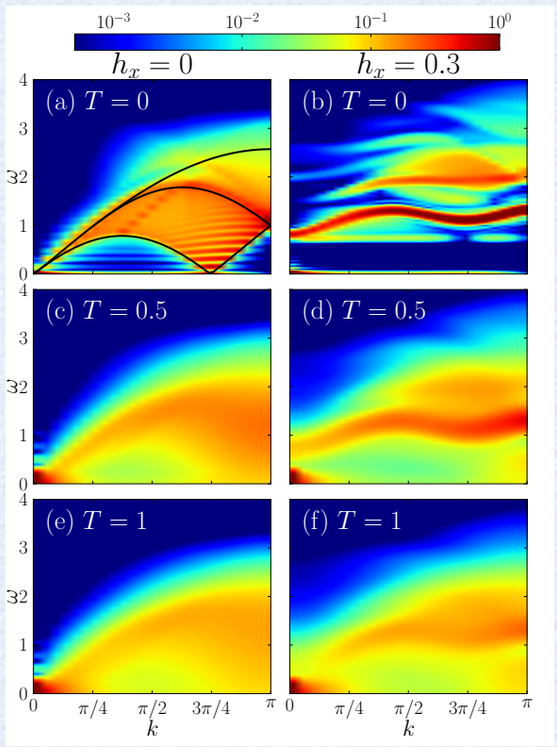
[A.C. Tiegel, S.R. Manmana, T. Pruschke, and A. Honecker, PRB **90**, 060406(R) (2014)]

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

Schrödinger equation:

time dependent

$$i\hbar\frac{\partial}{\partial t}\left|\psi\right\rangle = \hat{H}\left|\psi\right\rangle$$

time independent

$$\hat{H}\left|\psi\right\rangle = E\left|\psi\right\rangle$$

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m_i}\vec{\nabla}_i^2 + \sum_{\langle i,j\rangle}\hat{V}(\vec{x}_i,\vec{x}_j)$$

Example: Coulomb-interaction

$$\hat{V}(\vec{x}_i,\vec{x}_j) \sim \frac{\hat{n}_i\,\hat{n}_j}{|\vec{x}_i - \vec{x}_j|}$$

Quantum Many Body Systems: Entanglement

I) Superposition of states is *also* a possible state

II) Entanglement: (spin-1/2 particles, e.g., electrons)

possible states:

$$|\psi\rangle = \begin{cases} |\uparrow\rangle \otimes |\uparrow\rangle \\ |\uparrow\rangle \otimes |\downarrow\rangle \\ |\downarrow\rangle \otimes |\uparrow\rangle \\ |\downarrow\rangle \otimes |\downarrow\rangle \end{cases}$$

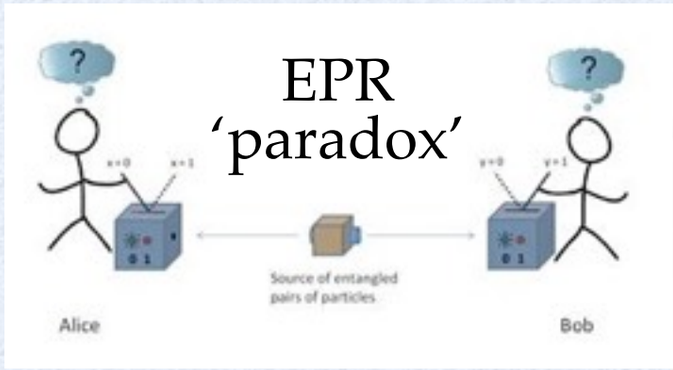
"classical", "product state"

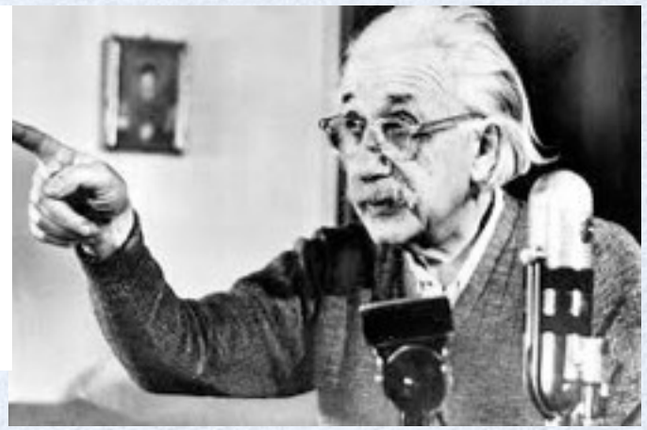
$$|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle \otimes |\uparrow\rangle + |\downarrow\rangle \otimes |\downarrow\rangle)$$

"entangled": not a product state

Schrödingers cat

Einstein: "spooky action at a distance"





Quantum Many Body Systems: Correlation Effects & Statistics

I) Correlated states:

"mean-field" picture of independent particles breaks down

$$\langle n_i n_j \rangle \neq \langle n_i \rangle \langle n_j \rangle$$

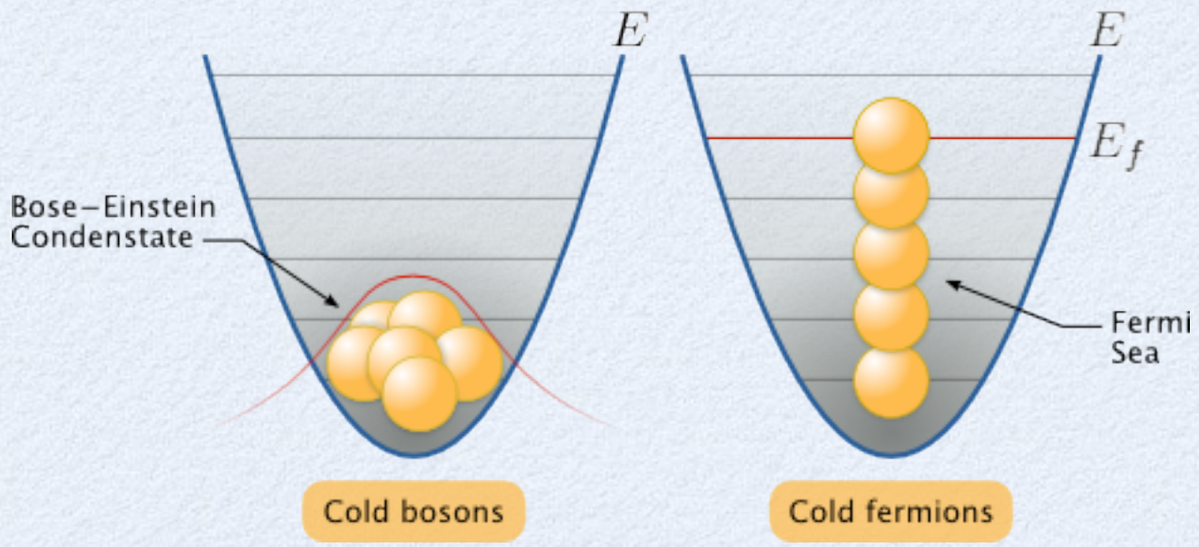
➠ Particles at sites i and j 'influence' each other

a) because of entanglement

b) because of mutual interactions.

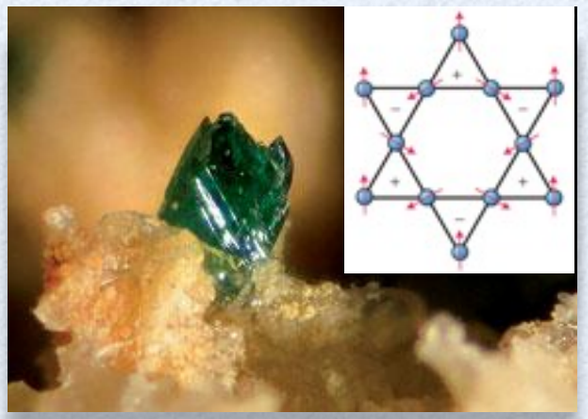
II) Exchange statistics:

Behavior at low temperatures:



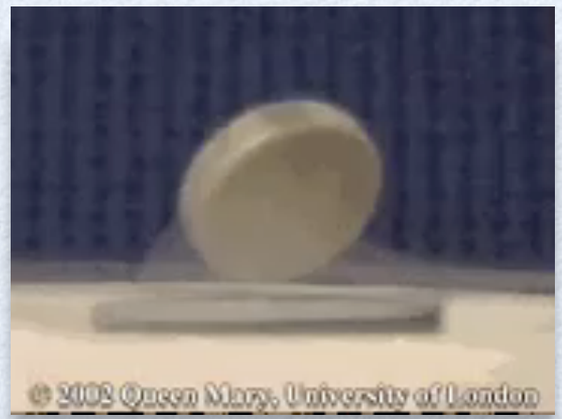
Realization of Strongly Correlated Systems in Nature and in the Lab

Quantum Magnetism of natural Minerals
(Herbertsmithite, Azurite,...): “Spin-liquids”?

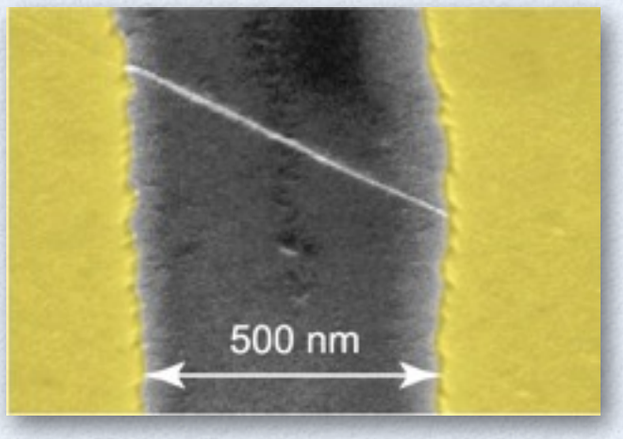


$$\hat{H} = -\sum_i \frac{\hbar^2}{2m_i}\vec{\nabla}_i^2 + \sum_{\langle i,j\rangle} \hat{V}(\vec{x}_i, \vec{x}_j)$$

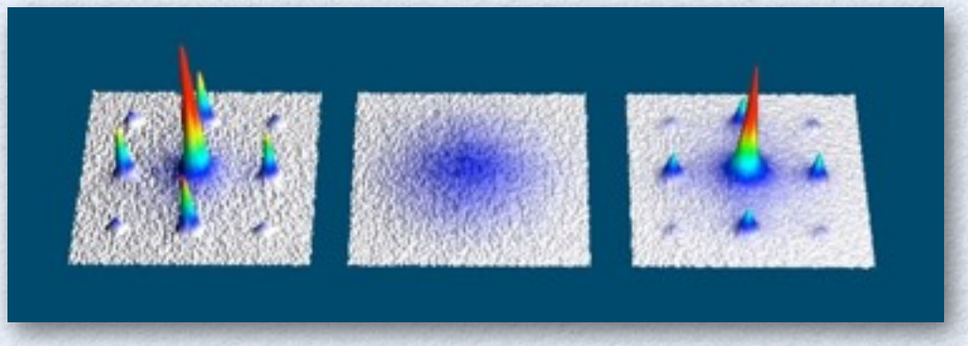
Synthetisized Materials:
High-Temperature Superconductors



Goal:
Identify new states of Matter



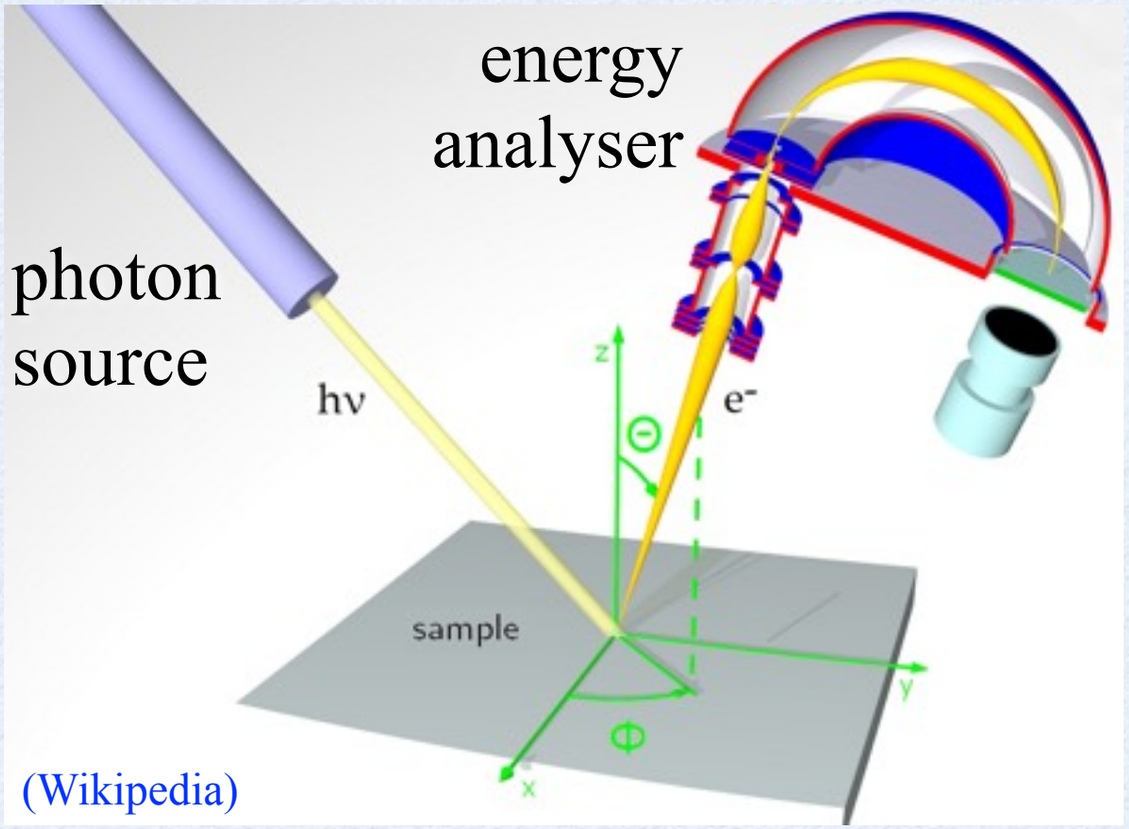
Quantum Wires, Nano Systems:
Transport Properties



Ultracold Gases (Optical Lattices):
Superfluids and Mott-Insulators

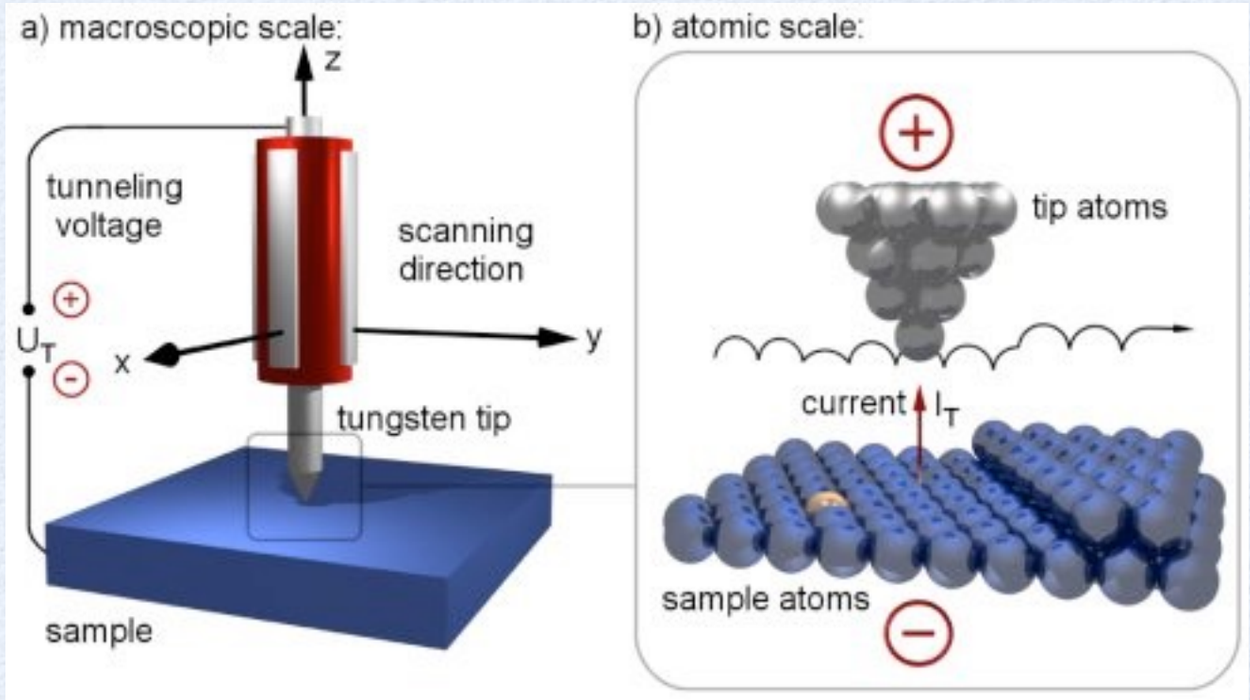
Excitations in Quantum Many-Body Systems: Dynamical Spectral Functions

angle-resolved photoemission (ARPES)



(Wikipedia)

scanning-tunneling spectroscopy



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

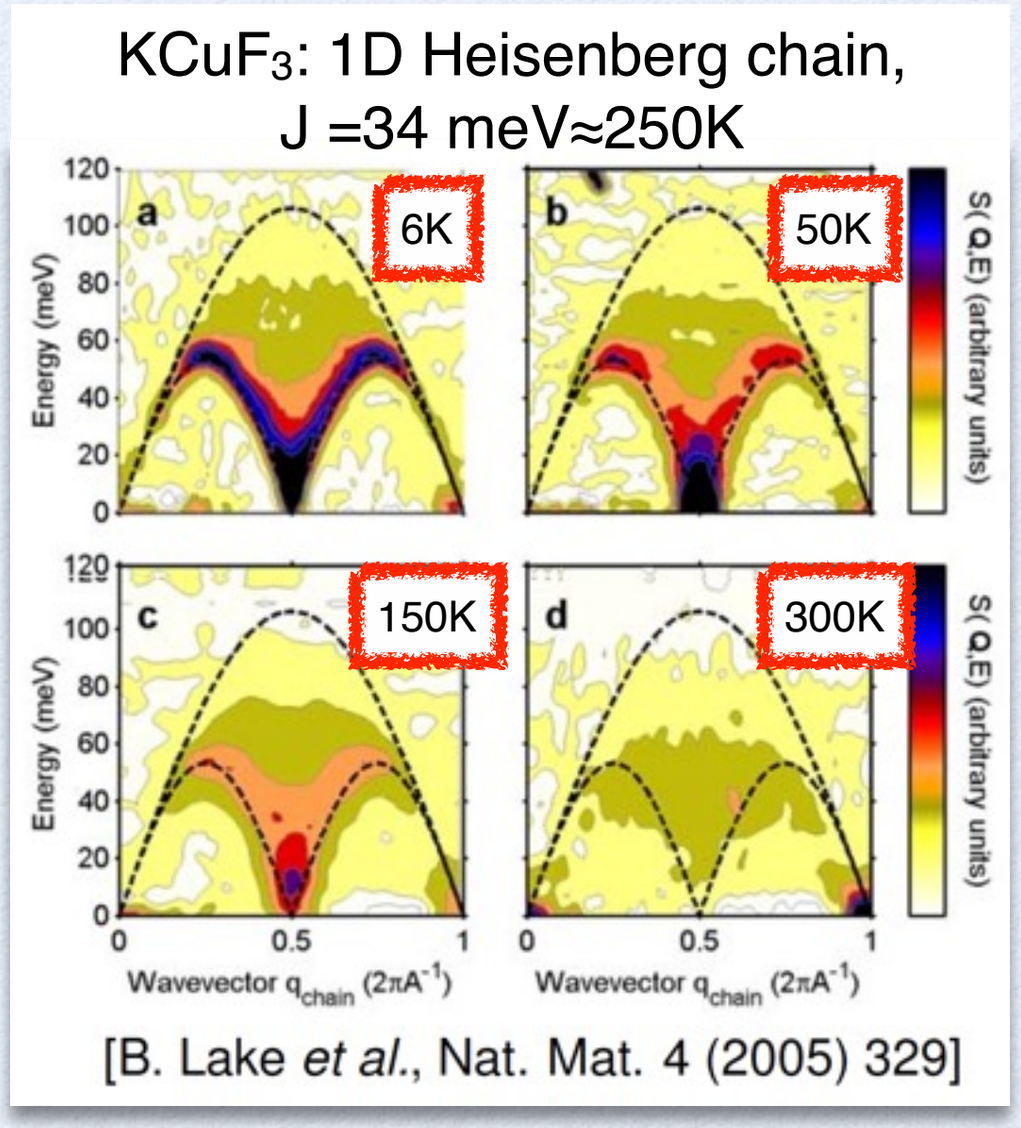
Linear response: measure quantities of type:

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

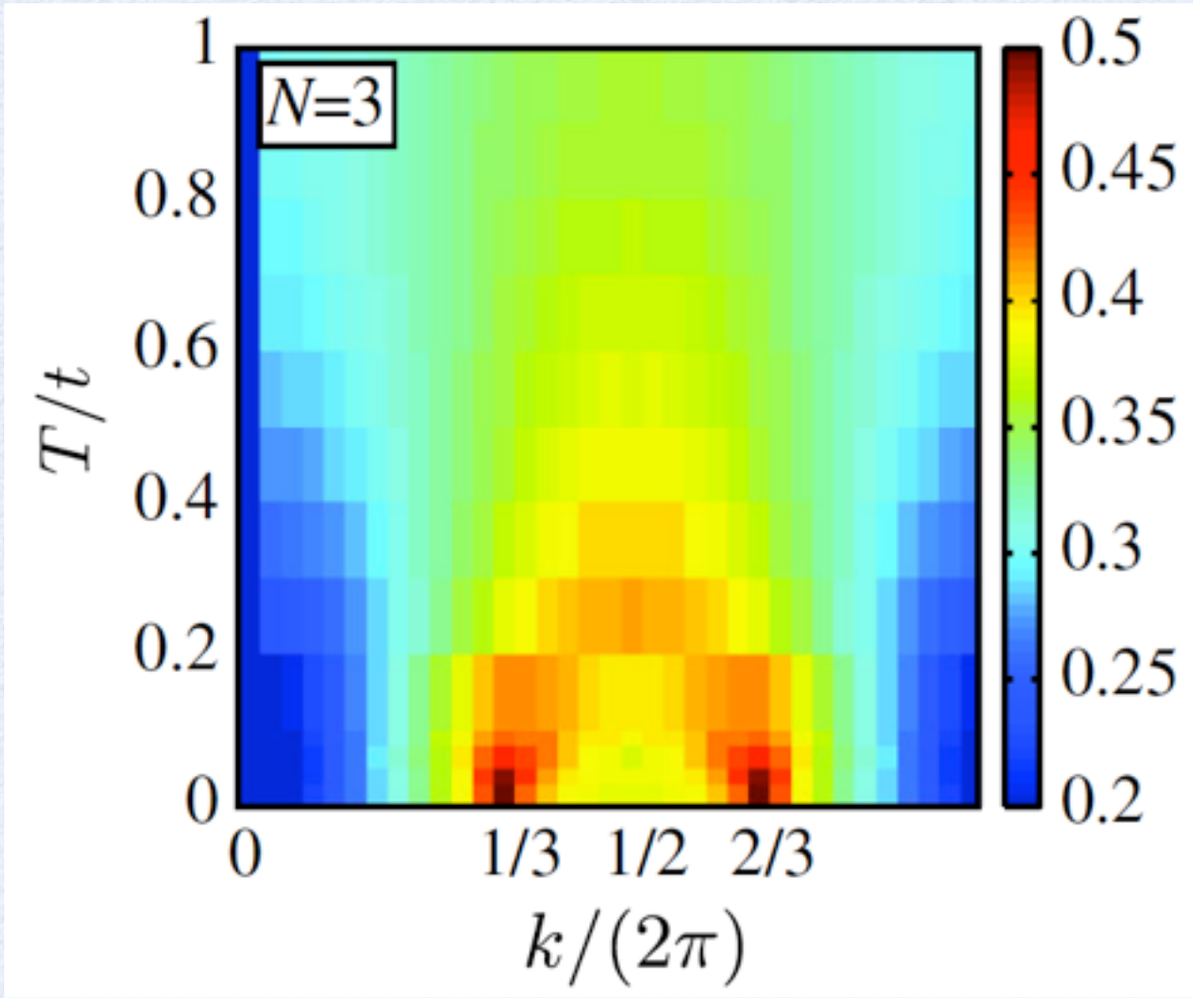
➠ insights into (local) density of states, excitations of the system, structure factors

Dynamical spectral functions: finite temperatures

Materials (neutron scattering):



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

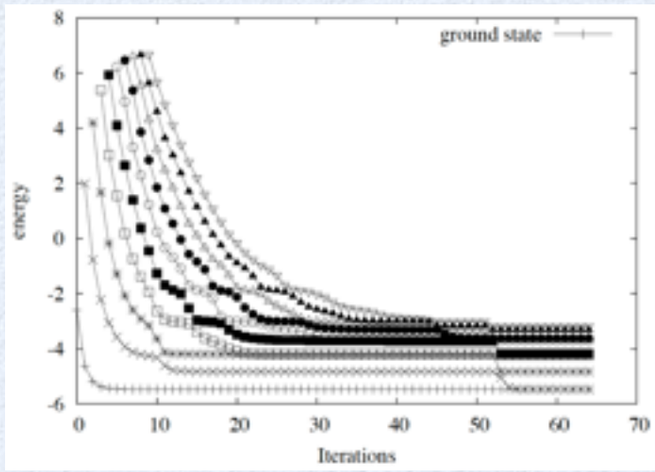


Theoretical Approach: Numerical Methods

Alternatives to 'analytical' methods:
"numerically exact" ↔ "perturbative" or "mean-field"

[Janus Supercomputer, Boulder]

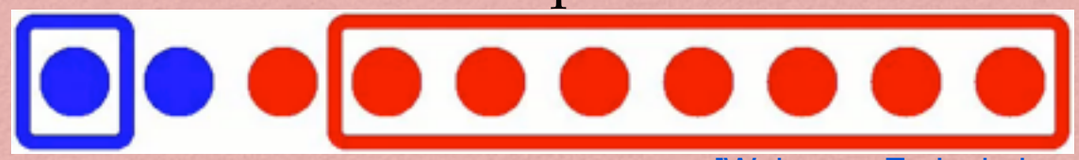
- Exact Diagonalization:
  ground state wave function via complete or iterative diagonalization of the Hamiltonian



Problem: exponentially growing Hilbert space
(e.g., spin-1/2 on L sites ➠ 2^L states)

- Density Matrix Renormalization Group (DMRG):
  (Quasi-)one-dimensional systems,
  truncation of the Hilbert space.

Also out-of-equilibrium!



[Webpage E. Jeckelmann]

Problem: Systems with strong entanglement ("area law")

- Further important methods: Quantum-Monte-Carlo, Numerical Renormalization Group

- "Semi-analytical" approaches: Functional Renormalization Group, Flow Equations, PCUTs,...

Dynamical correlation functions: $T = 0$ vs. $T > 0$

Dynamical correlation functions at T = 0:

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

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

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

DMRG:
Density Matrix Renormalization Group

Basic idea: data compression ("quantum version")

Original – 2.4 MB

Compressed 10x
257 KB

Compressed 20x
122 KB

Graphics (acoustics, signal transmission, etc.):

Example:
Fourier transform the signal and ignore modes which cannot be resolved (by the ear, the screen ,...).

➠ Good or even excellent quality, but with *much* smaller amount of data

DMRG: Density Matrix Renormalization Group

S.R. White, PRL (1992); U. Schollwöck, RMP (2005)/Ann. Phys. (2011); R.M. Noack & S.R. Manmana, AIP (2005)

Schmidt-decomposition:

$$|\psi\rangle = \sum_{j=1}^{\dim\mathcal{H}} w_j \, |\alpha\rangle_j \, |\beta\rangle_j \approx \sum_{j=1}^{m} w_j \, |\alpha\rangle_j \, |\beta\rangle_j$$

Approximation:
$m \ll \dim\mathcal{H}$
(e.g., 1000 sites: $\dim\mathcal{H} = 2^{1000}$, $m = 1000$)

$|\alpha\rangle_j$, $|\beta\rangle_j$: eigenstates of the reduced density matrix of A or B

- Very powerful for obtaining ground states in 1D
- Extension to non-equilibrium systems opened new direction of research

A. Daley et al, J.Stat. (2004); S.R. White & A.E. Feiguin, PRL (2004); S.R. Manmana et al., AIP (2005)

Key: Entanglement Entropy $\quad S = -\sum_j w_j^2 \log w_j^2$

➥ Measures information exchange and entanglement between A and B

➥ zero for *product states,* maximal for *maximally entangled states*

➥ the larger the entanglement in the system, the larger value of m needed

Problem in 2D:

"area law of entanglement growth" - m can grow exponentially with width of the systems

➥ frontier of today's efforts.

DMRG as Matrix Product State: Basic Idea

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

Wave function of a generic many-body system (e.g. S=1/2 chain):

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_N} c_{\sigma_1,\ldots,\sigma_N} |\sigma_1 \ldots \sigma_N\rangle$$

➟ 2^N coefficients (complex numbers)

Rewrite:

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_N} \mathbf{A}^{\sigma_1}\mathbf{A}^{\sigma_2}\cdots\mathbf{A}^{\sigma_{N-1}}\mathbf{A}^{\sigma_N} |\sigma_1 \ldots \sigma_N\rangle$$

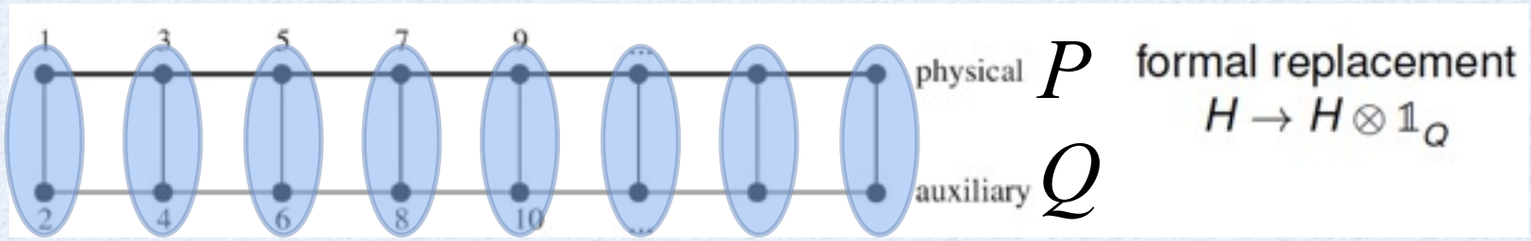
➟ 2N matrices

- can be 'truncated' (very efficient optimization in 1D)
- variational algorithms to 'optimize' each matrix (DMRG,...)

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)]

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)

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

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 $W \to [-1,1]$

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

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

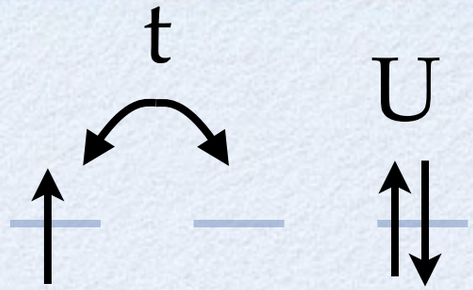
$$g_n^J = \frac{(N-n+1)\cos\frac{\pi n}{N+1} + \sin\frac{\pi n}{N+1}\cot\frac{\pi}{N+1}}{N+1}$$

"Jackson damping"

Effective Models for Quantum Magnets

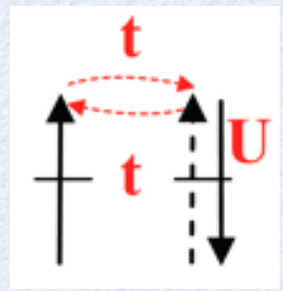
Starting point : Hubbard model

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



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

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



Real materials: additional spin-orbit coupling

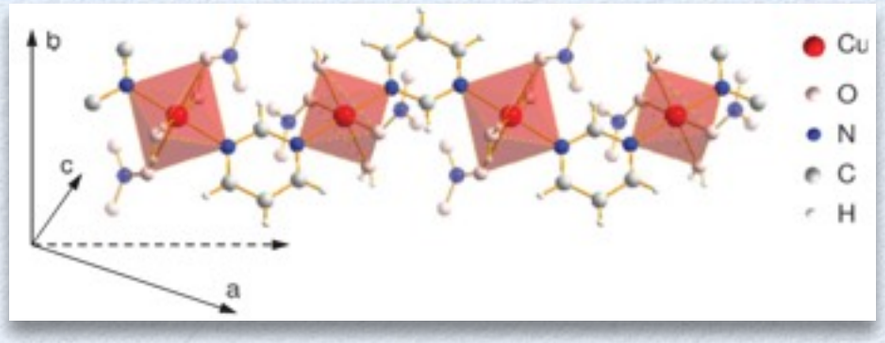
$$\sim \lambda \, \vec{L} \cdot \vec{S} \quad \lambda \ll 1 \qquad \vec{D} \cdot \left(\vec{S}_1 \times \vec{S}_2 \right) \qquad |\vec{D}| \sim \lambda$$

- 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:



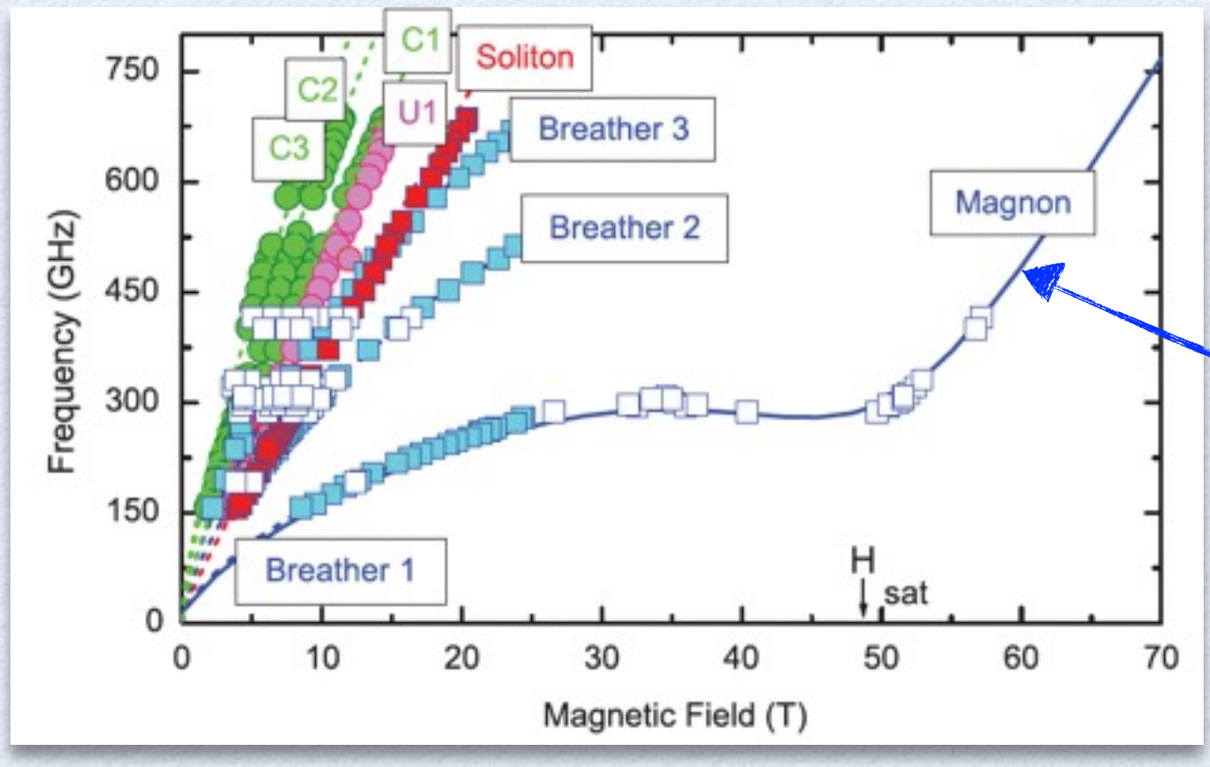
[S. Zvyagin et al., PRB(R) (2011)]

(Quasi-)1D Heisenberg AFM, described by

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

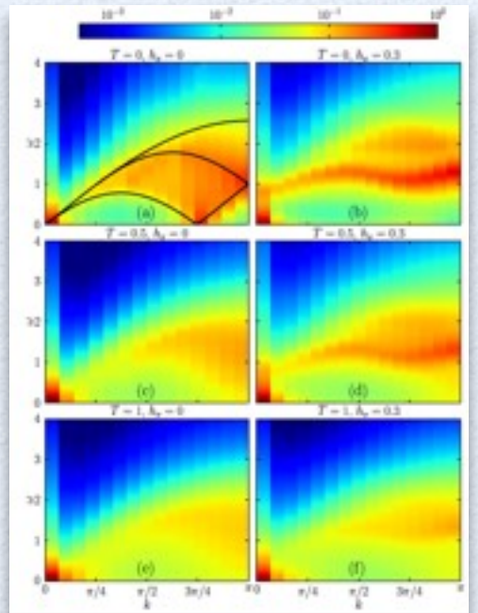
effect of staggered g-tensor + DM interaction

ESR spectrum in magnetic field:

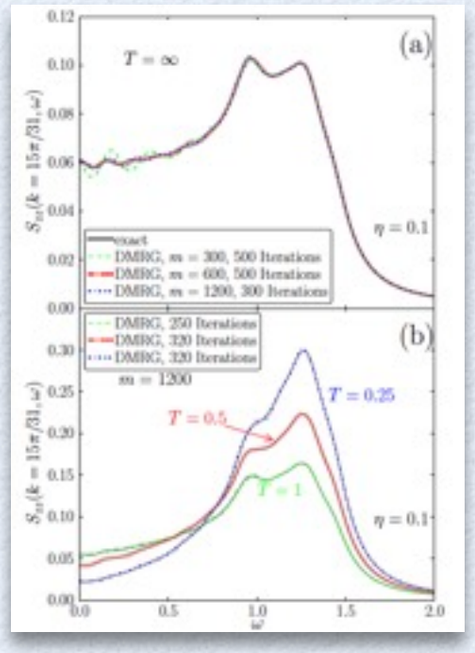


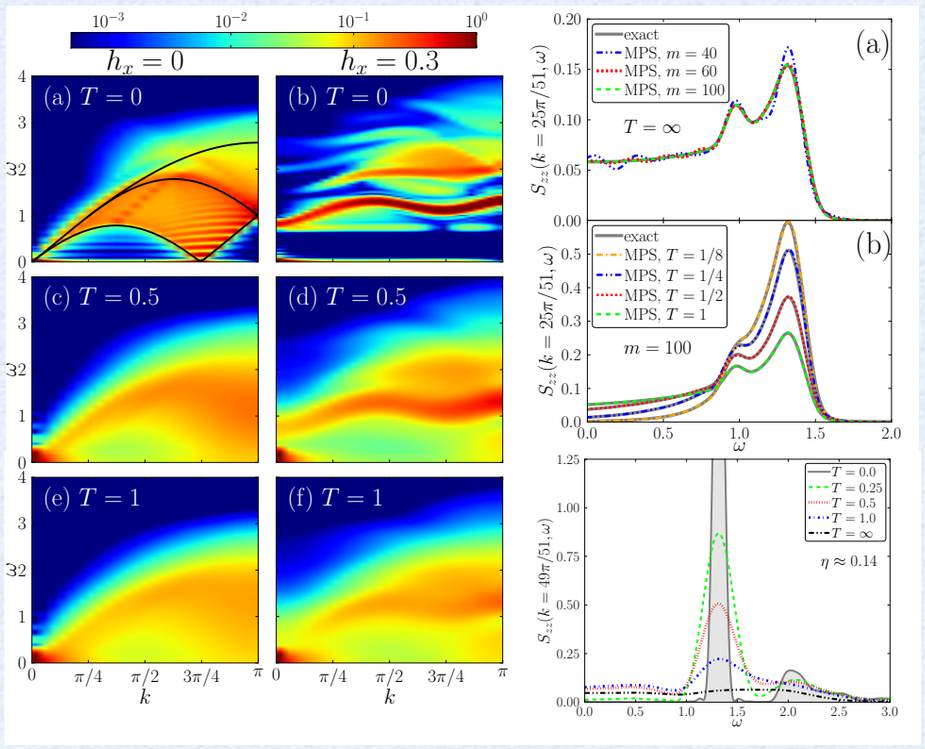
DMRG results

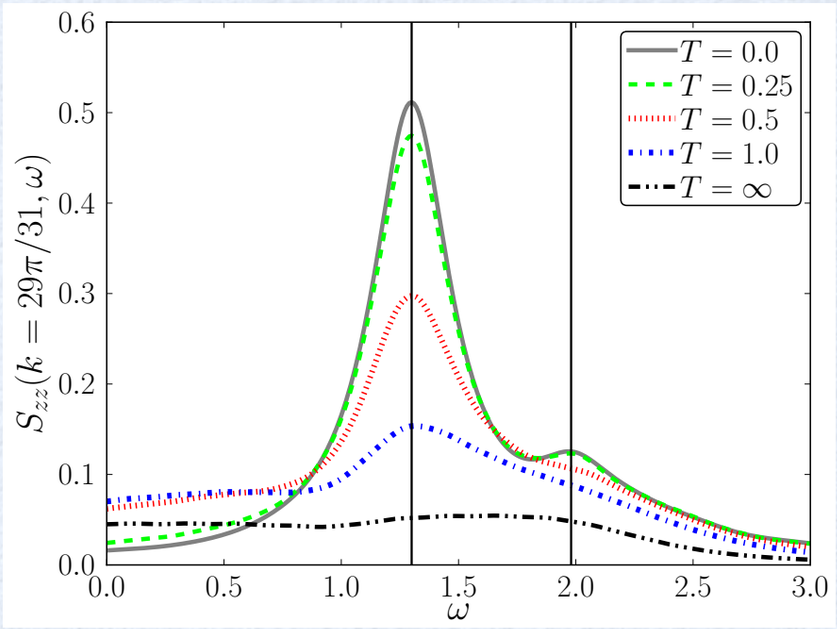
Liouvillian finite-T approach



Proof of Principle Calculations!







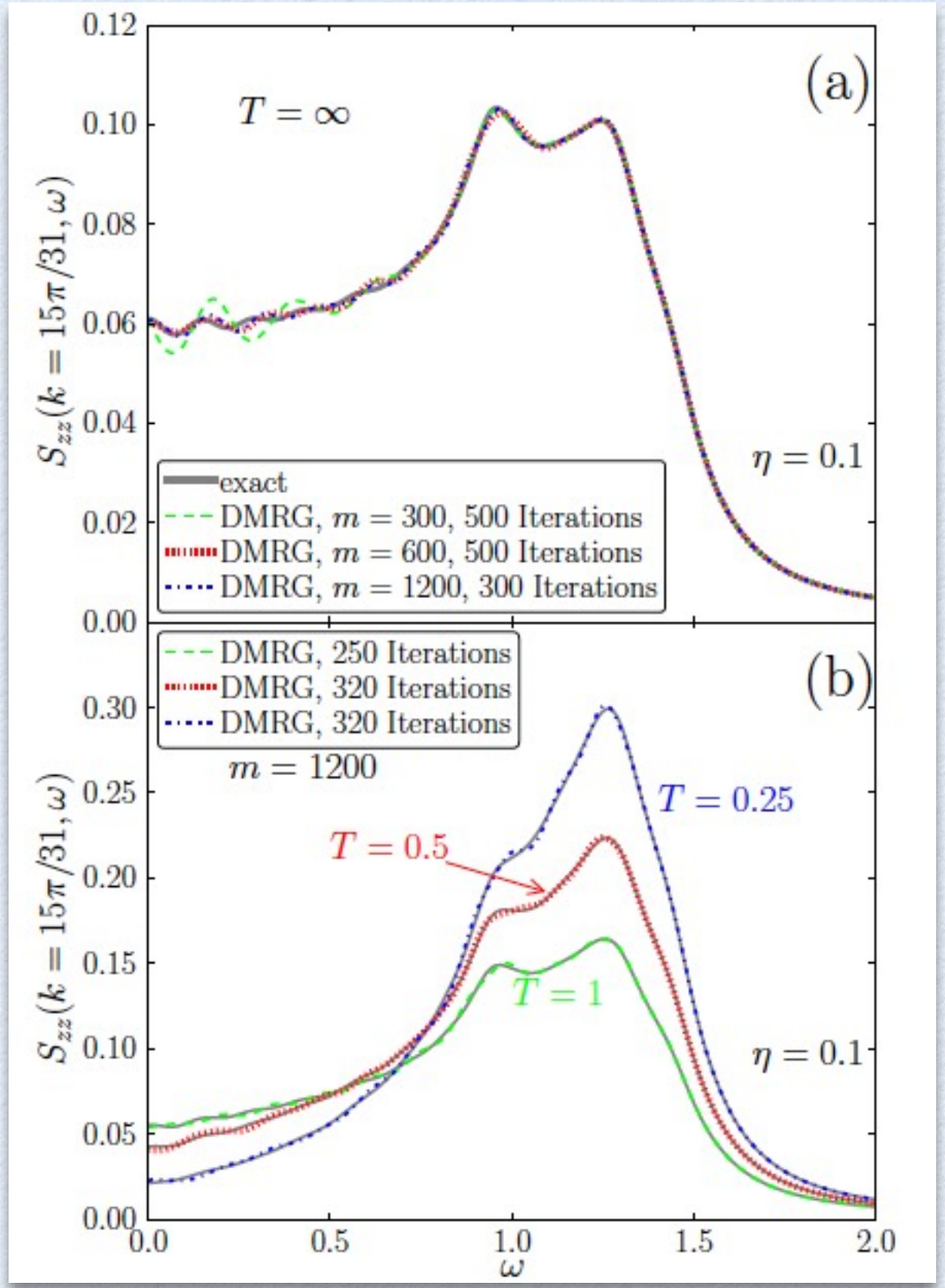
Liouvillian finite-T approach: comparison to exact results

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!



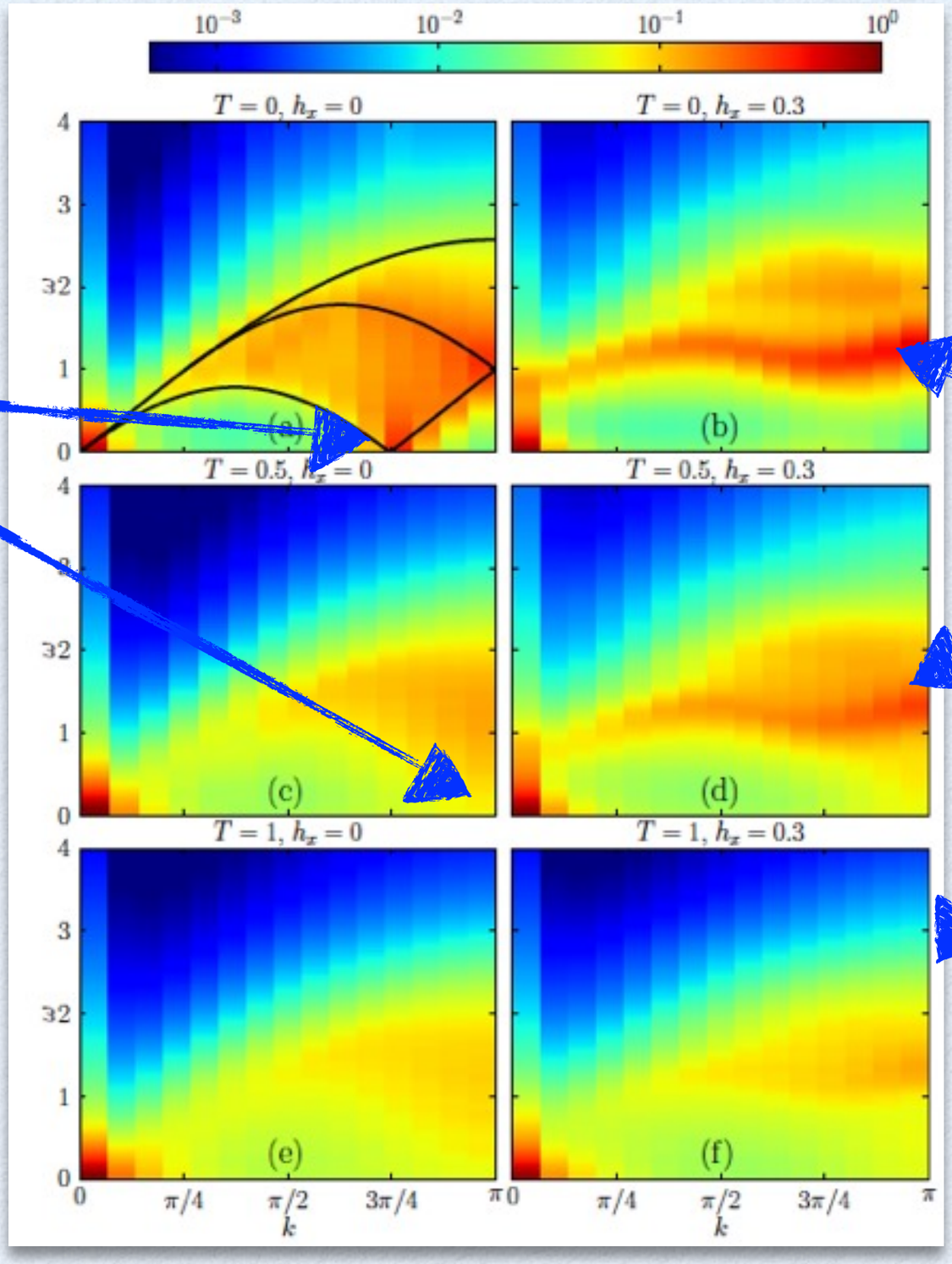
Liouvillian finite-T approach: Heisenberg antiferromagnet in magnetic field

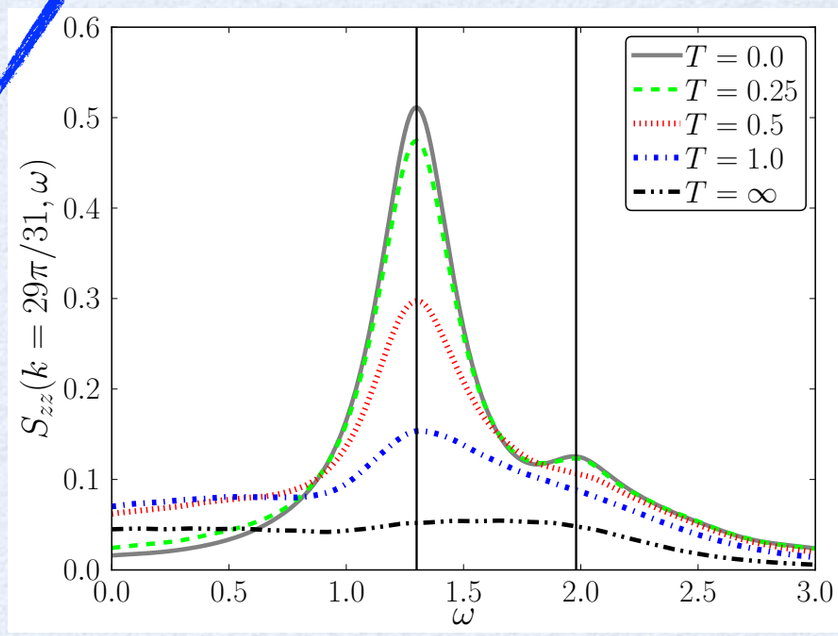
no DM

with DM

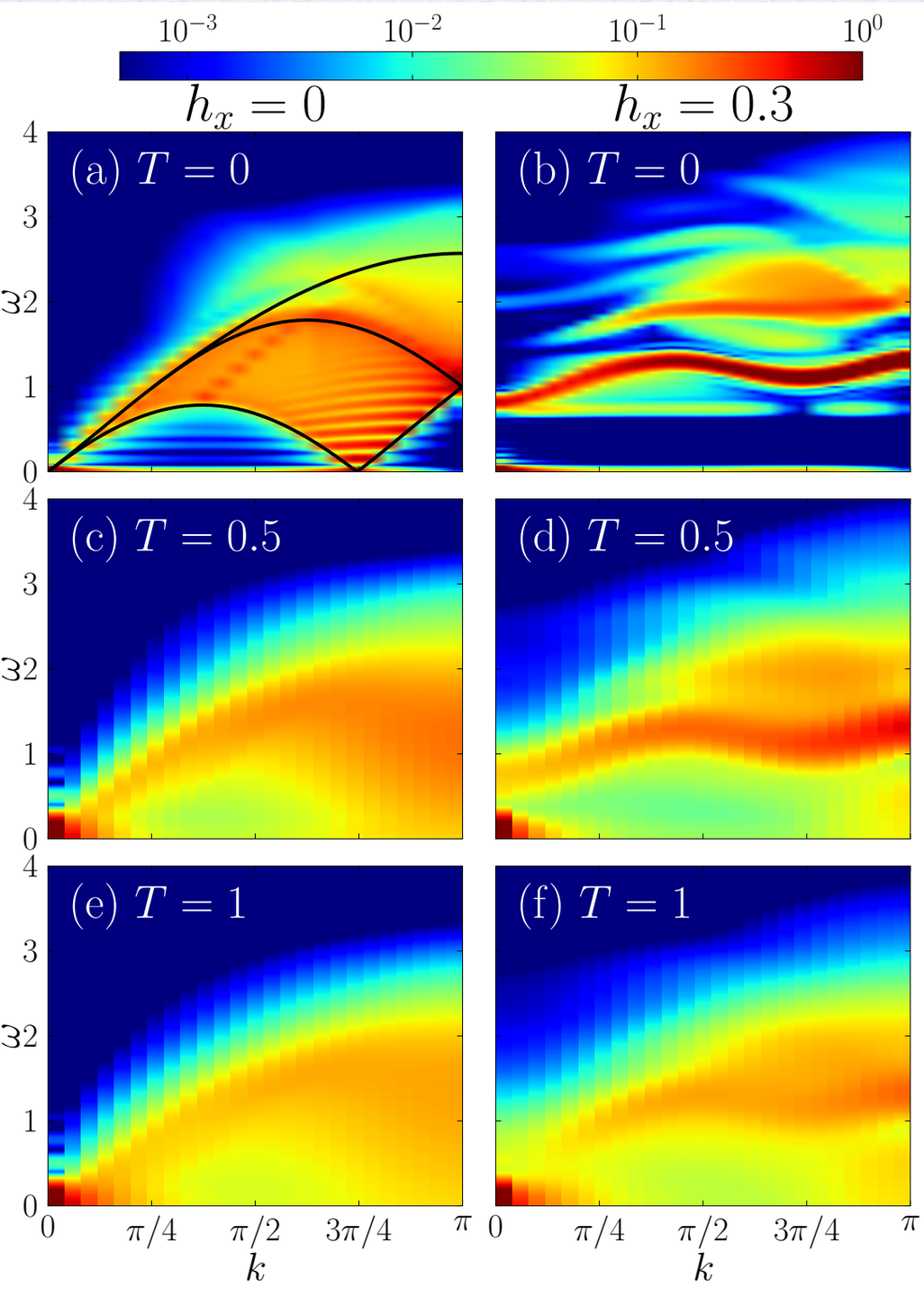
'Melting' of a Luttinger liquid

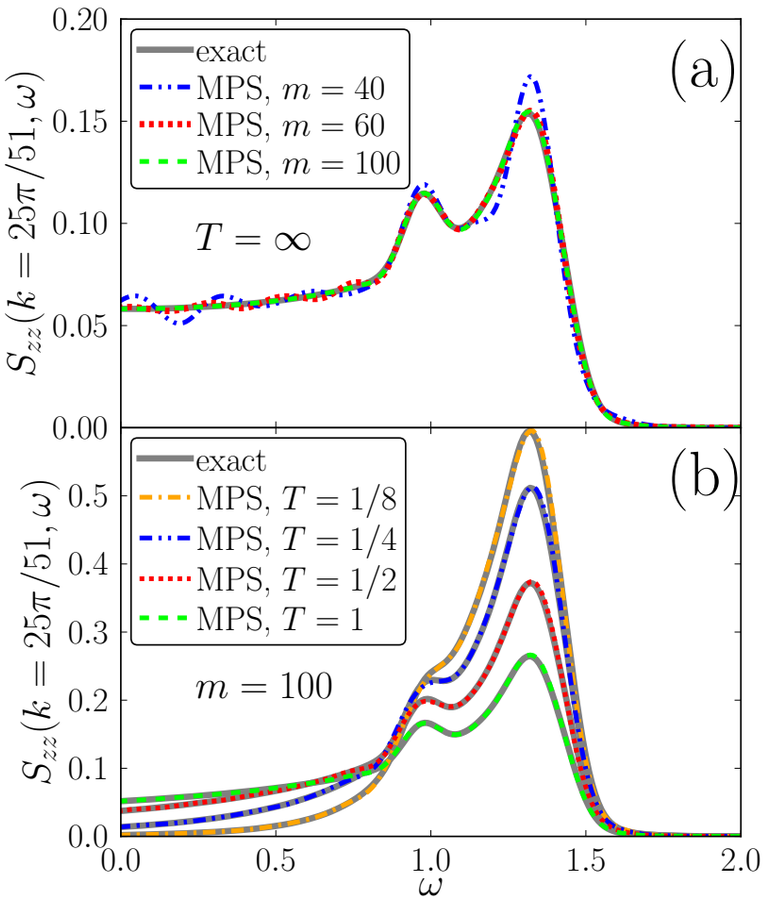
Formation of bands, thermal broadening

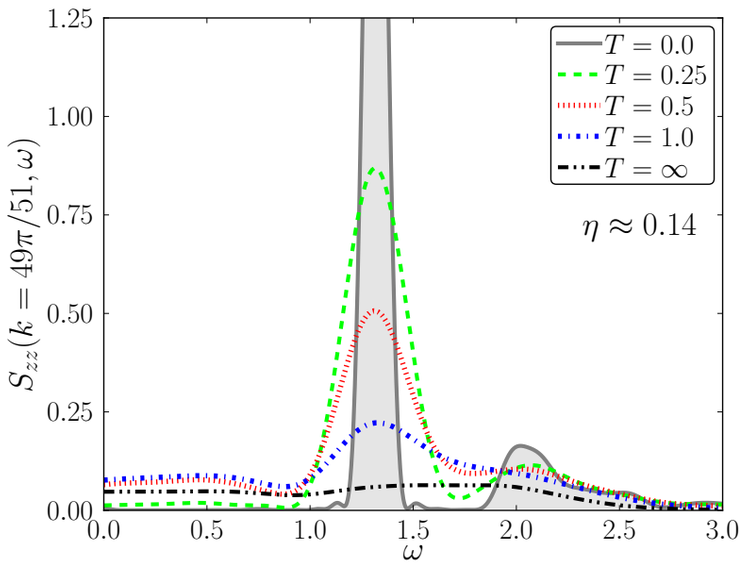




Liouvillian finite-T approach: using the Chebyshev expansion







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

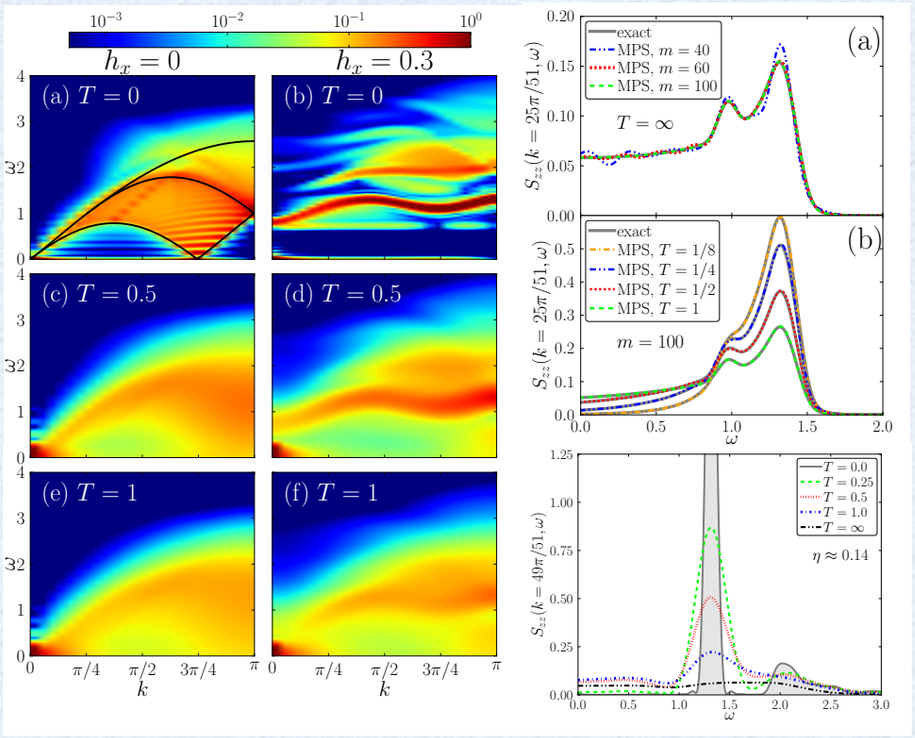
Conclusions

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, DMFT impurity solver, ...?)

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)