MPS-based quantum impurity solvers for DMFT
DMFT + DMRG

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Uni Hamburg, 16 Oct 2014

Motivation
Why use DMRG as impurity solver for DMFT?

Where is DMRG better than Quantum Monte Carlo?

- EQ: direct access to frequency-dependent observables / access T=0
- NEQ: no *phase* problem ▷ longer simulation times

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- EQ: homogeneous energy resolution / better scaling with number of bands
- NEQ: no application of NRG yet

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Why hasn't it been used up to now?

- Lanczos: instable and not precise García, Hallberg & Rozenberg, PRL (2004)
- DDMRG: computationally 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)

Outline

- Matrix product states: efficiently represent many-body wave functions of finite-size systems

- From finite-size systems to the thermodynamic limit

- Solving equilibrium DMFT using “CheMPS”

- Solving nonequilibrium DMFT using a time evolution algorithm

Matrix product states

Review: Schollwöck, Annals of Physics (2011)

Product state of local states (compare e.g. *Gutzwiller mean-field*)

$$
\begin{aligned}
|\psi\rangle &= \prod_{i=1\dots L}^{\otimes} \left(a^{\uparrow_i} |\uparrow_i\rangle + a^{\downarrow_i} |\downarrow_i\rangle\right), \quad a^{\sigma_i} \in \mathbb{C} \\
&= \sum_{\boldsymbol{\sigma}} \Big(\prod_{i=1\dots L} a^{\sigma_i} \Big) |\boldsymbol{\sigma}\rangle, \quad \boldsymbol{\sigma} = (\sigma_i)_{i=1}^{L}
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▷ of all possible many body states (superpositions $\sum_{\boldsymbol{\sigma}} c_{\boldsymbol{\sigma}} |\boldsymbol{\sigma}\rangle$, $c_{\boldsymbol{\sigma}} \in \mathbb{C}$), those with *zero* entanglement are realized

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Extend the ansatz by replacing $a^{\sigma_i} \in \mathbb{C}$ with $A^{\sigma_i} \in \mathbb{C}^{m_i \times m_{i+1}}$, $m_1 = 1$, $m_{L+1} = 1$.

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▷ No longer factorizes into product of local states ▷ entangled!

Matrix product states

Review: Schollwöck, Annals of Physics (2011)

- **Manage (truncate) matrix dimensions**:
  Weight of a Fock state $|\boldsymbol{\sigma}\rangle$ in $|\psi\rangle$ (almost) invariant under (truncated) SVD

$$c_{\boldsymbol{\sigma}} = \prod_{\sigma_i \in \boldsymbol{\sigma}} A^{\sigma_i} = \prod_{\sigma_i \in \boldsymbol{\sigma}} U^{\sigma_i} S^{\sigma_i} \left(V^{\sigma_i}\right)^{\dagger}$$

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- **DMRG**: Vartiational ground state search (minimize Rayleigh quotient)

$$\partial_{A_{\mu\nu}^{\sigma_i *}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = 0$$

  solved efficiently as ansatz is linear in $A_{\mu\nu}^{\sigma_i *}$.
  Important: Short-range interactions $\Rightarrow$ low entanglement

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- **Time evolution**
  Represent $\exp(-iHt)$ in Krylov subspace $\{|t_0\rangle, H|t_0\rangle, H^2|t_0\rangle, \ldots\}$.

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Thermodynamic limit from finite-size system

Extract *continuous* spectral function $\rho(\omega)$ of *thermodynamic limit* from a finite system with *discrete* energy levels?

Spectral function at $T = 0$

$$\begin{aligned}\rho(\omega) &= -\frac{1}{\pi}\operatorname{Im} G(\omega),\\ &= \sum_n w_n \delta(\omega - (E_n - E_0)), \qquad w_n = |\langle E_n | a^\dagger | E_0 \rangle|^2\end{aligned}$$

of single-particle Green's function

$$G(\omega) = \langle E_0 | a \frac{1}{\omega + i0^+ - (H - E_0)} a^\dagger | E_0 \rangle.$$

Thermodynamic limit from finite-size system

Review: Lin, Saad & Yang, ArXiv (2013)

Method 1 discrete representation of $\rho(\omega) = \sum_n w_n \delta(\omega - E_n)$

$$\rho_{\mathsf{discr}}(\omega) = \sum_n \frac{w_n}{\Delta_n} \chi\Big(\frac{\omega - E_n}{\Delta_n}\Big), \quad \Delta_n = \frac{1}{2}(E_{n+1} - E_{n-1}), \quad \chi \text{ indicator function}$$

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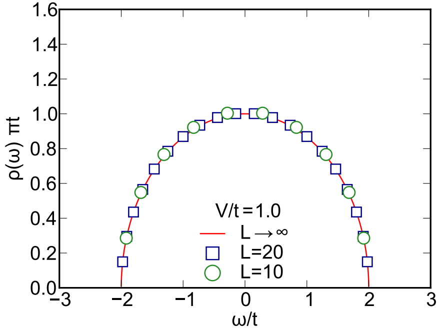

Example free SIAM

hybrid. $t_0 = V$, hopping $t_{i>0} = t$

$w_n = |\langle E_n | a_0^\dagger | E_0 \rangle|^2 \Rightarrow \rho(\omega) = \text{LDOS}$

$$H = -\sum_{i=0}^{L-2} t_i (a_i^\dagger a_{i+1} + \text{h.c.})$$

Features

- for $\omega = E_n$, rapid pointwise convergence to thermodynamic limit
- **but**: necessitates *precise* knowledge of poles and weights

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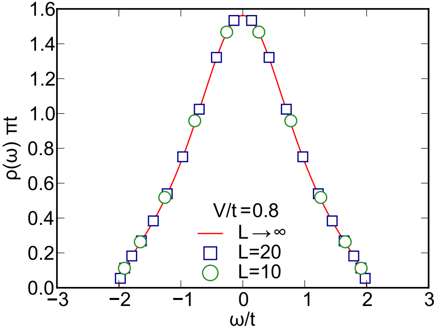

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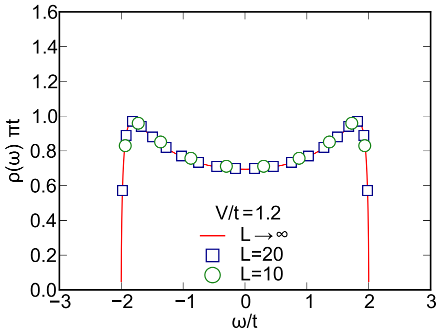

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Method 2 Broadened version of $\rho(\omega) = \sum_n w_n \delta(\omega - E_n)$

$$\rho_\eta(\omega) = \sum_n w_n h_\eta(\omega - E_n)$$

with either $h^g_\eta(x) = \frac{1}{\sqrt{2\pi}\eta} e^{-\frac{x^2}{2\eta^2}}$ (Gaussian) or $h^l_\eta = \frac{1}{\pi}\frac{1}{x^2+\eta^2}$ (Lorentzian).

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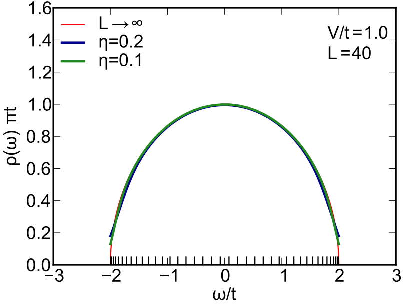

Features

- *uniform* convergence for $\eta \to 0$ and $L \to \infty$ requires larger systems than *pointwise* approach
- can be generated by expansions in smooth functions, without the *precise* knowledge of spectrum and weights

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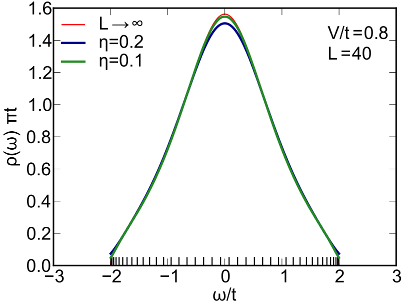

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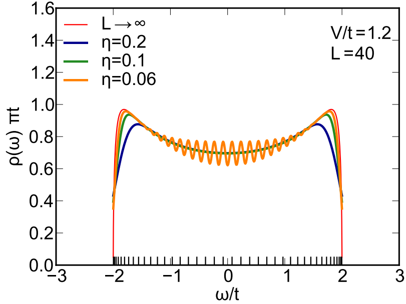

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Chebyshev expansion of spectral function

Weiße, Wellein, Alvermann & Fehske, RMP (2006)/Holzner, Weichselbaum, McCulloch, Schollwöck & von Delft, PRB (2011)

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

Recursive
$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$
$$T_0(x) = 1 \qquad T_1(x) = x$$

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

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Expand $\delta(x - H)$ in Chebyshev polynomials $\delta_N(\omega) = \sum_{n=1}^{N} \frac{T_n(\omega)}{\sqrt{1-\omega^2}} T_n(H)$

$$\rho_N(\omega) = \langle t_0 | \delta_N(\omega - H) | t_0 \rangle, \quad |t_0\rangle = a^\dagger |E_0\rangle$$

Evaluate $T_n(H)|t_0\rangle$ recursively / "Probe" spectrum of H in vicinity of $|E_0\rangle$

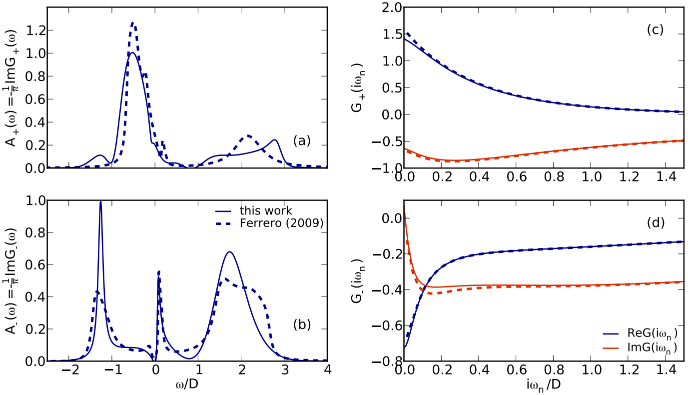
$|t_n\rangle = 2H|t_{n-1}\rangle - |t_{n-2}\rangle$ iterative MPS compression

$|t_1\rangle = H|t_0\rangle$ $|E_0\rangle$ by standard DMRG calculation

Two-site cluster DCA

Wolf, McCulloch, Parcollet & Schollwöck, PRB (2014a) / CTQMC by Ferrero, Cornaglia, De Leo, Parcollet, Kotliar & Georges, PRB (2009)

Model: Hole-doped Hubbard model on 2 dimensional square lattice



During Chebyshev recursion, as well as during time evolution, entanglement is generated and limits the accessible "time" (number of Chebyshev vectors).

What is the fundmental problem?

Wolf, McCulloch, Parcollet & Schollwöck, PRB (2014a) / Wolf, McCulloch & Schollwöck, ArXiv (2014b)

Must represent hybridization function $\Lambda(t, t')$ of impurity problem with veritable quantum degrees of freedom / cannot be analytically evaluated as in CTQMC!

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Must represent hybridization function $\Lambda(t,t')$ of impurity problem with veritable quantum degrees of freedom / cannot be analytically evaluated as in CTQMC!

▷ Choose the least-entangled representation for these quantum degrees of freedom

$$H^{\text{star}} = H_{\text{imp}} + H_{\text{bath}} + H_{\text{hyb}},$$

$$H_{\text{bath}} = \sum_{l=1}^{L_b} \sum_{\sigma} \epsilon_l c^\dagger_{l\sigma} c_{l\sigma},$$

$$H_{\text{hyb}} = \sum_{l=1}^{L_b} \sum_{\sigma} \left(V_l c^\dagger_{0\sigma} c_{l\sigma} + \text{H.c.} \right),$$

$$H^{\text{chain}} = H_{\text{imp}} + H_{\text{pot}} + H_{\text{kin}},$$

$$H_{\text{pot}} = \sum_{l=1}^{L_b} \sum_{\sigma} \widetilde{\epsilon}_l c^\dagger_{l\sigma} c_{l\sigma},$$

$$H_{\text{kin}} = \sum_{l=0}^{L_b-1} \sum_{\sigma} \left(\widetilde{V}_l c^\dagger_{l+1,\sigma} c_{l\sigma} + \text{H.c.} \right).$$

$$\Lambda^{\text{star}}(\omega) = \sum_{l=1}^{L_b} \frac{|V_l|^2}{\omega - \epsilon_l}$$

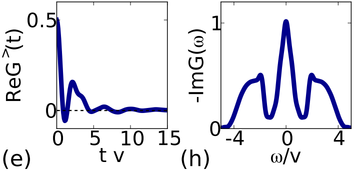
$$\Lambda^{\text{chain}}(\omega) = \cfrac{|\widetilde{V}_0|^2}{\omega - \widetilde{\varepsilon}_1 - \cfrac{|\widetilde{V}_1|^2}{\omega - \widetilde{\varepsilon}_2 - \cfrac{\cdots}{\omega - \widetilde{\varepsilon}_{L_b-1} - \cfrac{|\widetilde{V}_{L_b-1}|^2}{\omega - \widetilde{\varepsilon}_{L_b}}}}},$$

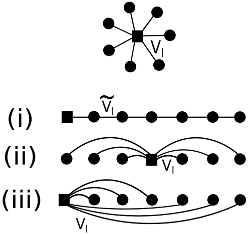
Different entanglement in star and chain geometry

Wolf, McCulloch & Schollwöck, ArXiv (2014b)

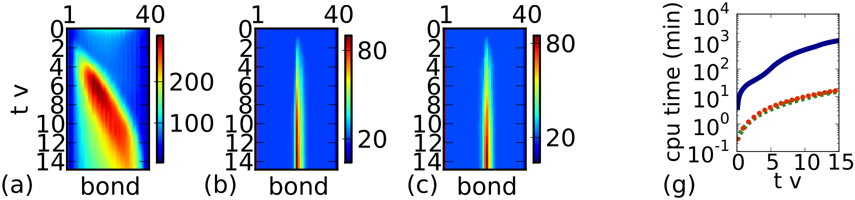
Model: DMFT for single-band Hubbard model on Bethe lattice

- ▷ Compute Green function





▷ Very different matrix dimension growth in different geometries



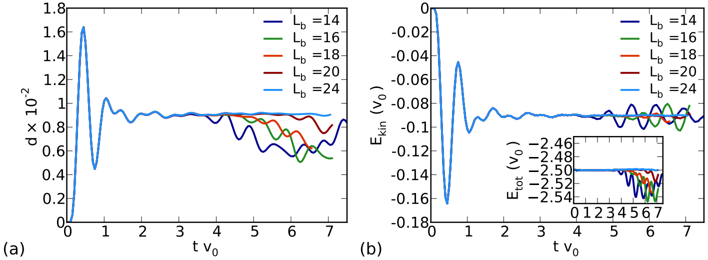
Non-equilibrium DMFT

Wolf, McCulloch & Schollwöck, ArXiv (2014b)

Model: single-band Hubbard model on Bethe lattice
▷ quench from atomic limit $v = 0$ to $v = v_0$

Nonequilibrium Hamiltonian representation by Gramsch, Balzer, Eckstein & Kollar, PRB (2013)

Up to now: exact diagonalization ▷ $t_{\text{max}} \sim 3/v_0$ for $U/v_0 = 10$
Using MPS: $t_{\text{max}} \sim 7/v_0$ for $U/v_0 = 10$



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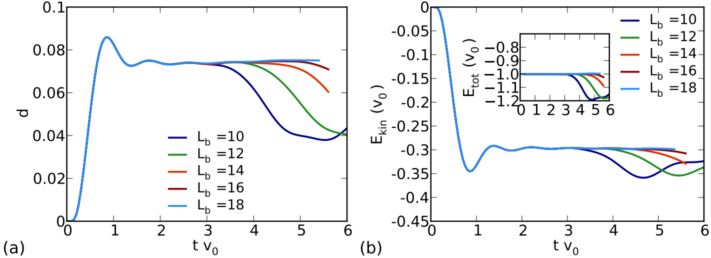
Up to now: exact diagonalization ▷ $t_{\text{max}} \sim 3/v_0$ for $U/v_0 = 4$

Using MPS: $t_{\text{max}} \sim 5.5/v_0$ for $U/v_0 = 4$



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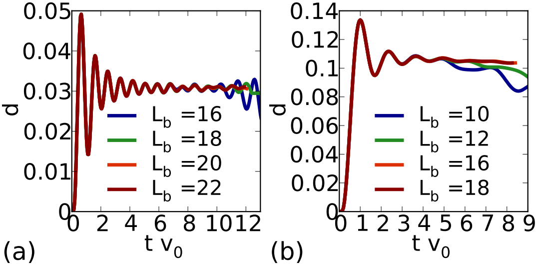
Nonequilibrium Hamiltonian representation by Gramsch, Balzer, Eckstein & Kollar, PRB (2013)

With known hybridization function (no self-consistency) Balzer, Li, Vendrell & Eckstein, ArXiv (2014)



Summary and Outlook

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- DMFT with DMRG + CheMPS much more efficient than previous MPS methods
- Entanglement depends strongly on representation of impurity model ▷ star geometry favorable
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- in equilibrium: apply these results to three-band models ▷ conductivities
- in nonequilibrium: treat quenches with correlated initial states

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Thanks for your attention!

Balzer, K., Z. Li, O. Vendrell & M. Eckstein, 2014, ArXiv , 1407.6578.

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, ArXiv , 1405.67281405.6728.

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.

Holzner, A., A. Weichselbaum, I. P. McCulloch, U. Schollwöck & J. von Delft, 2011, Phys. Rev. B **83**, 195115.

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, ArXiv 1308.5467.

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

Schollwöck, U., 2011, Annals of Physics **326**, 96.

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

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, ArXiv , 1410.3342.