MPS-based quantum impurity solvers

DMFT + DMRG

F. Alexander Wolf

with M. Eckstein, O. Parcollet, I. P. McCulloch and U. Schollwöck

Arnold Sommerfeld Center for Theoretical Physics, LMU Munich

Würzburg, 28 Feb 2015

Outline

Measure spectral functions

- Finite size ▷ thermodynamic limit
- Analytically continue on real-time axis
- How to span the subspace using MPS?

DMFT with MPS

- Self-consistency – entanglement?
- Geometry of impurity problem – entanglement?

Results

- Equilibrium: two-patch DCA
- Non-equilibrium: quench from atomic limit

Why consider DMRG as impurity solver for DMFT?

Advantages over QMC

- EQ: direct access to frequency-dependent observables
- EQ/NEQ: no sign-problem

Why consider DMRG as impurity solver for DMFT?

Advantages over QMC

- EQ: direct access to frequency-dependent observables
- EQ/NEQ: no sign-problem

Advantages over NRG

- EQ: homogeneous energy resolution
- NEQ: no application of NRG yet

Why consider DMRG as impurity solver for DMFT?

Advantages over QMC

- EQ: direct access to frequency-dependent observables
- EQ/NEQ: no sign-problem

Advantages over NRG

- EQ: homogeneous energy resolution
- NEQ: no application of NRG yet

Why hasn't it been used up to now?

- Lanczos: instable and imprecise García, Hallberg & Rozenberg, PRL (2004)
- DDMRG: extremely expensive Nishimoto & Jeckelmann, JPhysCondMat, 2 papers (2004), Karski, Raas & Uhrig, PRB (2005), Karski, Raas & Uhrig, PRB (2008)
- Chebyshev and time evolution: much faster and precise Ganahl, Thunström, Verstraete, Held & Evertz, PRB (2014b), Ganahl, Aichhorn, Thunström, Held, Evertz & Verstraete, arXiv (2014a), Wolf, McCulloch, Parcollet & Schollwöck, PRB (2014a), Wolf, McCulloch & Schollwöck, PRB (2014b)

Spectral functions: finite size ▷ thermodynamic limit

Lin, Saad & Yang, arxiv:1308.5467 (2013) e.g. Wolf, Justiniano, McCulloch & Schollwöck, arXiv:1501.07216 (2015)

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

Continuous spectral function of thermodynamic limit from discrete spectral function of finite system?

$$A(\omega) = \langle\psi_0|\delta(\omega - (H - E_0))|\psi_0\rangle, \quad |\psi_0\rangle = c^\dagger|E_0\rangle = \text{single-part. excit.}$$

Spectral functions: finite size $\triangleright$ thermodynamic limit

Lin, Saad & Yang, arxiv:1308.5467 (2013) e.g. Wolf, Justiniano, McCulloch & Schollwöck, arXiv:1501.07216 (2015)

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

Continuous spectral function of thermodynamic limit from discrete spectral function of finite system?

$$A(\omega) = \langle \psi_0 | \delta(\omega - (H - E_0)) | \psi_0 \rangle, \quad |\psi_0\rangle = c^\dagger |E_0\rangle = \text{single-part. excit.}$$

Expand $A(\omega)$ in "oscillatory functions" $p_n(\omega)$, truncate this expansion!

$$A(\omega) \simeq \sum_{n=0}^{N} c_n p_n(\omega) \qquad \text{error } \simeq c_N \text{ for exp. conv.}$$

Spectral functions: finite size ▷ thermodynamic limit

Lin, Saad & Yang, arxiv:1308.5467 (2013) e.g. Wolf, Justiniano, McCulloch & Schollwöck, arXiv:1501.07216 (2015)

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

Continuous spectral function of thermodynamic limit from discrete spectral function of finite system?

$$A(\omega) = \langle\psi_0|\delta(\omega - (H - E_0))|\psi_0\rangle, \quad |\psi_0\rangle = c^\dagger|E_0\rangle = \text{single-part. excit.}$$

Expand $A(\omega)$ in "oscillatory functions" $p_n(\omega)$, truncate this expansion!

$$A(\omega) \simeq \sum_{n=0}^{N} c_n p_n(\omega) \qquad \text{error } \simeq c_N \text{ for exp. conv.}$$

- $p_n(\omega) = e^{i\omega\frac{n}{a}}$

  $\Rightarrow c_n = \langle\psi_0|e^{-i(H-E_0)\frac{n}{a}}|\psi_0\rangle$ time evolve

- $p_n(\omega) = T_n(\omega)$

  $\Rightarrow c_n' = \langle\psi_0|T_n(\frac{1}{a}(H - E_0))|\psi_0\rangle$ Chebyshev recurse

Spectral functions: finite size ▷ thermodynamic limit

Lin, Saad & Yang, arxiv:1308.5467 (2013) e.g. Wolf, Justiniano, McCulloch & Schollwöck, arXiv:1501.07216 (2015)

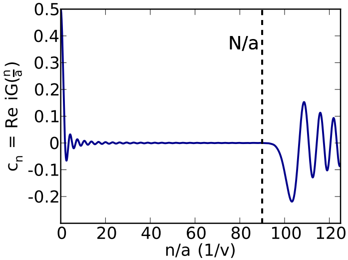
Weiße, Wellein, Alvermann & Fehske, RMP 78, 275 (2006)

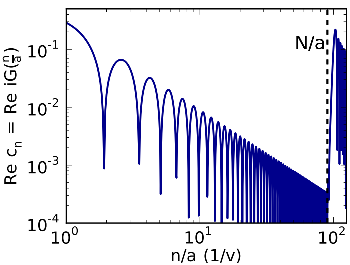
Continuous spectral function of thermodynamic limit from discrete spectral function of finite system?

$$A(\omega) = \langle\psi_0|\delta(\omega - (H - E_0))|\psi_0\rangle, \quad |\psi_0\rangle = c^\dagger|E_0\rangle = \text{single-part. excit.}$$

Expand $A(\omega)$ in "oscillatory functions" $p_n(\omega)$, truncate this expansion!

$$A(\omega) \simeq \sum_{n=0}^{N} c_n p_n(\omega) \qquad \text{error } \simeq c_N \text{ for exp. conv.}$$





Spectral functions: finite size ▷ thermodynamic limit

Lin, Saad & Yang, arxiv:1308.5467 (2013) e.g. Wolf, Justiniano, McCulloch & Schollwöck, arXiv:1501.07216 (2015)

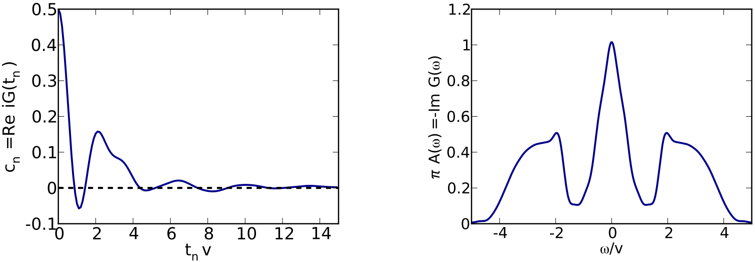
Weiße, Wellein, Alvermann & Fehske, RMP 78, 275 (2006)

Continuous spectral function of thermodynamic limit from discrete spectral function of finite system?

$$A(\omega) = \langle \psi_0 | \delta(\omega - (H - E_0)) | \psi_0 \rangle, \quad |\psi_0\rangle = c^\dagger |E_0\rangle = \text{single-part. excit.}$$

Expand $A(\omega)$ in "oscillatory functions" $p_n(\omega)$, truncate this expansion!

$$A(\omega) \simeq \sum_{n=0}^{N} c_n p_n(\omega) \qquad \text{error } \simeq c_N \text{ for exp. conv.}$$



Spectral functions: analytic continuation

Wolf, Justiniano, McCulloch & Schollwöck, arXiv:1501.07216 (2015)

Note that expansion coefficients are analytic functions of n for $n \in \mathbb{C}$

$$c_n = \langle \psi_0 | e^{-i(H-E_0)\frac{n}{a}} | \psi_0 \rangle \qquad \text{exponential}$$

$$c'_n = \langle \psi_0 | \cos(n \arccos \tfrac{1}{a}(H-E_0)) | \psi_0 \rangle \qquad \text{Chebyshev polynomial}$$

Find surrogate function $g(n)$ that agrees with c_n on $\{0, 1, ..., N\}$

$\Rightarrow g(n)$ describes c_n also for $n \to \infty$.

Spectral functions: analytic continuation

Wolf, Justiniano, McCulloch & Schollwöck, arXiv:1501.07216 (2015)

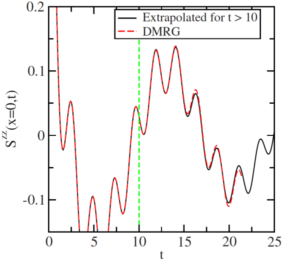
Note that expansion coefficients are analytic functions of n for $n \in \mathbb{C}$

$$c_n = \langle \psi_0 | e^{-i(H-E_0)\frac{n}{a}} | \psi_0 \rangle \qquad \text{exponential}$$

$$c'_n = \langle \psi_0 | \cos(n \arccos \tfrac{1}{a}(H - E_0)) | \psi_0 \rangle \qquad \text{Chebyshev polynomial}$$

Find surrogate function $g(n)$ that agrees with c_n on $\{0, 1, ..., N\}$

$\Rightarrow g(n)$ describes c_n also for $n \to \infty$.



Agreement in L_2 norm for short "times" ensures agreement for long times.

White & Affleck, PRB 77 134437 (2008)

Spectral functions: analytic continuation

Wolf, Justiniano, McCulloch & Schollwöck, arXiv:1501.07216 (2015)

Note that expansion coefficients are analytic functions of n for $n \in \mathbb{C}$

$$c_n = \langle\psi_0|e^{-i(H-E_0)\frac{n}{a}}|\psi_0\rangle \qquad \text{exponential}$$

$$c'_n = \langle\psi_0|\cos(n \arccos \tfrac{1}{a}(H-E_0))|\psi_0\rangle \qquad \text{Chebyshev polynomial}$$

Find surrogate function $g(n)$ that agrees with c_n on $\{0, 1, ..., N\}$

$\Rightarrow g(n)$ describes c_n also for $n \to \infty$.

Fit function that accounts for the functional form of c_n

$$g(n) = \sum_j \alpha_j e^{i\omega_j n}$$

▷ *linear prediction:* recursive reformulation leads to *linear fit*

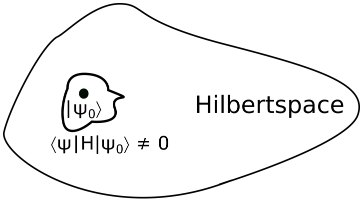
$$g(n) = \sum_j a_j g(n-j)$$

▷ for Chebyshev Ganahl, Thunström, Verstraete, Held & Evertz, Phys. Rev. B 90, 045144 (2014b)

Spectral functions: entanglement point of view

Wolf, Justiniano, McCulloch & Schollwöck, arXiv:1501.07216 (2015)

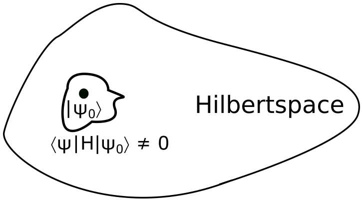
- Low entanglement of single-particle excitation $|\psi_0\rangle$
- Neighborhood of $|\psi_0\rangle$
  $\big\{|\psi\rangle : \langle\psi|H|\psi_0\rangle \neq 0\big\}$
- How to span this neighborhood?



Spectral functions: entanglement point of view

Wolf, Justiniano, McCulloch & Schollwöck, arXiv:1501.07216 (2015)

- Low entanglement of single-particle excitation $|\psi_0\rangle$
- Neighborhood of $|\psi_0\rangle$ $\{|\psi\rangle : \langle\psi|H|\psi_0\rangle \neq 0\}$
- How to span this neighborhood?



Immediate idea

- Orthogonal basis states "around" $|\psi_0\rangle$ most efficiently span this neighborhood (*Lanczos*)

$$|\psi_{n+1}\rangle = (H - \alpha_n)|\psi_n\rangle - \beta_n|\psi_{n-1}\rangle,$$

where α_n, β_n such that $\langle\psi_n|\psi_m\rangle = \delta_{nm}$

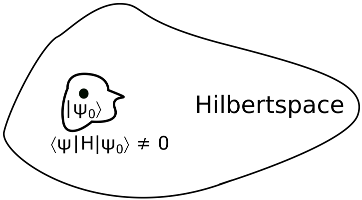
▷ But this simply is unstable, all the more, using MPS.

Dargel, Wöllert, Honecker, McCulloch, Schollwöck & Pruschke, PRB 85 205119 (2012)

Spectral functions: entanglement point of view

Wolf, Justiniano, McCulloch & Schollwöck, arXiv:1501.07216 (2015)

- Low entanglement of single-particle excitation $|\psi_0\rangle$
- Neighborhood of $|\psi_0\rangle$
  $\{|\psi\rangle : \langle\psi|H|\psi_0\rangle \neq 0\}$
- How to span this neighborhood?

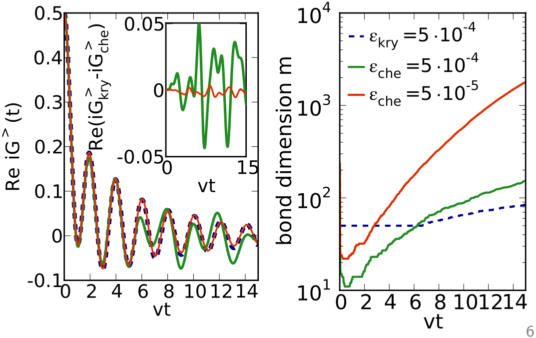


Stable alternatives

- Chebyshev recurse from $|\psi_0\rangle$ ▷ expand $A(\omega)$ in Chebyshev polynomials first MPS

  Holzner *et al.*, PRB 83 195115

- Time-propagate $|\psi_0\rangle$
  ▷ Fourier expand $A(\omega)$

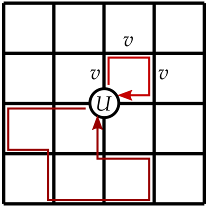


DMFT: self-consistency from entanglement point of view

Wolf, McCulloch & Schollwöck, PRB 90, 23513 (2014b)

Consider SIAM that is parametrized by the *hybridization function*

$$\Lambda(\omega) = v^2 G(\omega) \quad \text{or} \quad \Lambda(t) = v^2 G(t)$$

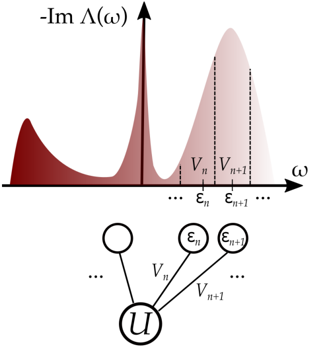


DMFT: self-consistency from entanglement point of view

Wolf, McCulloch & Schollwöck, PRB 90, 23513 (2014b)

Consider SIAM that is parametrized by the *hybridization function*

$$\Lambda(\omega) = v^2 G(\omega) \quad \text{or} \quad \Lambda(t) = v^2 G(t)$$



DMFT: self-consistency from entanglement point of view

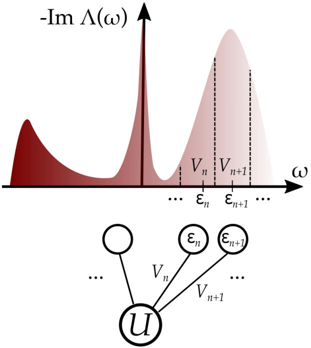
Wolf, McCulloch & Schollwöck, PRB 90, 23513 (2014b)

Consider SIAM that is parametrized by the *hybridization function*

$$\Lambda(\omega) = v^2 G(\omega) \quad \text{or} \quad \Lambda(t) = v^2 G(t)$$

▷ Solving the self-consistency in frequency space generally requires computing $|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$ for $t \to \infty$.

▷ $|\psi(\infty)\rangle$ is highly entangled. DDMRG *a priori* involves this point.



DMFT: self-consistency from entanglement point of view

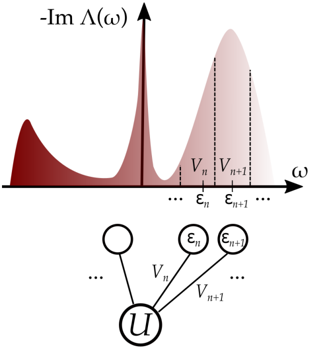
Wolf, McCulloch & Schollwöck, PRB 90, 23513 (2014b)

Consider SIAM that is parametrized by the *hybridization function*

$$\Lambda(\omega) = v^2 G(\omega) \quad \text{or} \quad \Lambda(t) = v^2 G(t)$$

▷ Solving the self-consistency in frequency space generally requires computing $|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$ for $t \to \infty$.

▷ $|\psi(\infty)\rangle$ is highly entangled. DDMRG *a priori* involves this point.



Remark (i) If Fourier transform can be avoided: *much* easier!
▷ NEQDMFT starting from uncorrelated initial state solved on time-slices. Gramsch, Balzer, Eckstein & Kollar, PRB 88, 235106 (2013)

DMFT: self-consistency from entanglement point of view

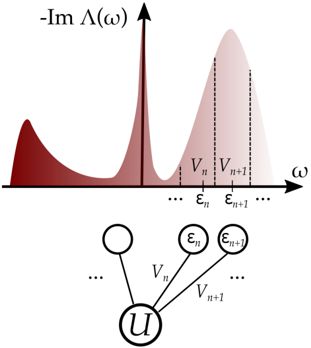
Wolf, McCulloch & Schollwöck, PRB 90, 23513 (2014b)

Consider SIAM that is parametrized by the *hybridization function*

$$\Lambda(\omega) = v^2 G(\omega) \quad \text{or} \quad \Lambda(t) = v^2 G(t)$$

▷ Solving the self-consistency in frequency space generally requires computing $|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$ for $t \to \infty$.

▷ $|\psi(\infty)\rangle$ is highly entangled. DDMRG *a priori* involves this point.



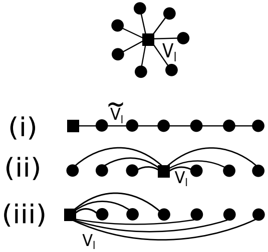
Remark (i) If Fourier transform can be avoided: *much* easier!
▷ NEQDMFT starting from uncorrelated initial state solved on time-slices. Gramsch, Balzer, Eckstein & Kollar, PRB 88, 235106 (2013)

Remark (ii) When solving the self-consistency iteratively in frequency space: successively increase resolution by going from short times to longer times ▷ exponential speed-up

DMFT: entanglement from geometry point of view

Wolf, McCulloch & Schollwöck, PRB 90, 23513 (2014b)

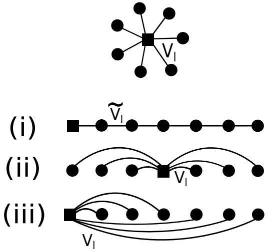
▷ Lower entanglement: star or chain geometry?

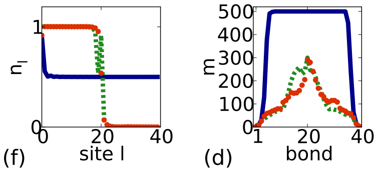


DMFT: entanglement from geometry point of view

Wolf, McCulloch & Schollwöck, PRB 90, 23513 (2014b)

▷ Lower entanglement: star or chain geometry?



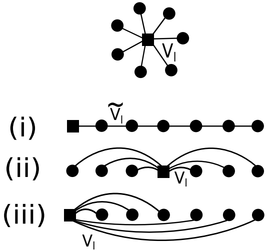


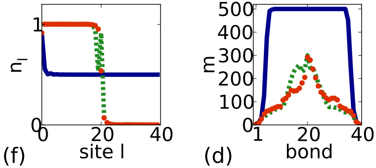
quickly converging DMRG algorithm
Hubig, McCulloch, Schollwöck & Wolf, arXiv:1501.05504 (2015)

DMFT: entanglement from geometry point of view

Wolf, McCulloch & Schollwöck, PRB 90, 23513 (2014b)

▷ Lower entanglement: star or chain geometry?

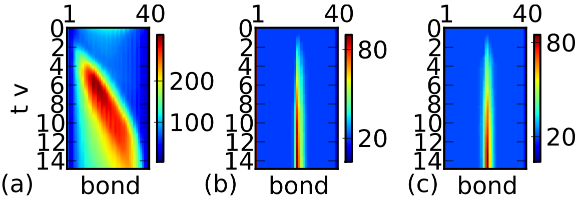




quickly converging DMRG algorithm

Hubig, McCulloch, Schollwöck & Wolf, arXiv:1501.05504 (2015)

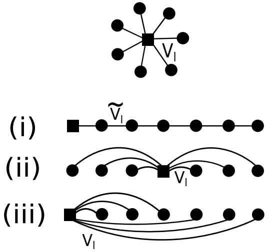
▷ Highly different bond dimension growth in different geometries

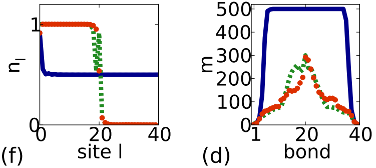


DMFT: entanglement from geometry point of view

Wolf, McCulloch & Schollwöck, PRB 90, 23513 (2014b)

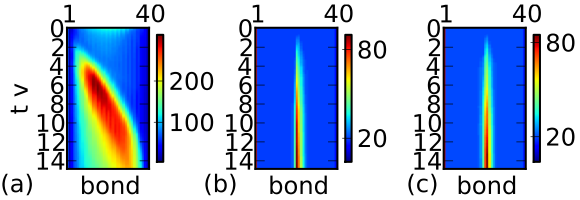
▷ Lower entanglement: star or chain geometry?

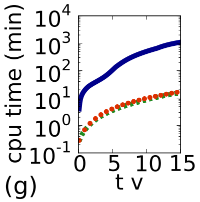




quickly converging DMRG algorithm
Hubig, McCulloch, Schollwöck & Wolf, arXiv:1501.05504 (2015)

▷ Highly different bond dimension growth in different geometries



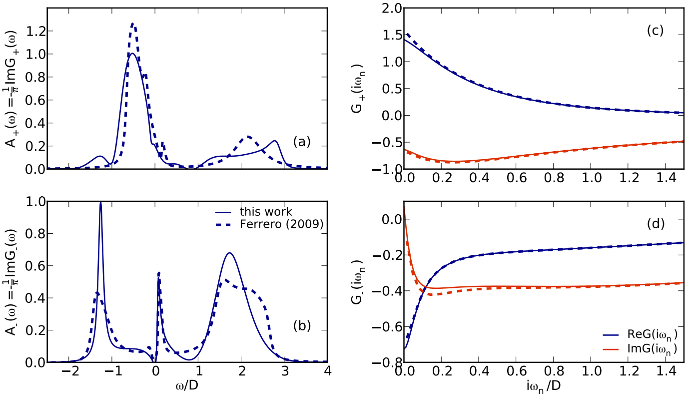


Results: two-site cluster DCA

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

CTQMC by Ferrero, Cornaglia, De Leo, Parcollet, Kotliar & Georges, PRB 80, 064501 (2009)

Model: Hole-doped Hubbard model on 2 dim. square lattice



▷ Pseudo-gap well reproduced

Results: non-equilibrium DMFT

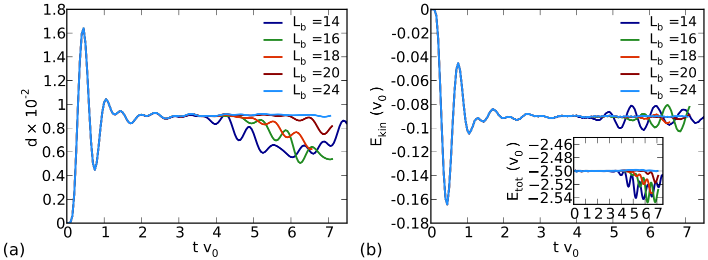
MPS solution Wolf, McCulloch & Schollwöck, PRB 90, 23513 (2014b)

Hamiltonian representation Gramsch, Balzer, Eckstein & Kollar, PRB 88, 235106 (2013)

Model: single-band Hubbard model on Bethe lattice

▷ quench from atomic limit $v = 0$ to $v = v_0$

Strong interactions: $U = 10v_0$
Exact diagonalization: $t_{\text{max}} \sim 3/v_0$
MPS: $t_{\text{max}} \sim 7/v_0$



Results: non-equilibrium DMFT

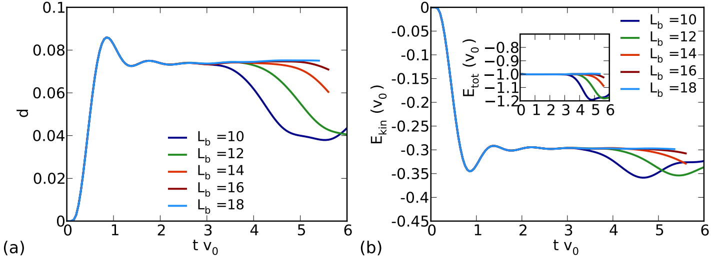
MPS solution Wolf, McCulloch & Schollwöck, PRB 90, 23513 (2014b)

Hamiltonian representation Gramsch, Balzer, Eckstein & Kollar, PRB 88, 235106 (2013)

Model: single-band Hubbard model on Bethe lattice

▷ quench from atomic limit $v = 0$ to $v = v_0$

Intermediate interactions: $U = 4v_0$
Exact diagonalization: $t_{\mathsf{max}} \sim 3/v_0$
MPS: $t_{\mathsf{max}} \sim 5.5/v_0$



Summary and Outlook

Summary

- Time evolution or Chebyshev polynomials to compute spectral functions combined with analytic continuation on the “real-time” domain
- Exploit the self-consistency from an entanglement point of view
- Star geometry much less entangled than chain geometry

Summary and Outlook

Summary

- Time evolution or Chebyshev polynomials to compute spectral functions combined with analytic continuation on the “real-time” domain
- Exploit the self-consistency from an entanglement point of view
- Star geometry much less entangled than chain geometry

Outlook

- further understand entanglement properties of impurity problems
- in equilibrium: apply these results to three-band models and compute conductivities
- in nonequilibrium: treat quenches with correlated initial states

Summary and Outlook

Summary

- Time evolution or Chebyshev polynomials to compute spectral functions combined with analytic continuation on the “real-time” domain
- Exploit the self-consistency from an entanglement point of view
- Star geometry much less entangled than chain geometry

Outlook

- further understand entanglement properties of impurity problems
- in equilibrium: apply these results to three-band models and compute conductivities
- in nonequilibrium: treat quenches with correlated initial states

Thank you!

Dargel, P. E., A. Wöllert, A. Honecker, I. P. McCulloch, U. Schollwöck & T. Pruschke, 2012, Phys. Rev. B **85**, 205119.

Ferrero, M., P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar & A. Georges, 2009, Physical Review B **80**, 064501.

Ganahl, M., M. Aichhorn, P. Thunström, K. Held, H. G. Evertz & F. Verstraete, 2014a, preprint 1405.6728.

Ganahl, M., P. Thunström, F. Verstraete, K. Held & H. G. Evertz, 2014b, Phys. Rev. B **90**, 045144.

García, D. J., K. Hallberg & M. J. Rozenberg, 2004, Phys. Rev. Lett. **93**, 246403.

Gramsch, C., K. Balzer, M. Eckstein & M. Kollar, 2013, Phys. Rev. B **88**, 235106.

Hubig, C., I. P. McCulloch, U. Schollwöck & F. A. Wolf, 2015, 1501.05504.

Karski, M., C. Raas & G. S. Uhrig, 2005, Phys. Rev. B **72**, 113110.

Karski, M., C. Raas & G. S. Uhrig, 2008, Phys. Rev. B **77**, 075116.

Lin, L., Y. Saad & C. Yang, 2013, 1308.5467.

Nishimoto, S. & E. Jeckelmann, 2004, J. Phys.: Condens. Matter **16**, 613.

Weiße, A., G. Wellein, A. Alvermann & H. Fehske, 2006, Rev. Mod. Phys. **78**, 275.

White, S. R. & I. Affleck, 2008, Phys. Rev. B **77**, 134437.

Wolf, F. A., J. A. Justiniano, I. P. McCulloch & U. Schollwöck, 2015, 1501.07216.

Wolf, F. A., I. P. McCulloch, O. Parcollet & U. Schollwöck, 2014a, Phys. Rev. B **90**, 115124.

Wolf, F. A., I. P. McCulloch & U. Schollwöck, 2014b, Phys. Rev. B **90**, 235131.