MPS-based quantum impurity solvers

DMFT + DMRG

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Chan Group, Princeton University, May 13 2015

Overview: quantum embedding techniques

DMFT, CDMFT, DCA

- CTQMC Gull, Millis, Lichtenstein, Rubtsov, Troyer & Werner, RMP 83, 349 (2011)
- NRG Bulla, Costi & Pruschke, RMP 80, 395 (2008)
- ED Caffarel & Krauth, PRL 72, 1545 (1994) / Granath & Strand, PRB 86, 115111 (2012) / Lu, Höppner, Gunnarsson & Haverkort, PRB 90, 085102 (2014)
- Truncated CI Zgid, Gull & Chan, PRB 86, 165128 (2012)
- DMRG García, Hallberg & Rozenberg, PRL 93, 246403 (2004)

DMET

- Knizia & Chan, PRL 109, 186404 (2012)
- dynamic formulation Booth & Chan, arXiv:1309.2320 (2013)

Overview: DMFT + DMRG

Why not successful? ▷ wrong algorithmic approaches

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- Chebyshev and Fourier expansions: cheaper and precise

  Ganahl, Thunström, Verstraete, Held & Evertz, PRB 90, 045144 (2014b)

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  FAW, McCulloch, Parcollet & Schollwöck, PRB 90, 115124 (2014a) ▷ two-site cluster!

  FAW, McCulloch & Schollwöck, PRB 90, 235131 (2014b) ▷ entanglement and non-EQ!

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  Balzer, FAW, McCulloch, Werner & Eckstein, arXiv:1504.02461 (2015)

Outline

- Overview: impurity solvers and quantum embedding
- Compute Green's / spectral functions using MPS: algorithms, cost, error control, computability
- DMFT: bath discretization, bath geometry and long range Hamiltonian
- Benchmark: two-site DCA in different setups

Compute Green's / spectral functions using MPS

FAW, McCulloch & Schollwöck, PRB 90, 235131 (2014b)

Let $|\psi_0\rangle = a^\dagger |E_0\rangle$ be a single-particle excitation:

$$A(\omega) = \langle \psi_0 | \delta\big(\omega - (H - E_0)\big) | \psi_0 \rangle$$

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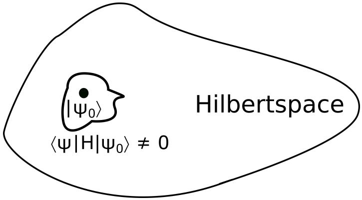
- $|\psi_0\rangle$ is lowly entangled.
- Need to compute neighborhood of $|\psi_0\rangle$

$$\{\ |\psi\rangle\ |\ \langle\psi|H|\psi_0\rangle \neq 0\ \}$$



- **Hope** that there is a basis for this neighborhood that is not too strongly entangled!
- How to construct this basis?

Compute Green's / spectral functions using MPS

- DDMRG: solve $$G_\eta(\omega) = \langle\psi_0| \underbrace{\frac{1}{\omega + i\eta - (H - E_0)}|\psi_0\rangle}_{= |\mathsf{cv}_\eta(\omega)\rangle}$$

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- Lanczos: represent H in orthog. Krylov basis $[1, H, H^2, \ldots]|\psi_0\rangle$

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

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- Chebyshev expansion: $A(\omega) \sim \sum_n \langle\psi_0|\psi_n\rangle \cos(n \arccos(\omega))$

$$|\psi_n\rangle = \cos(n \arccos H')|\psi_0\rangle$$

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

MPS: Holzner, Weichselbaum, McCulloch, Schollwöck & von Delft, PRB 83, 195115 (2011)

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- Fourier expansion: $A(\omega) \sim \sum_n \langle\psi_0|\psi_n\rangle e^{i\omega t_n}$

$$|\psi_n\rangle = e^{-i(H-E_0)t_n}|\psi_0\rangle$$

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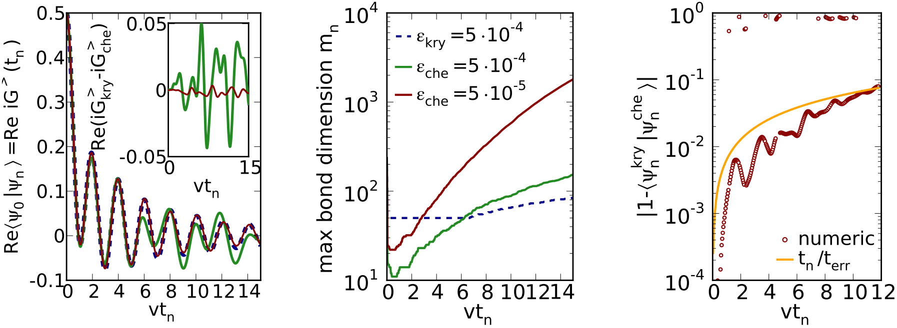

Evaluate expansions of Green's functions / Computability

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- Truncate expansion after n_{max} time steps

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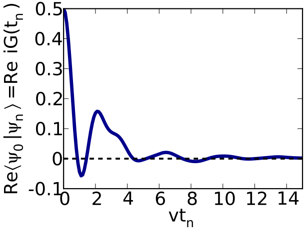

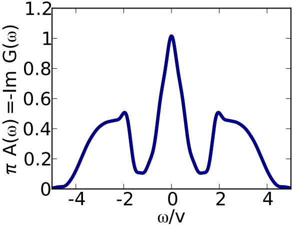

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Can we reach high enough values of n_{max}?

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Can we reach high enough values of n_{max}?

Convergence $\langle\psi_0|\psi_n\rangle \to 0$ depends on degree of differentiability of $A(\omega)$

- smooth ▹ exponential convergence
- step function ▹ $\frac{1}{t_n}$ convergence
- singular ▹ no convergence

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What does this mean in practice?

- Real axis $A(\omega)$ ▷ *van Hove kinks* smoothed out for fermionic interacting systems → fast convergence except at criticality

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- Imag axis $G(i\omega)$ ▷ metallic phase $\to$ algebraic convergence / insulating phase $\to$ exponential

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Can we reach high enough values of n_{max}?

Real axis $A(\omega)$

$$|\psi_n\rangle = e^{-i(H-E_0)t_n}|\psi_0\rangle$$

- entanglement explodes, but convergence is often reached earlier

Imag axis $G(i\omega)$

$$|\psi_n\rangle = e^{-(H-E_0)\tau_n}|\psi_0\rangle$$

- no entanglement generated, can compute arbitrarily long times
- metallic phase: very long times have to be computed
- insulating phase: only extremely short times need to be computed

Evaluate expansions of Green's functions / Computability

What if entanglement explodes before convergence?

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Windowing / broadening approach: enforce convergence

$$A_\eta(\omega) \sim \sum_n \langle \psi_0 | \psi_n \rangle e^{i\omega t_n} e^{-(\eta\, t_n)^2/2}$$

- broadened version $A_\eta(\omega)$ of $A(\omega)$ conserves sum rules
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Linear prediction (extrapolation) White & Affleck, PRB 77, 134437 (2008)

- analytically continue to convergence FAW et al., PRB 91, 115144 (2015)
- enhance resolution
- requires exponential convergence

Outline

- Overview: impurity solvers and quantum embedding
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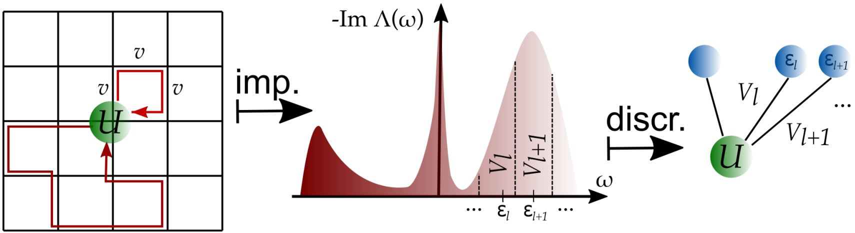
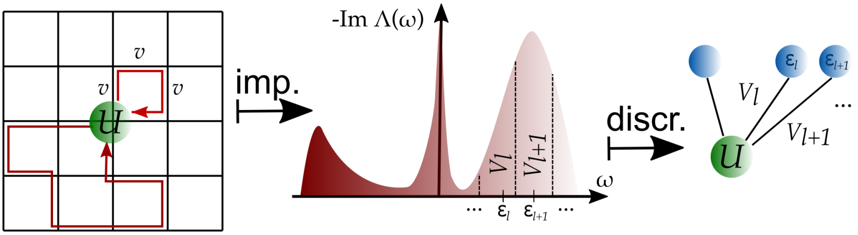
- DMFT: bath discretization, bath geometry and long range Hamiltonian
- Benchmark: two-site DCA in different setups

DMFT: optimal bath discretization



DMFT: optimal bath discretization



Imag axis

- minimize $\sum_{\omega_n} \left| \Lambda_{\mu\nu}(i\omega_n) - \sum_l \frac{V_{\mu l} V^*_{\nu l}}{i\omega_n - \varepsilon_l} \right|^2$ Caffarel & Krauth, PRL 72, 1545 (1994)
- unstable for many bath sites and/or off-diagonal couplings?

  Liebsch & Ishida, J. Phys.: Condens. Matter 24, 053201 (2012) Go & Millis, PRL 114, 016402 (2015)
- extremely fast convergence: 8 bath sites suffice for perfect fit!

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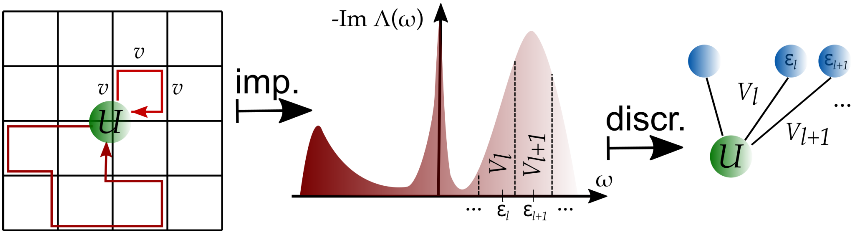


Real axis

- discretization strategy Bulla, Costi & Pruschke, RMP 80, 395 (2008)

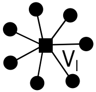
$$|V_{\mu l}|^2 = \int_{\omega_l}^{\omega_{l+1}} d\omega \, (-\mathrm{Im}\Lambda_{\mu\mu}(\omega)), \;\; \varepsilon_l = \frac{1}{|V_{\mu l}|^2} \int_{\omega_l}^{\omega_{l+1}} d\omega \, \omega(-\mathrm{Im}\Lambda_{\mu\mu}(\omega))$$

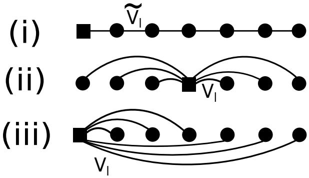
- orthogonal polynomial strategy e.g. Shenvi, Schmidt, Edwards & Tully, PRA 78, 022502 (2008)
- no notion of optimality! no off-diagonal $\Lambda_{ij}(\omega)$ de Vega & FAW (in progress)
- much slower convergence: many bath sites needed!

DMFT: geometry of bath

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

star or chain?





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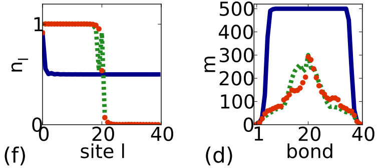
ground state

- star: local, lowly entangled
- chain: delocalized, highly entangled



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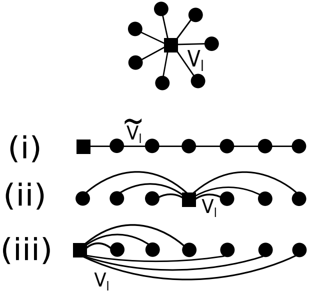

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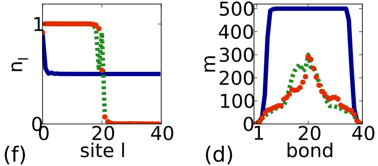

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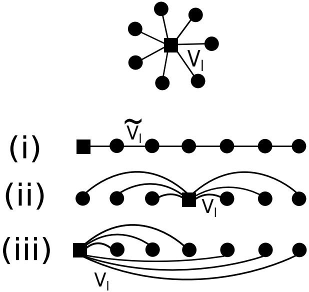
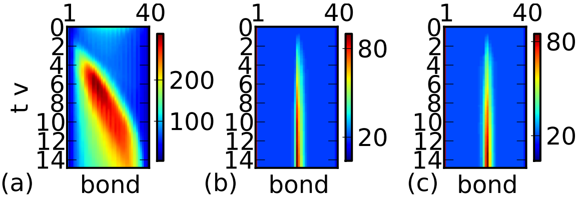


time evolution



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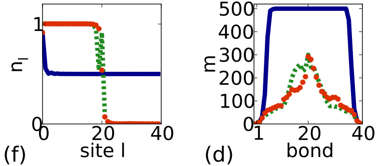

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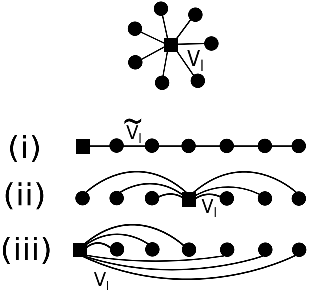

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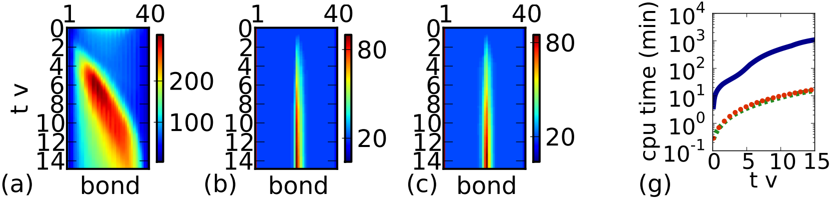
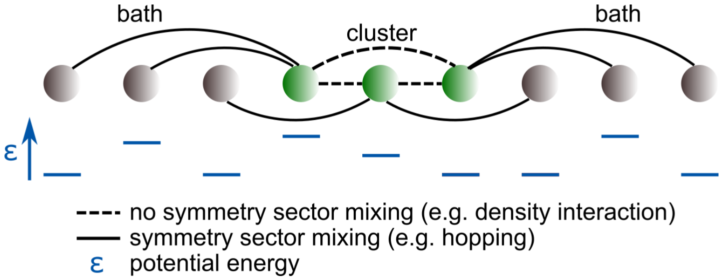


DMFT: beast of an Hamiltonian



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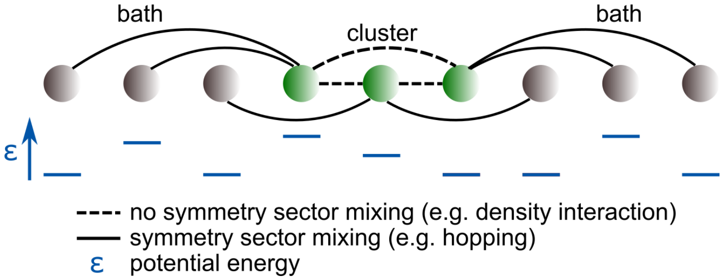

How to optimize the ground state?

- use perturbation techniques

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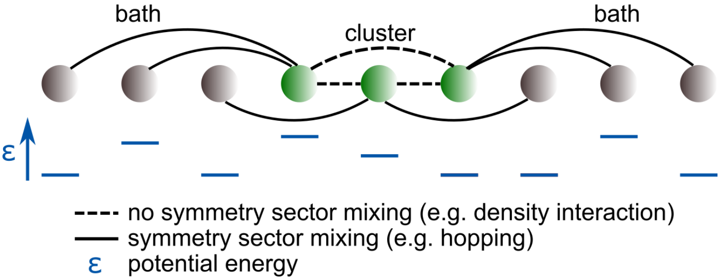

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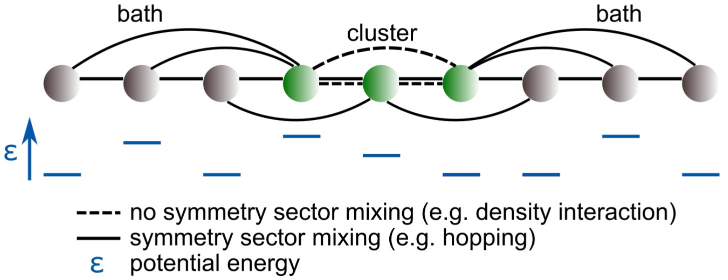

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- use additional hoppings / annealing

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Benchmark: two-site cluster DCA in K-space repres.

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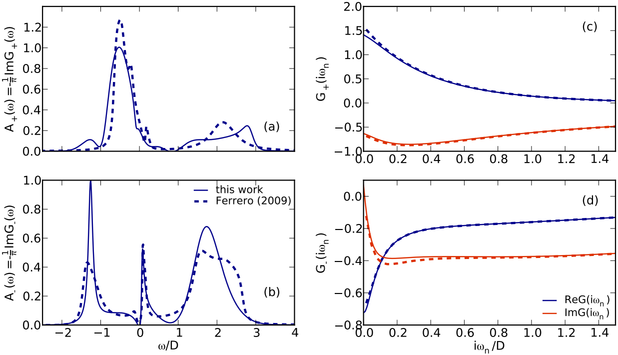
CTQMC by Ferrero, Cornaglia, De Leo, Parcollet, Kotliar & Georges, PRB 80, 064501 (2009)

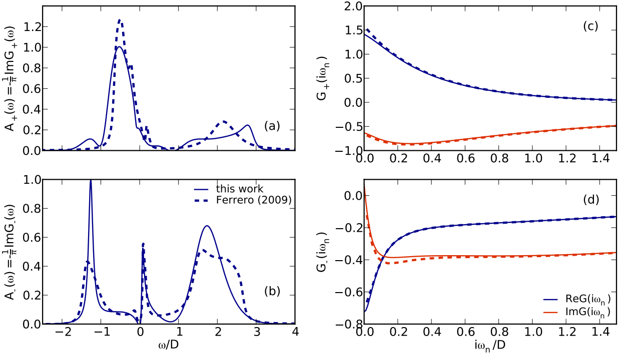
- model: hole-doped (4%) Hubbard model on 2 dim. square lattice
- spectral function: adaptive Chebyshev expansions, linear prediction
- bath discretization: linear discretization, $L_b/L_c = 30 - 40$
- geometry: chain
- cpu time: $\sim$ 60 min ground state, 300 min spectral function



Benchmark: two-site cluster DCA in K-space repres.

FAW, McCulloch, Parcollet & Schollwöck, PRB 90, 115124 (2014a)
CTQMC by Ferrero, Cornaglia, De Leo, Parcollet, Kotliar & Georges, PRB 80, 064501 (2009)

- model: hole-doped (4%) Hubbard model on 2 dim. square lattice
- spectral function: time evolution
- bath discretization: linear discretization, $L_b/L_c = 30 - 40$
- geometry: star
- cpu time: $\sim$ 60 min ground state, 40 min spectral function

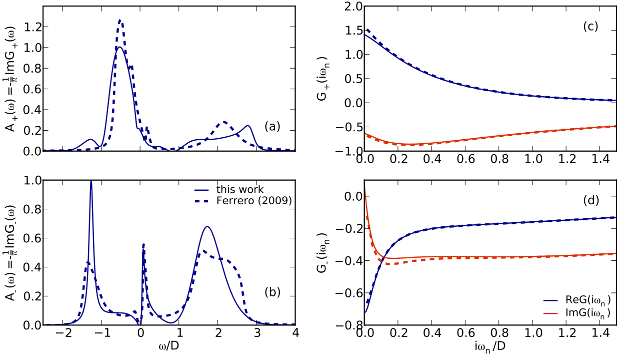


Benchmark: two-site cluster DCA in K-space repres.

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

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

- model: hole-doped (4%) Hubbard model on 2 dim. square lattice
- Matsubara Green's function: imag time evolution
- bath discretization: fitting, $L_b/L_c = 8$
- geometry: star
- cpu time: $\sim$ 15 min ground state, 15 min/60 min Green's function



Thanks to collaborators

- U. Schollwöck (LMU Munich)
- M. Eckstein (Max Planck and U. Hamburg)
- A. Go (Columbia U.)
- A. Millis (Columbia U.)
- O. Parcollet (CEA Saclay)
- I.P. McCulloch (U. Queensland)
- C. Hubig (LMU Munich)

Summary and Outlook

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- star geometry much less entangled than chain geometry
- real axis: small clusters exactly
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Thank you!

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