Spectral functions and time evolution from the Chebyshev recursion

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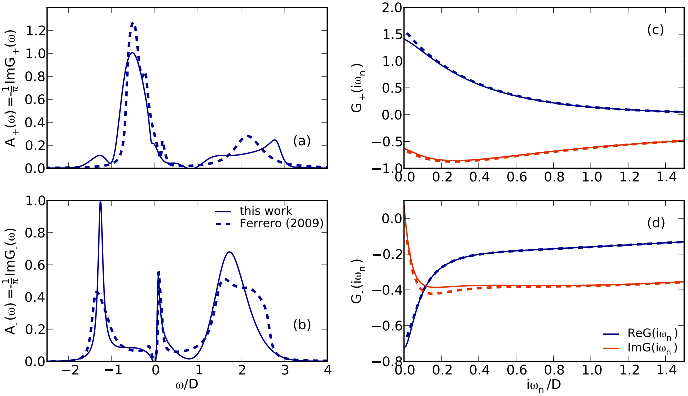
LMU, Group Seminar Theoretical Nanophysics, 3 Dec 2014

Motivation: two-site cluster DCA

Wolf, McCulloch, Parcollet & Schollwöck, PRB 90 115124 (2014a)

Model: Hole-doped Hubbard model on 2 dim square lattice, CTQMC by Ferrero, Cornaglia, De Leo, Parcollet, Kotliar & Georges, PRB 80 064501 (2009)



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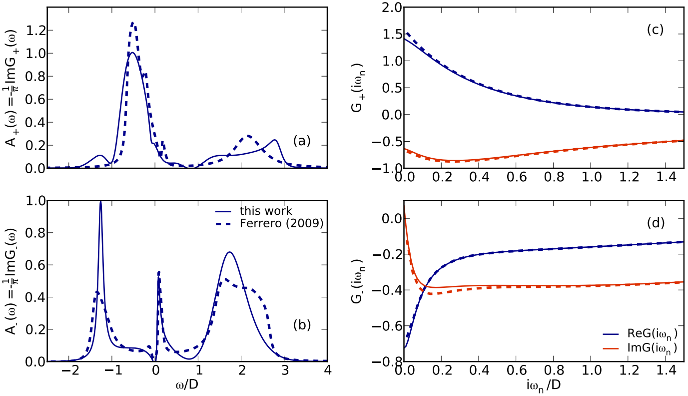

Fundamental problem of method: during Chebyshev recursion entanglement is generated ▷ accessible order or recursion limited (analogous to time evolution)

Chebyshev expansion of spectral function

Weiße, Wellein, Alvermann & Fehske, RMP 78 275 (2006)

Chebyshev Polynomials

$$T_n(x) = \cos\left(n \arccos(x)\right)$$

Recursive

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$

$$T_1(x) = x \qquad T_0(x) = 1$$

Orthogonal

$$\int_{-1}^{1} \frac{dx}{\sqrt{1-x^2}} T_m(x) T_n(x) \propto \delta_{mn}$$

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Global spectral function of $\mathcal{H}$ gives probability to find an eigenvalue at x

$$A_{\mathsf{glob}}(x) = \frac{1}{\dim \mathcal{H}} \mathsf{Tr}\, \delta(x - \mathcal{H}) = \frac{1}{\dim \mathcal{H}} \sum_n \delta(x - \mathcal{E}_i)$$

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Local spectral function gives probability to find eigenvalues at x under the *strong* constraint that eigenstates at x are *close* to a state $|t_0\rangle$ (non-zero overlap $\langle t_0 | E_n \rangle$)

$$A(x) = \langle t_0 | \delta(x - \mathcal{H}) | t_0 \rangle = \sum_n \left| \langle t_0 | E_n \rangle \right|^2 \delta(x - \mathcal{E}_i)$$

Expand $\delta(x - \mathcal{H})$ in Chebyshev polynomials

Weiße, Wellein, Alvermann & Fehske, RMP 78 275 (2006)

Expansion coefficient

$$\int dx\, T_n(x)\delta(x - \mathcal{H}) = T_n(\mathcal{H})$$

Sum to infinity

$$\delta(x - \mathcal{H}) \sim \frac{1}{\sqrt{1 - x^2}} \sum_{n=1}^{\infty} T_n(\mathcal{H}) T_n(x)$$

Insert this in spectral function

$$A(x) = \langle t_0 | \delta(x - \mathcal{H}) | t_0 \rangle \sim \frac{1}{\sqrt{1 - x^2}} \sum_{n=1}^{\infty} T_n(x) \langle t_0 | T_n(\mathcal{H}) | t_0 \rangle$$

Use recursive definition to compute $|t_n\rangle = T_n(\mathcal{H})|t_0\rangle$

$$|t_n\rangle = 2\mathcal{H}|t_{n-1}\rangle - |t_{n-2}\rangle$$
$$|t_1\rangle = \mathcal{H}|t_0\rangle$$

Comments on Chebyshev recursion with MPS

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$$|t_n\rangle = 2\mathcal{H}|t_{n-1}\rangle - |t_{n-2}\rangle$$
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▷ starting from a weakly entangled state $|t_0\rangle$, one evolves farer and farer away into a highly-entangled sector Wolf, McCulloch, Parcollet & Schollwöck, PRB 90 115124 (2014a)

▷ need to adjust matrix dimensions ▷ only finite expansion order n can be reached

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Fundamental problem: All MPS methods suffer from entanglement growth!

▷ Time evolution $e^{-iHt}|t_0\rangle$: only short times

▷ Dynamic DMRG: only high values of *broadening parameter* (*regulizer*) η

▷ *Lanczos* recursion and *Chebyshev* recursion: only low expansion orders

Is there are a way to escape this?

Analyticity of Green functions

Spectral function is

$$A(x) = -\lim_{\eta \to 0} \frac{1}{\pi} \mathsf{Im}\, G(x + i\eta)$$

where $G(x + i\eta)$ is analytic in upper half plane.

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Example: Knowledge of $G(z)$ on the imaginary-frequency axis: fit Padé approximation (continued fraction) to it and reconstruct $\lim_{\eta \to 0} G(x + i\eta)$ on the real axis.

Analytical continuation on the real-time axis

Laplace series is a suitable set of functions to fit $G(t)$ on real axis.

$$f(t) = \sum_j \alpha_j e^{(i\omega_j - \eta_j)t}$$

▷ Allow j to run over all eigen states ▷ Fourier series: $\omega_j \sim E_j$ and $\eta_j = 0$

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▹ Instead: target effective peak structure corresponding to excitations (aggolmeration of poles / eigenvalues) ▹ much less terms in $\sum_j$ ... which are now *damped* ▹ Laplace series

▹ Analytical continuation: If there is a method to determine the parameters in $f(t)$ that make it equal to some local *exact* data of $G(t)$, then we can use $f(t)$ to reconstruct $G(t)$ for *all* times.

Linear prediction

Non-linear fitting problem is hard to solve!

$$f(t) = \sum_{j=1}^{p} \alpha_j e^{(i\omega_j - \eta_j)t}, \qquad \eta_j > 0.$$

Note the following property of $f(t)$, which emerges if we discretize time linearly

$$f(t_n) = \sum_{j=1}^{p} a_j f(t_{n-j}), \quad |a_j| < 1.$$

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Demand that numerical data $G(t_n)$ and $f(t_n)$ agree on domain $[t_0, t_1]$ that is accessible to the numerical method, i.e. minimize

$$\sum_{t_n \in [t_0, t_1]} \left| G(t_n) - \sum_{j=1}^{p} a_j G(t_{n-j}) \right|^2$$

▷ This linear fitting problem (determine parameters a_j) can be easily solved!

Example: simple low energy excitations

White & Affleck, PRB 77 134437 (2008)   Barthel, Schollwöck & White, PRB 79 245101 (2009)

Low energy excitiations

- ▷ determine long-time behavior $\propto e^{(i\omega-\eta)t}$ where $\eta \ll 1$
- ▷ determine sharp features in spectral function $\propto \frac{\eta}{\pi}\frac{1}{\eta^2+(x-\omega)^2}$

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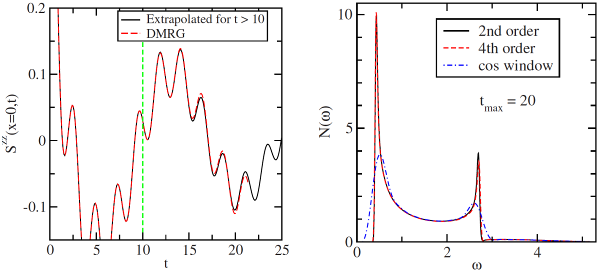
For a general single-particle excitation of the ground state

▷ for short times, eigenstates from the whole single-particle bandwidth contribute!

▷ at long times, only a superposition of few $\propto e^{(i\omega-\eta)t}$ survive

Linear prediction *obviously* applies for magnons in Heisenberg model!



Linear prediction of Chebyshev expansion

Linear prediction in time ▷ extrapolate coefficients $G(t_n)$ of Fourier expansion of $A(x)$

By analogy? / Ad hoc: Why not try linear predicition for coefficients μ_n of Chebyshev expansion of $A(x)$? Ganahl, Thunström, Verstraete, Held & Evertz, PRB 79 045144 (2014)

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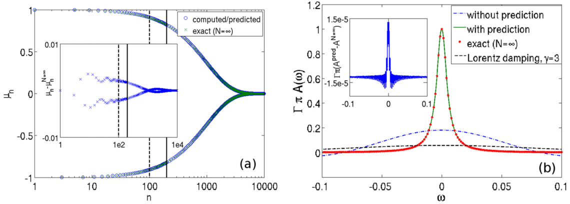

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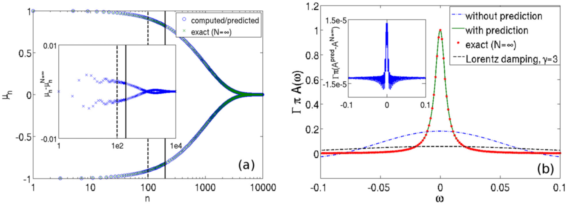

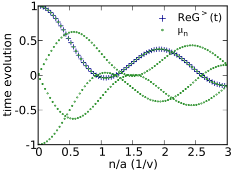

▷ In the setup they considered, Chebyshev expansion is equivalent to Fourier expansion!

General problem:

▷ (Complex) analyticity “hard” (impossible) to define for a discrete sequence μ_n

▷ Seeing linear prediction as analytical continuation not straight-forward to justify!

Linear prediction of Chebyshev expansion

Another view point: Convergence theory for Chebyshev expansions.

▷ Roughly: Chebyshev expansion of $f(x)$ convergences exponentially if $f(x)$ smooth and algebraically if $f(x)$ discontinuous. Boyd, Chebyshev and Fourier spectral methods (2001)

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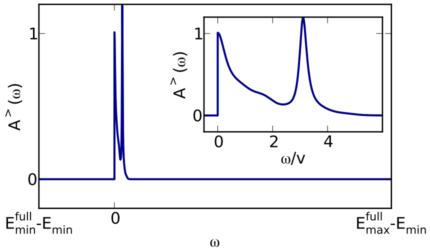
▷ Exponential convergence is compatible with linear prediciton!

But: spectral function is *in general at least* discontinuous. Although in the thermodynamic limit, the delta functions merge to a sectionwise smooth function

$$A^{>}(x) = \sum_n \left|\langle t_0^{>} | E_n \rangle\right|^2 \delta(x - E_i)$$

the weights $\left|\langle t_0^{>} | E_n \rangle\right|^2$ can produce discontinuities.



Chebyshev expansion of fermionic Green function

For a fermionic particle-like Green function, defined by choosing $|t_0^>\rangle = c^\dagger|E_0\rangle$, the discontinuity can be lifted by adding the hole parts $|t_0^<\rangle = c|E_0\rangle$

$$A(x) = A^>(x) + A^<(-x)$$

▷ Chebyshev expansion of $A(x)$ much better controlled than the one of $A^>(x)$ Holzner, Weichselbaum, McCulloch, Schollwöck & von Delft, PRB 83 195115 (2011)

▷ accessible to linear predicition Ganahl, Thunström, Verstraete, Held & Evertz, PRB 90 045144 (2014)

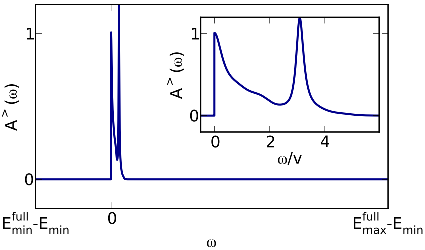
Observe: Discontinuity produced by weights $\left|\langle t_0^>|E_n\rangle\right|^2$ if $|t_0^>\rangle$ involves ground state at $x = 0$ can **also** be lifted by defining

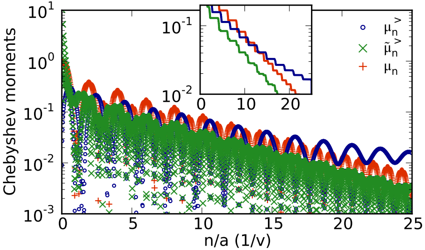
$$\widetilde{A}^>(x) = A^>(x) - A^>(0).$$

Chebyshev expansion of fermionic Green function

$$A(x) = A^{>}(x) + A^{>}(-x) \qquad \widetilde{A}^{>}(x) = A^{>}(x) - A^{>}(0)$$

The Chebyshev expansions of both continuous redefinitions converge exponentially!





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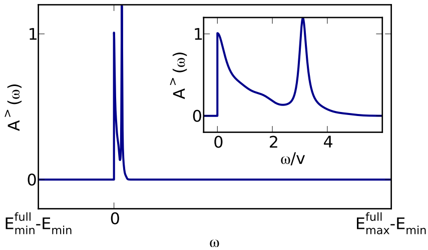

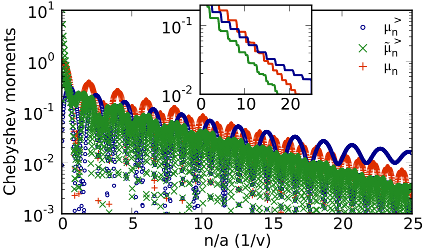

▷ We can hence apply linear predicition to both of these redefinitions.

▷ Only problem: prior to linear predicition, the value of $A^>(0)$ is unknown. Luckily, the corresponding self-consistency equation can be stably solved iteratively.

Chebyshev expansion of fermionic Green function

What is the advantage of using $\widetilde{A}(x)$ over $A(x)$?

$$A(x) = A^{>}(x) + A^{>}(-x) \qquad \widetilde{A}^{>}(x) = A^{>}(x) - A^{>}(0)$$

▷ **Different view** on recursion over H: *Probe* spectrum of H in vicinity of $|t_0\rangle$ by subsequent applications of H

▷ MPS: each application of H to the test vectors $|t_n\rangle$ produces entanglement

▷ **Fundamental question**: find the recursion (algorithm) that extracts most information about spectrum of H *per application* of H?

▷ Jorge: Lanczos better than Chebyshev (among other results)

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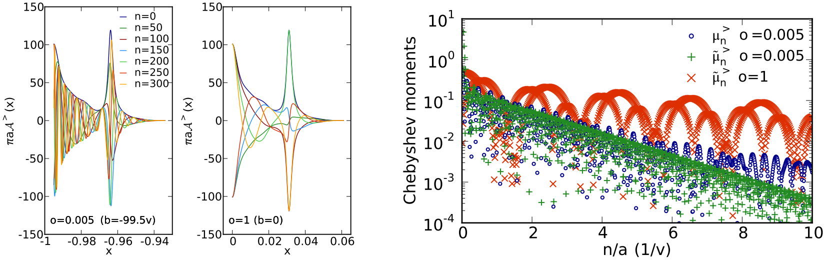
▷ Among all **possible setups of Chebyshev recursions**, which one is optimal? ▷ Wolf, McCulloch, Parcollet & Schollwöck, PRB 90 115124 (2014a)

Here:

▷ $A(\omega)$ is only available in the least-optimal setup of Chebyshev recursions (which we can now show is the one that is equivalent to time evolution)

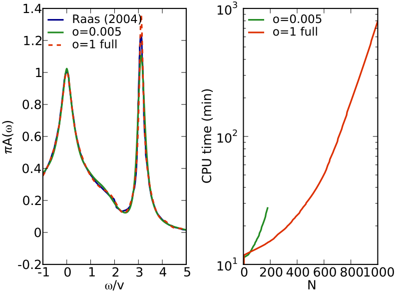
▷ $A^{>}(\omega)$ is available in the optimal setup (resolution increased by factor ~ 6)!



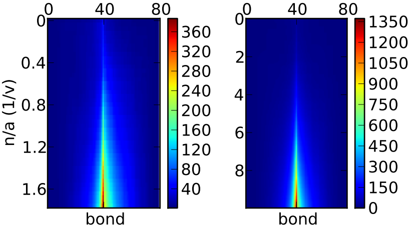
Orders of magnitude speed-up for MPS computations

▷ To reach the same error level, an expansion order of about $\sim \frac{1}{6}$ of the original setup suffices.

▷ Due to the exponential time scale, this means a huge speedup. In the following example, a factor 30.



Bond dimensions



Outlook

Path 1: Combine several results on the computation of spectral functions to treat multi-band problems in DMFT applications.

- Correct way of treating recursions with MPS: adaptive bond dimensions
  Wolf, McCulloch, Parcollet & Schollwöck, PRB 90 115124 (2014a)
- Optimal Chebyshev recursion w.r.t. entanglement production
  Wolf, McCulloch, Parcollet & Schollwöck, PRB 90 115124 (2014a)
- Linear prediction for Chebyshev expansions
  Ganahl, Thunström, Verstraete, Held & Evertz, PRB 90 045144 (2014)
- Least entangled geometry for representation of impurity problems
  Wolf, McCulloch & Schollwöck, arXiv:1410.3342 (2014b)
- Exploit optimal Chebyshev recursion for linear prediction
  this work

Path 2: Use equialence of time evolution and Chebyshev expansion to use the Chebyshev recursion as a new *time evolution* that only involves action of H (MPO representation known) and not of e^{-iHt} (no MPO representation known). this work

Summary

- Chebyhsev recursion efficient way to compute spectral functions
- from precise knowledge of $G(t)$ on a small domain $[t_0, t_1]$ reconstruct $G(t)$ for all times
- linear prediction is, due to linearity, a *practically feasble* algorithm to extract precise information about $G(t)$ on $[t_0, t_1]$
- linear prediction can also be applied to Chebyshev expansions
- lift discontinuity of spectral functions to use optimal Chebyshev setup
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Thanks for your attention!

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