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

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Numerics for Correlated Systems in Göttingen: Talk to these people

I.) Matrix Product States:  Alexander Tiegel  ➔ Poster P10  Thomas Köhler  ➔ Poster P14

II.) VCA/CPT for spin systems:  Benjamin Lenz  ➔ Poster P9

III.) QMC/Dual Fermions:  René Kerkdyk  ➔ Talk F7 (Tomorrow)  Patrick Haase  ➔ Poster P4

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**Dynamical correlation functions:**

**DMRG approach for \( T > 0 \)?**

Main question of this talk:

*Direct* computation of dynamical spectral functions via DMRG at \( T > 0 \)?


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

\[L = \mathcal{H}_P \otimes I_Q - I_P \otimes \mathcal{H}_Q\]

- here: proof of principle results (no optimized code)
- flexibility of approaches to resolvent
- *high* resolution, small errors
- works at all frequencies
- no further input needed (e.g. linear prediction)
Excitations in Quantum Many-Body Systems: Dynamical Spectral Functions

angle-resolved photoemission (ARPES)  
scanning-tunneling spectroscopy

Linear response: measure quantities of type:

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

insights into (local) density of states, excitations of the system, structure factors
Dynamical spectral functions: finite temperatures

Materials (neutron scattering):

KCuF$_3$: 1D Heisenberg chain,
J =34 meV≈250K

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

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

[L. Bonnes et al., PRL 109, 205305 (2012)]
Dynamical spectral functions: Cluster Perturbation Theory for Spins

\[ G^{-1} = G_0^{-1} - V \]
\[ G_{CPT}(k, \omega) = \frac{1}{L} \sum_{i,j=1}^{L} G_{ij}(Q, \omega)e^{-ik(r_i-r_j)} \]
\[ \mathcal{H} = -J \sum_i \left( \frac{1}{2}(S_i^+S_{i+1}^- + S_i^-S_{i+1}^+) + S_i^zS_{i+1}^z \right) \]


1D Heisenberg model

Bethe ansatz (L=400)

CPT (L=20)

Klauser et al. (2011)
**Dynamical correlation functions:**

$\mathcal{T} = 0$ vs. $\mathcal{T} > 0$

**Dynamical correlation functions at $T = 0$:**

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

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

**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:

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

\[ \Rightarrow \varrho_T = e^{-H/T} = \text{Tr}_Q | \Psi_T \rangle \langle \Psi_T | \]

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

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

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)]

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

(backward evolution in Q by Karrasch et al.)

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

[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”**


**Liouville space description of thermofields and their generalisations**

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**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.

Use continued fraction expansion (CFE)

\[ G_A(z) = -\frac{1}{\pi} \text{Im} \left\langle \psi_0 \left| A^\dag \frac{1}{z-L} A \right| \psi_0 \right\rangle = -\frac{1}{\pi} \text{Im} \frac{\left\langle \Psi_0 \left| A^\dag A \right| \Psi_0 \right\rangle}{z-a_0 - \frac{b_1^2}{z-a_1 - \frac{b_2^2}{z-\cdots}}} \]

Via Lanczos recursion

\[ |f_0\rangle = A |\Psi_0\rangle, \quad |f_{n+1}\rangle = L |f_n\rangle - a_n |f_n\rangle - b_n^2 |f_{n-1}\rangle \]

\[ a_n = \frac{\left\langle f_n | L | f_n \right\rangle}{\left\langle f_n | f_n \right\rangle}, \quad b_{n+1}^2 = \frac{\left\langle f_{n+1} | f_{n+1} \right\rangle}{\left\langle f_n | f_n \right\rangle}, \quad b_0 = 0 \]
Dynamical correlation functions: 
Chebyshev recursion

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

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

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

\[ W : \text{bandwidth of } \mathcal{L} \]

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

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

\[ g_n : \text{damping factors } \to \text{ Gaussian broadening } \eta \sim 1/N \]

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

“Jackson damping”

[MPS: A. Holzner et al., PRB 83, 195115 (2011); A. Weiße et al., RMP 78, 275 (2006)]
Effective Models for Quantum Magnets

Starting point: Hubbard model

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

Heisenberg exchange: 2\textsuperscript{nd} order perturbation theory for \( U >> t \)

\[ J \vec{S}_1 \cdot \vec{S}_2 \quad J = \frac{4t^2}{U} \]

Real materials: additional spin-orbit coupling

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

- Heisenberg term symmetric under permutations, SU(2) invariant
- Dzialoshinskii-Moriya-Term antisymmetric, breaks SU(2) invariance
- Typically \( D \sim 1 - 10\% J \)

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

\[ \mathcal{H} = \sum_j [JS_j \cdot S_{j+1} - HS_j^z - h (-1)^j S_j^z] \]

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)

Time evolution approaches: linear prediction

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

real time behavior: linear prediction

Fourier space:
Time evolution approaches: linear prediction

Comparison to experiments: KCuF$_3$

[B. Lake et al., PRL (2013)]
Exact results for analytically solvable XX-model:
Time evolution approaches: linear prediction

Time evolution with MPS:

Difference to linear prediction from $t=2$

Difference to linear prediction from $t=4$
Work directly in frequency space: Liouvillian finite-\(T\) approach.

Proof of Principle Calculations!
Liouvillian finite-$T$ approach: comparison to exact results

Continued fraction expansion:

$$H_{XX} = J \sum_{i}^{L-1} (S^x_i S^x_{i+1} + S^y_i S^y_{i+1})$$

$$S^\alpha_k = \sqrt{\frac{2}{L+1}} \sum_{i=1}^{L} \sin(k i) S^\alpha_i$$

Excellent agreement with exact results!
**Liouvillian finite-\(T\) approach:**

**Heisenberg antiferromagnet in magnetic field**

**Chebyshev approach:**

**no DM**

‘Melting’ of a Luttinger liquid

**with DM**

Formation of bands, thermal broadening

\[
\begin{align*}
T &= 0 \\
T &= 0.5 \\
T &= 1
\end{align*}
\]

\[
\begin{align*}
\hbar x &= 0 \\
\hbar x &= 0.3
\end{align*}
\]
Conclusions

Go to Liouville space and work directly in frequency space:

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

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)