The DMRG method and applications

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Outline

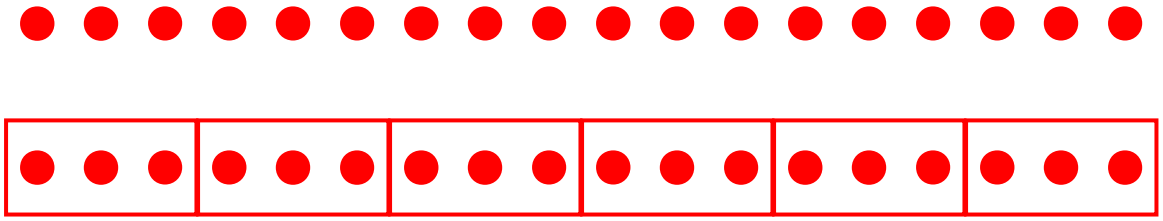
- Basic facts
- The Density Matrix projection
- The DMRG Method
- Example: Heisenberg model
- Quantum information interpretation
- Applications and extensions
- Dynamical DMRG: Lanczos method

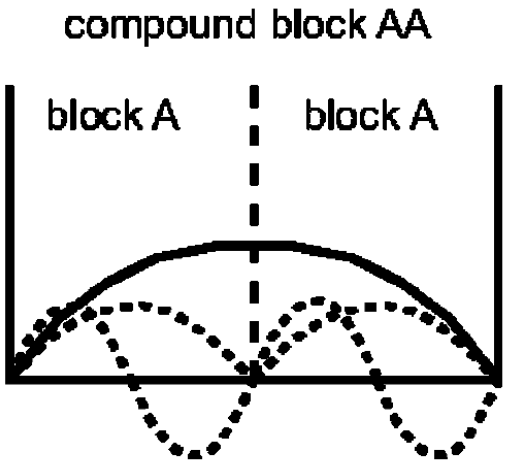
  Correction vector method
- Application to the Dynamical Mean Field Theory (DMFT)

Example: Heisenberg model

$H = J \sum_i \mathbf{S}_i \mathbf{S}_{i+1}$

N sites, 2^N states





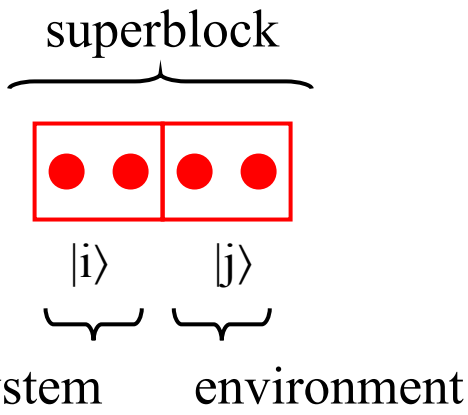
Tight-binding model

By keeping the lowest-lying energy states, poor results

White and Noack (92): several boundary conditions $\Longrightarrow$ improvement

How to get a more systematic way of reducing the Hilbert space?
Using the density matrix:

N=4 sites



$$|\psi_0\rangle = \sum_{i,j=1}^{M} \psi_{ij}|i\rangle|j\rangle$$

Full density matrix: $\rho = |\psi_0\rangle\langle\psi_0|$

Reduced density matrix: $\rho_{ii'} = \sum_j \rho_{ij,i'j} = \sum_j \langle j|\langle i|\psi_0\rangle\langle\psi_0|i'\rangle|j\rangle = \sum_j \psi_{ij}\psi_{i'j}$

Tr(ρ)=1

The Density Matrix projection ⟶ optimal states in the system

$$|\psi_0\rangle = \sum_{i,j=1}^{M} \psi_{ij}|i\rangle|j\rangle$$ a state of the superblock

Wanted: variational wave function in optimal basis: $|\alpha\rangle = \sum_{i=1}^{m} u_{\alpha i}|i\rangle$

$$|\hat{\psi}_0\rangle = \sum_{\alpha=1}^{m}\sum_{j=1}^{M} a_{\alpha j}|\alpha\rangle|j\rangle$$ m≤M

such that

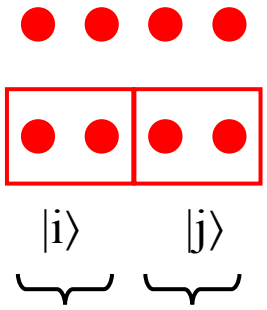
$$||\psi_0\rangle - |\hat{\psi}_0\rangle|^2 = 1 - 2\sum_{\alpha ij} \psi_{ij}a_{\alpha j}u_{\alpha i} + \sum_{\alpha j} a_{\alpha j}^2$$ is minimal w.r.t. $\boldsymbol{a_{\alpha j}}$

$$\Longrightarrow \quad \sum_i \psi_{ij}u_{\alpha i} = a_{\alpha j}$$

Reduced density matrix of the system: $\rho_{ii'} = \sum_j \rho_{ij,i'j} = \sum_j \langle j|\langle i|\psi_0\rangle\langle\psi_0|i'\rangle|j\rangle = \sum_j \psi_{ij}\psi_{i'j}$

we obtain: $1 - \sum_{\alpha ii'} u_{\alpha i}\rho_{ii'}u_{\alpha i'} = 1 - \sum_{\alpha=1}^{m}\omega_\alpha$ $\qquad \rho_{ii'} = \sum_l p_l \sum_j \psi_{l,ij}\psi_{l,i'j}$

DMRG: Density Matrix Renormalization Group (S. White 1992)

1) 

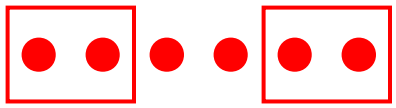
$H \rightarrow |\psi\rangle$

$$|\psi\rangle = \sum_{ij=1}^{M} \psi_{ij} |i\rangle|j\rangle$$

2) Define the system´s reduced DM: $\rho = \mathrm{Tr}_j |\psi\rangle\langle\psi|$ $\qquad \rho_{ii'} = \sum_j \psi_{ij}^* \psi_{i'j}$

3) Diagonalize $\rho = \begin{pmatrix} \ddots & & \\ & \omega_\alpha & \\ & & \ddots \end{pmatrix}_{MxM}$ where $\sum_{\alpha=1}^{M} \omega_\alpha = 1$

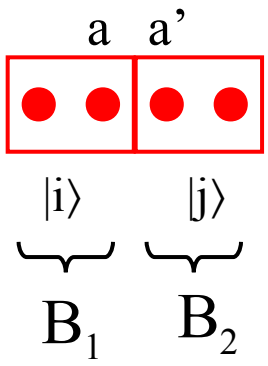
4) Keep only *m* largest-eigenvalue states⇒ truncation error $\propto 1 - \sum_{\alpha=1}^{m} \omega_\alpha$

5) Rotate and Enlarge: 

6) Go to 1

Example: Heisenberg model

$$H = \sum_i \mathbf{S}_i \mathbf{S}_{i+1} = S_i^z S_{i+1}^z + \frac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)$$



$$[H_{B_1 B_2}]_{ij;\, i'j'} = [H_{B_1}]_{ii'}\delta_{jj'} + [H_{B_2}]_{jj'}\delta_{ii'} + [S_a^z]_{ii'}[S_{a'}^z]_{jj'}$$

$$+ \frac{1}{2}[S_a^+]_{ii'}[S_{a'}^-]_{jj'} + \frac{1}{2}[S_a^-]_{ii'}[S_{a'}^+]_{jj'}$$

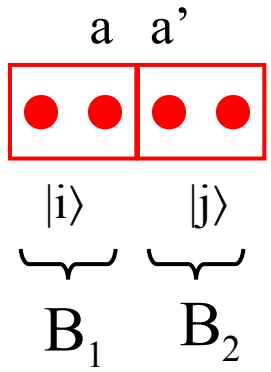
↑ …… 1
↓ …… 0

Basis in B_1 {00, 10, 01, 11}

B_2

$$H = S_i^z S_{i+1}^z + \frac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)$$

$$H_{B1} = \quad H_{B2} = \begin{pmatrix} 1/4 & & & \\ & -1/4 & 1/2 & \\ & 1/2 & -1/4 & \\ & & & 1/4 \end{pmatrix}$$



$$S_{a\ B1}^{z} = \begin{pmatrix} -1/2 & & & \\ & -1/2 & & \\ & & 1/2 & \\ & & & 1/2 \end{pmatrix} \qquad S_{a\ B2}^{z} = \begin{pmatrix} -1/2 & & & \\ & 1/2 & & \\ & & -1/2 & \\ & & & 1/2 \end{pmatrix}$$

$$S_{a\ B1}^{+} = \begin{pmatrix} 0 & & & \\ & 0 & & \\ 1 & & 0 & \\ & 1 & & 0 \end{pmatrix} \qquad S_a^- = (S_a^+)^\dagger$$

$$S_{a',\ B2}^{z} = \begin{pmatrix} -1/2 & & & \\ & 1/2 & & \\ & & -1/2 & \\ & & & 1/2 \end{pmatrix} \qquad \ldots \text{ etc}$$

$$H_{B1} \times \delta_{B2} = \begin{pmatrix} 1/4 & & & \\ & -1/4 & 1/2 & \\ & 1/2 & -1/4 & \\ & & & 1/4 \end{pmatrix} \times \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} 1/4 & & \\ & -1/4 & 1/2 \\ & 1/2 & -1/4 \end{pmatrix} & & & \\ & \begin{pmatrix} 1/4 & & \\ & -1/4 & 1/2 \\ & 1/2 & -1/4 \end{pmatrix} & & \\ & & \begin{pmatrix} 1/4 & & \\ & -1/4 & 1/2 \\ & 1/2 & -1/4 \end{pmatrix} & \\ & & & \begin{pmatrix} 1/4 & & \\ & -1/4 & 1/2 \\ & 1/2 & -1/4 \end{pmatrix} \end{pmatrix}$$

Same for $\delta_{B1} \times H_{B2}$

Basis for $B_1 x B_2$: {0000, 1000, 0100, 1100,
0010, 1010, 0110, 1110,
0001, 1001, 0101, 1101,
0011, 1011, 0111, 1111}

$$S^{+}_{a\,B1} \times S^{-}_{a',\,B2} = \begin{pmatrix} 0 & & & \\ & 0 & & \\ 1 & & 0 & \\ & 1 & & 0 \end{pmatrix} \times \begin{pmatrix} & 1 & & \\ 0 & & 0 & \\ & & & 0 \\ & & & & 0 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} 0 & & \\ & 0 & \\ & & 0 \end{pmatrix} & \begin{pmatrix} 0 & & \\ & 0 & \\ 1 & & 0 \end{pmatrix} & & \\ & \begin{pmatrix} 0 & & \\ & 0 & \\ & & 0 \end{pmatrix} & \begin{pmatrix} 0 & & \\ & 0 & \\ 1 & & 0 \end{pmatrix} & \\ & & \begin{pmatrix} 0 & & \\ & 0 & \\ & & 0 \end{pmatrix} & \\ & & & \begin{pmatrix} 0 & & \\ & 0 & \\ & & 0 \end{pmatrix} \end{pmatrix}$$

$$[H_{B_1B_2}]_{ij;\,i'j'} = [H_{B_1}]_{ii'}\delta_{jj'} + [H_{B_2}]_{jj'}\delta_{ii'} + [S^z_a]_{ii'}[S^z_{a'}]_{jj'}$$

$$+ \frac{1}{2}[S^+_a]_{ii'}[S^-_{a'}]_{jj'} + \frac{1}{2}[S^-_a]_{ii'}[S^+_{a'}]_{jj'}$$

$H \rightarrow |\psi\rangle$ using Lanczos, Davidson or exact diagonalization

$$|\psi\rangle = \sum_{ij=1}^{M} \psi_{ij}|i\rangle|j\rangle$$

Remember:

Basis in B_1 {00, 10, 01, 11}≡ {i=1, 2, 3, 4}

B_2 {00, 10, 01, 11}≡ {j=1, 2, 3, 4}

Basis for $B_1 x B_2$: {0000, 1000, 0100, 1100,
0010, 1010, 0110, 1110,
0001, 1001, 0101, 1101,
0011, 1011, 0111, 1111}≡
{ij=11, 21, 31, 41,
12, 22, 32, 42,
13, 23, 33, 43,
14, 24, 34, 44}

So from here we can get the ψ_{ij} and form the reduced density matrix:

$$\rho_{ii'} = \sum_{j} \psi_{ij}{}^{*} \psi_{i'j}$$

Following the DMRG general iteration:

3) Diagonalize $\rho=\begin{pmatrix} \ddots & & \\ & \omega_\alpha & \\ & & \ddots \end{pmatrix}_{MxM}$ where $\sum_{\alpha=1}^{M} \omega_\alpha = 1$

4) Keep only *m* largest-eigenvalue states⇒ truncation error $\propto 1-\sum_{\alpha=1}^{m} \omega_\alpha$

Define rotation and reduction matrix O_{mxM} with new basis set.

5) RRR: Rotate, Reduce and Rename operators in block B1:

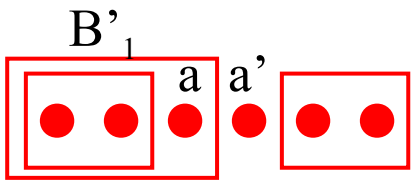
$H_{B1rot}=O^{\dagger}H_{B1}O$

$$\begin{pmatrix} O \\ 4x2 \end{pmatrix}$$

$$\begin{pmatrix} H_{B1} \\ 4x4 \end{pmatrix}\begin{pmatrix} \\ \end{pmatrix}$$

$$\begin{pmatrix} O^{\dagger} \\ 2x4 \end{pmatrix}\begin{pmatrix} H_{B1rot} \\ 2x2 \end{pmatrix}$$

6) Enlarge the system:



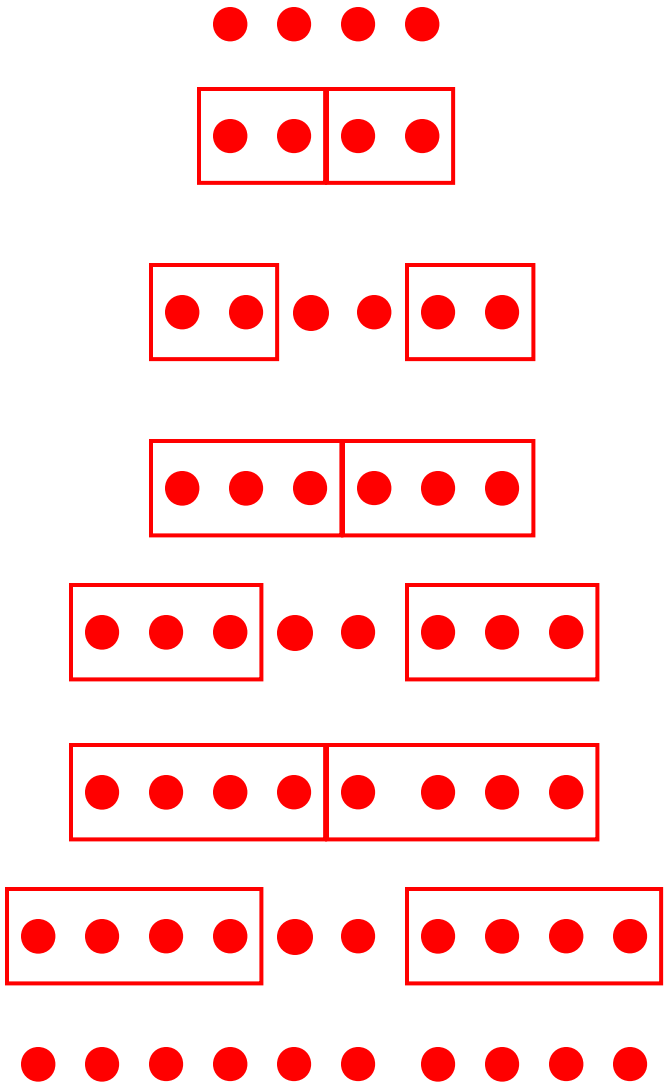
Define operators in the new enlarged B'_1 as: $H_{B'1}=H_{B1rot}x\delta_a + S.S_a\ldots$

And link operators: $S^z_{B'1}=\delta_{B'1}xS^z_a$ and same for $S^+_{B'1}$ and $S^-_{B'1}$

7) Start all over again

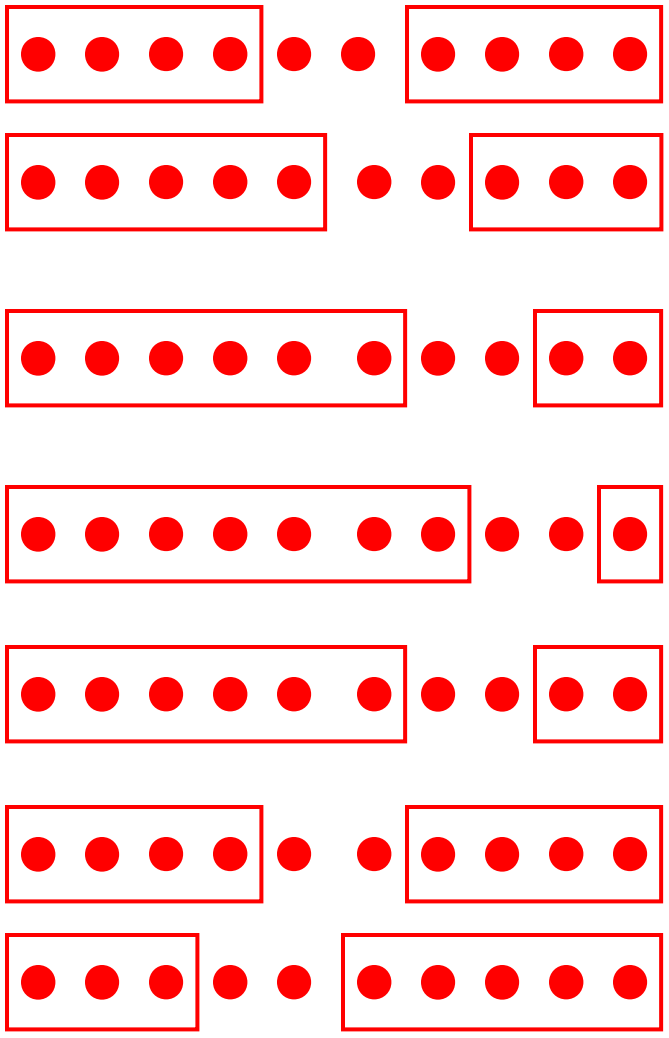
Schemes:

Infinite-system

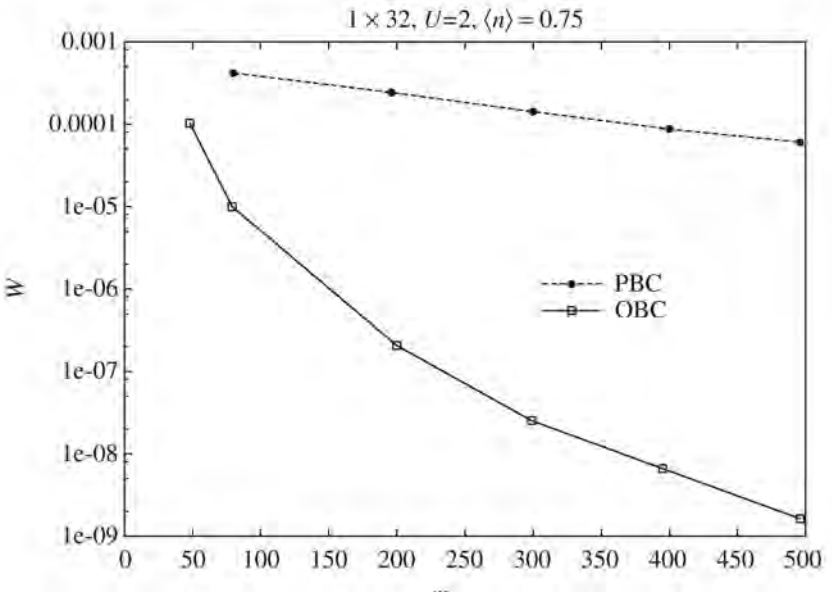


Finite-system

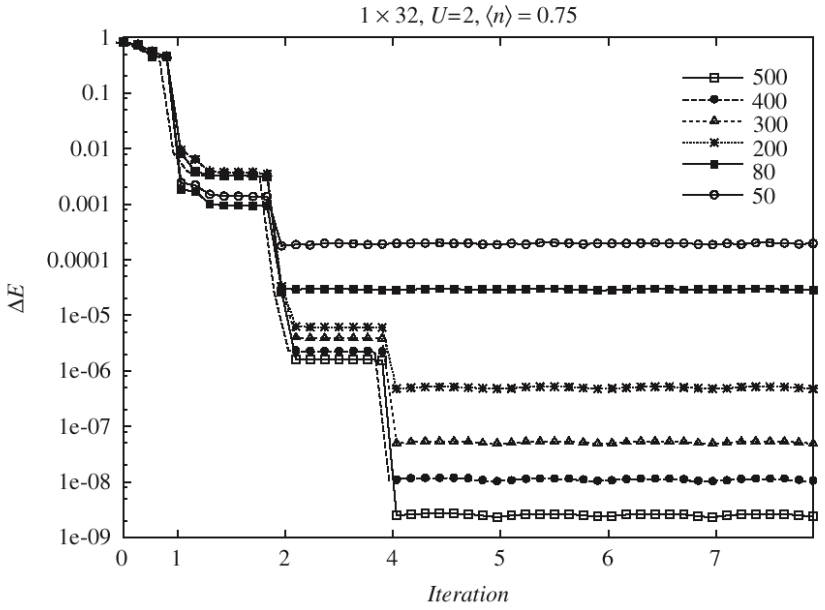
sweeps



Boundary conditions:

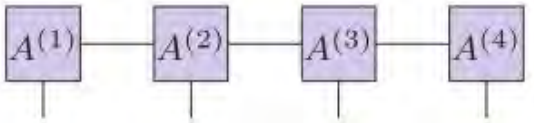


Finite-size sweeps:

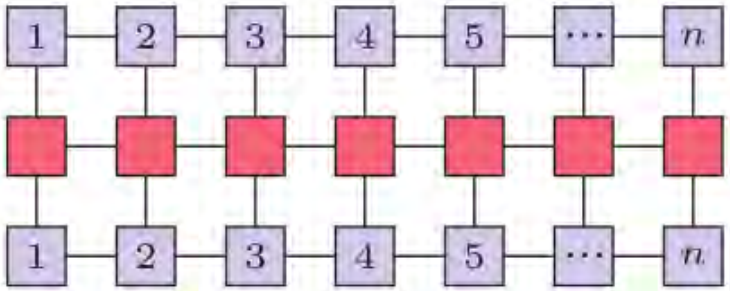


MPS

$$|\Gamma\rangle := \arg\min_{|\psi\rangle \in \mathcal{D}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

$|\psi\rangle =$ 

arg min 



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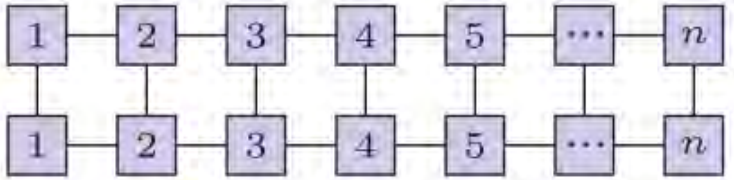
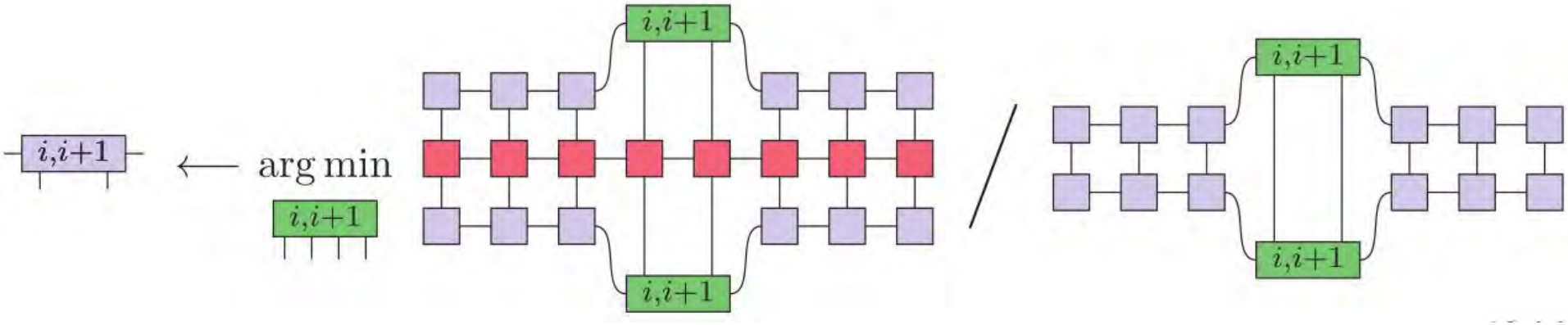


Highly nonlinear problem.
Looking for a self-consistent solution,
Solving one tensor at a time → DMRG1

DMRG2 = traditional DMRG



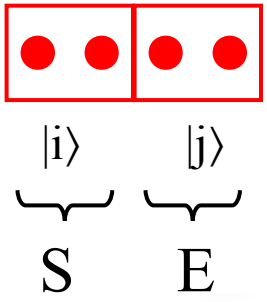
Equivalent to density-matrix-based compression

Quantum information interpretation: An interesting new perspective on Quantum Mechanics

"The most challenging and interesting problems in quantum dynamics involve understanding the behaviour of strongly-coupled many-body systems… Better ways of characterizing the features of many particle entanglement may lead to new and more effective methods for understanding the dynamical behaviour of complex quantum systems." John Preskill (2000)

(Gaite 2001, 2003; Latorre et al. 2003, Osborn et al. 2001...)

Entanglement between System (S) and Environment (E)



Diagonalized reduced density matrix: $\rho_S = \sum_{\alpha=1}^{\min(N_S, N_E)} \omega_\alpha |\alpha^S\rangle\langle\alpha^S|$

with rank $r \leq \min(N_S, N_E) \Longrightarrow$ Schmidt decomposition for the pure wf of the superblock:

$$|\psi\rangle = \sum_{\alpha=1}^{\min(N_S, N_E)} \sqrt{\omega_\alpha} |\alpha^S\rangle |\alpha^E\rangle$$

and $|\psi\rangle$ is entangled $\Leftrightarrow r > 1$

Von Neumann entropy (T=0!): $S_S = -\mathrm{Tr}\rho_S \log_2 \rho_S = -\sum_\alpha \omega_\alpha^S \log_2 \omega_\alpha^S$

DMRG works best for small S (e.g. state-product states in AKLT, dimers, open BC…)

Remarks on quantum information aspects in DMRG:

a) Critical systems: From conformal field theories: $S \alpha N^{d-1}$

and in d=1 S=k logN+const.

d is the dimensionality

S=number of q bits corresponding to the entanglement information so
m α 2^S states to be kept.
1d $\Longrightarrow$ m ~ N^k
2d $\Longrightarrow$ m ~ 2^N

b) 1d gapped systems: S saturates for N ~ ξ (correlation length) $\Longrightarrow$ better performance of the DMRG

General remarks:

- MPS (matrix product states), like in AKLT $\mathcal{H} = \sum_{i=1}^{N} \left[(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 + \alpha (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) \right]$
  DMRG is a variational approach within MPS

- Best performance for DMRG: open BC
  gapped systems (ω_α decay exponentially)
  MPS
- ω_α decay very slowly for D=2 and the entropy S_S grows with system size

- Symmetries: Total S_z ,charge, parity (strightforward)
  SU(2) total spin, momentum, other continuous symmetries

Applications and extensions

Applications:

- 1, “2D” and ladder spin systems
- 1D and ladder electron systems
- Kondo and Anderson 1D lattice models
- 1 and 2 impurity models
- Quantum Hall systems

Extensions:

- Small particles and nuclei
- Classical systems in D+1
- Non-hermitian Hamiltonians
- Finite temperature using transfer matrix
- Phonons, bosons and disorder
- Molecules and quantum chemistry
- Momentum representation
- Time-dependent problems
- Dynamical properties
- Application to DMFT

DMRG for dynamical properties

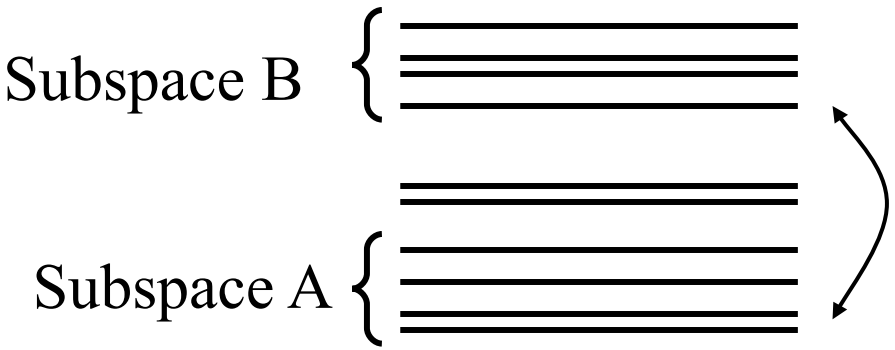
We want to calculate the following dynamical correlation function:

$$C_A(t\text{-}t') = \langle \psi_0 | A^\dagger(t) A(t') | \psi_0 \rangle$$

Fourier transforming:

$$C_A(\omega) = \sum_n |\langle \psi_n | A | \psi_0 \rangle|^2 \, \delta(\omega - (E_n - E_0))$$

$$G_A(\omega + i\,\eta) = \langle 0 | A^\dagger \frac{1}{E_0 + \omega + i\,\eta - H} A | 0 \rangle \qquad C_A(\omega) = -\frac{1}{\pi} \lim_{\eta \to 0^+} \mathcal{I}m\, G_A(\omega + i\,\eta)$$



K. H., PRB 52, 9827 (1995)

Lanczos dynamics

The Green's function:

$$G_A(\omega+i\,\eta)= \quad \langle 0|A^\dagger \frac{1}{E_0+\omega+i\,\eta-H} A|0\rangle$$

Can be written as follows:

$$G_A=\cfrac{\langle\psi_0|A^\dagger A|\psi_0\rangle}{z-a_0-\cfrac{b_1^2}{z-a_1-\cfrac{b_2^2}{z-a_2-\ldots\ldots}}}$$

where

$$\begin{cases} |f_{n+1}\rangle=H\,|f_n\rangle - a_n\,|f_n\rangle - b_n^2\,|f_{n-1}\rangle \\ |f_0\rangle= A|\psi_0\rangle \\ a_n= \langle f_n|\,H\,|f_n\rangle/\,\langle f_n|f_n\rangle \\ b_n^2= \langle f_n|f_n\rangle/\,\langle f_{n-1}|f_{n-1}\rangle; \qquad b_0=0 \end{cases}$$

$$\rho_{ii'} = \sum_l p_l \sum_j \psi_{l,ij}\psi_{l,i'j}$$

Correction vector dynamics

Target a particular energy $z=\omega+i\eta$

So that the Green's function is a product of two vectors:

$$G_A(z)= \langle 0|A^\dagger \frac{1}{z\text{-}H} A|0\rangle = \langle A|x(z)\rangle$$

where $$|x(z)\rangle= \frac{1}{z\text{-}H} A|0\rangle$$

Use as target states: $|0\rangle$

$A|0\rangle$

$$|x(z)\rangle= \frac{1}{z\text{-}H} A|0\rangle$$

Correction vector dynamics

$$|x(z)\rangle = \frac{1}{z-H} A|0\rangle \qquad z=\omega+i\eta$$

The correction vector $|x(z)\rangle$ is complex: $|x(z)\rangle = |x^r(z)\rangle + i|x^i(z)\rangle$

Multiplying and dividing by $(\omega - i\eta - H)$ we obtain:

$$((H-\omega)^2+\eta^2)\,|x^i(z)\rangle = -\eta A|0\rangle$$

and $\quad \eta|x^r(z)\rangle = (H-\omega)|x^i(z)\rangle$

A variational method to obtain $|x(z)\rangle$:

$$W_{A,\eta}(\omega, X) = \langle X|(H-w)^2 + \eta^2|X\rangle + \eta\langle\psi_0|A|X\rangle + \eta\langle X|A|\psi_0\rangle$$

$|X_{min}\rangle = |x^i(z)\rangle$ and $W_{A,\eta}(\omega, X_{min}) = -\pi\eta C_A(\omega+i\eta)$

(Ramasesha et al., 1989 & succ.; Kühner and White, 1999; Jeckelmann, 2002)

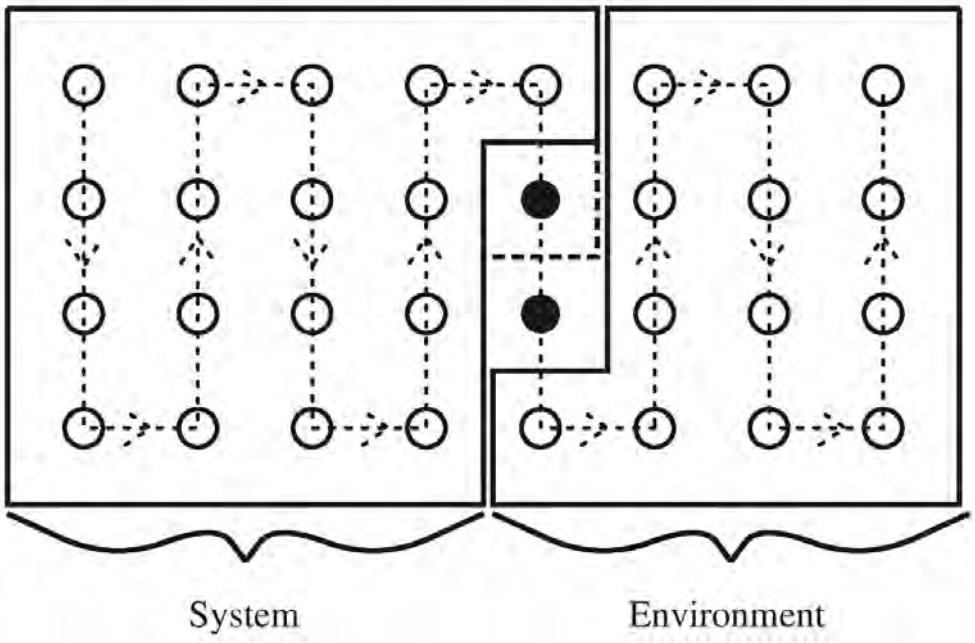
DMRG in two dimensions:

In 2D, ω_α decay slower $\Longrightarrow$more states to be kept (larger $\boldsymbol{m}$)

However;

- Larger systems than ED can be achieved: e.g. 4x20 t-J model
  9x9 and 10x7 t-J lattices

  24x11 Heisenberg lattice…
- Results for low T are more precise than with Monte Carlo



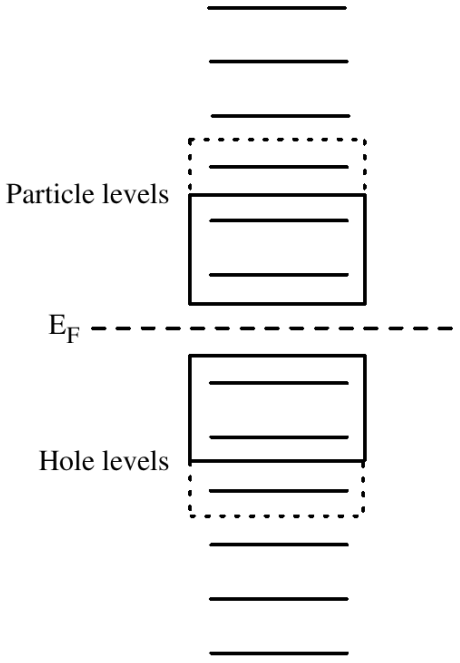
Momentum representation: (Xiang '96)

- Hamiltonian written in momentum space. Good for long-ranged models in real space
- Example: Hubbard model: a) real space $H = -t \sum_{\langle ij \rangle \sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$

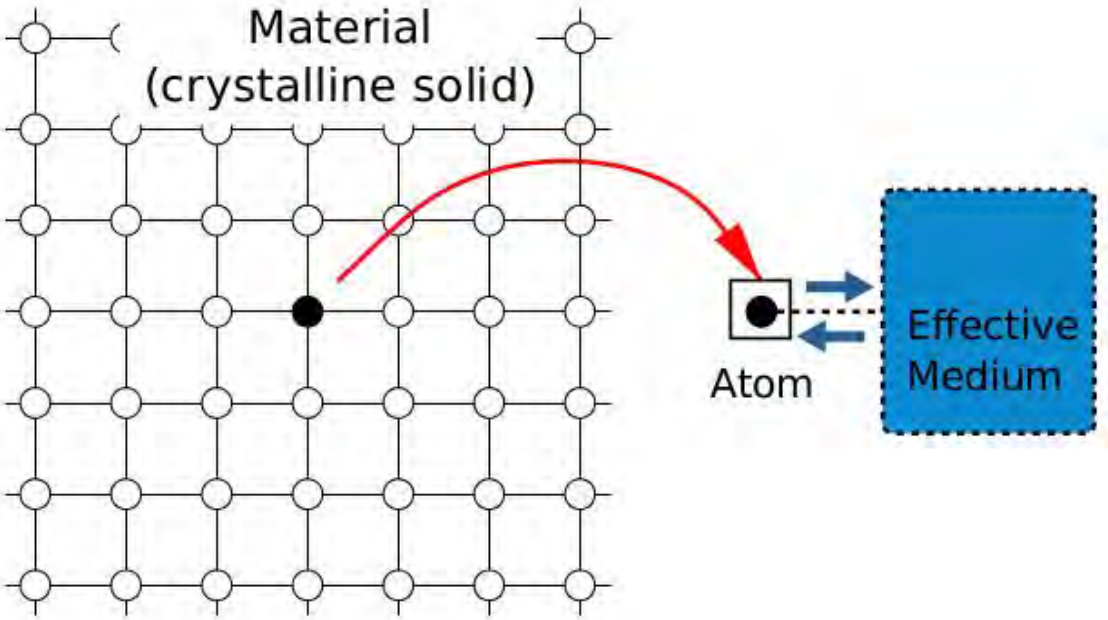
b) reciprocal space: $H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + \frac{U}{N} \sum_{\mathbf{p},\mathbf{k},\mathbf{q}} c^{\dagger}_{\mathbf{p}-\mathbf{q}\uparrow} c^{\dagger}_{\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\downarrow} c_{\mathbf{p}\uparrow}$

<u>Grains and nuclei:</u> (Dukelsky & Sierra '99)

general Hamiltonian: $H = \sum_{ij} T_{ij} c^{\dagger}_{i} c_{j} + \sum_{ijkl} V_{ijkl} c^{\dagger}_{i} c^{\dagger}_{j} c_{l} c_{k}$



Dynamical Mean Field Theory (DMFT)



Infinite dimensions

⇓

Local self-energy

⇓

$$\Sigma_{ij}(\omega) \approx \Sigma(\omega)\delta_{ij}$$

Georges, A., Kotliar, G., Krauth, W., Rozenberg, M. Rev. Mod. Phys. 68 , 13125 (1996)

Example 1: One-band Hubbard model on a square lattice (single imp)

$$H = t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i} n_i$$

i) Set $\Sigma(\omega) = 0$

ii) Obtain $G(\omega) = \frac{1}{N} \sum_{k} \left[\omega - t(\mathbf{k}) - \Sigma(\omega)\right]^{-1} = G_0\left(\omega - \Sigma(\omega)\right)$

iii) Calculate the hybridization $\Gamma(\omega) = \omega + \mu - \Sigma(\omega) - \left[G(\omega)\right]^{-1}$

iv) Fit the hybridization to define a Hamiltonian $\Gamma_d(\omega) = \sum_{i} \frac{v_i^2}{\omega - \lambda_i}$

v) Calculate $G_{imp}(\omega)$ ⟵ Impurity solver, e.g. DMRG

vi) Obtain $\Sigma(\omega) = \omega + \mu - \left[G_{imp}(\omega)\right]^{-1} - \Gamma_d(\omega)$

vii) Go to ii)

DMFT: Impurity solvers

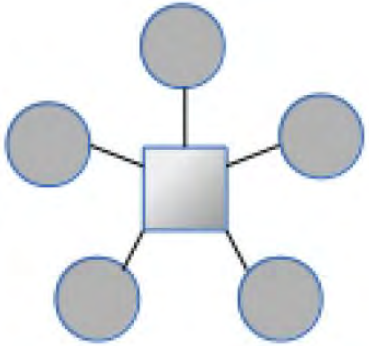
Several numerical impurity-solver methods:

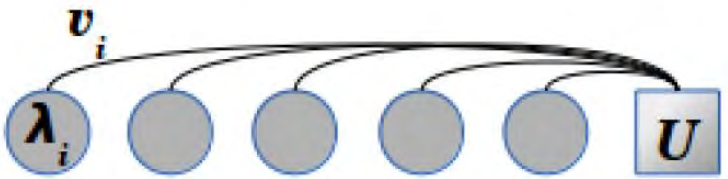
- IPT (Georges A. and Kotliar G., Phys. Rev. B 1992)
- ED (Caffarel M. and Krauth W., Phys. Rev. Lett. 1994)
- HFQMC (Zhang X. Y., Rozenberg M. J., Kotliar G., Phys. Rev. B 1993)
- NCA (Pruschke T., Cox D. L. and Jarrell M., Phys. Rev. Lett. 1993)
- NRG (Bulla R., Costi T. and Vollhardt D., Phys. Rev. B, 2001)

More recently:

- DMRG (Garcia, Hallberg, Rozenberg, PRL. 2004, PRB(RC) 2005;
Y. Núñez-Fernández and K. Hallberg, Front. Phys. 6:13 (2018);
Karski, Raas, Uhrig, 2005, F. Wolf, I. McCulloch and U. Schollwoeck 2014)
- CTQMC (review: Gull E., et al, Rev. Mod. Phys. 2011)
- FLEX (Kotliar et al, J. Phys.: Cond. Matt. 2004)
-TEBD for dynamics: Verstraete et al, PRB 2014
-CI techniques (Zgid et al, 2011, 2012)
- and several other methods...

Cluster DMFT+DMRG in the star geometry

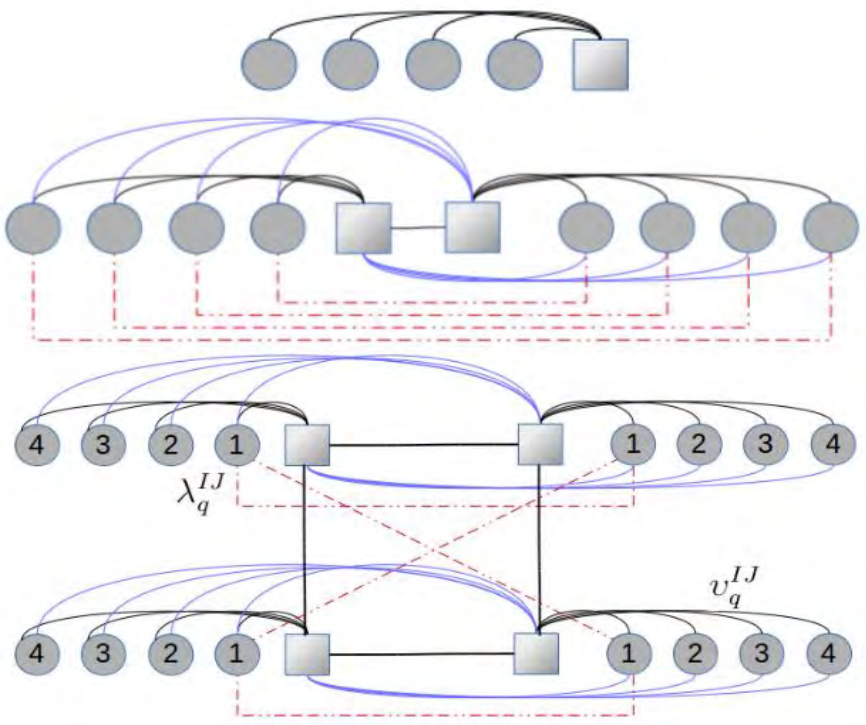




$$H_{imp} = H_{loc} + H_b$$

$$H_b = \sum_{i\sigma} \lambda_i b^\dagger_{i\sigma} b_{i\sigma} + \sum_{i\sigma} v_i \left[b^\dagger_{i\sigma} c_{0\sigma} + H.c. \right]$$

Complex “impurity” (multi-site, multi-band)



$$H_{imp} = \hat{h}_0^0 + \hat{V}_0 + H_b$$

$$H_b = \sum_{IJq\sigma} \lambda_q^{IJ} b_{Iq\sigma}^\dagger b_{Jq\sigma} + \sum_{IJq} v_q^{IJ} \left[b_{Iq\sigma}^\dagger c_{0J\sigma} + H.c. \right]$$

DFT+DMFT

DMFT needs two inputs:

- the non-interacting lattice Green function: $G_0(\omega)$
- the local interaction

DFT gives:

- the Kohn-Sham band structure: $E_\nu(\boldsymbol{k})$
- the effective Hamiltonian: $H_{\nu\nu'}(\boldsymbol{k})$

Idea:

- select bands close to the Fermi level
- obtain some localized Hamiltonian for them: $H^0_{\nu\nu'}(\boldsymbol{k})$

$$G_0(\omega) = \sum_{\boldsymbol{k}} [\omega \mathbf{1} - H^0(\boldsymbol{k})]^{-1}$$

Local interaction: $\hat{V}$

Advantages of using DMRG as the impurity solver:

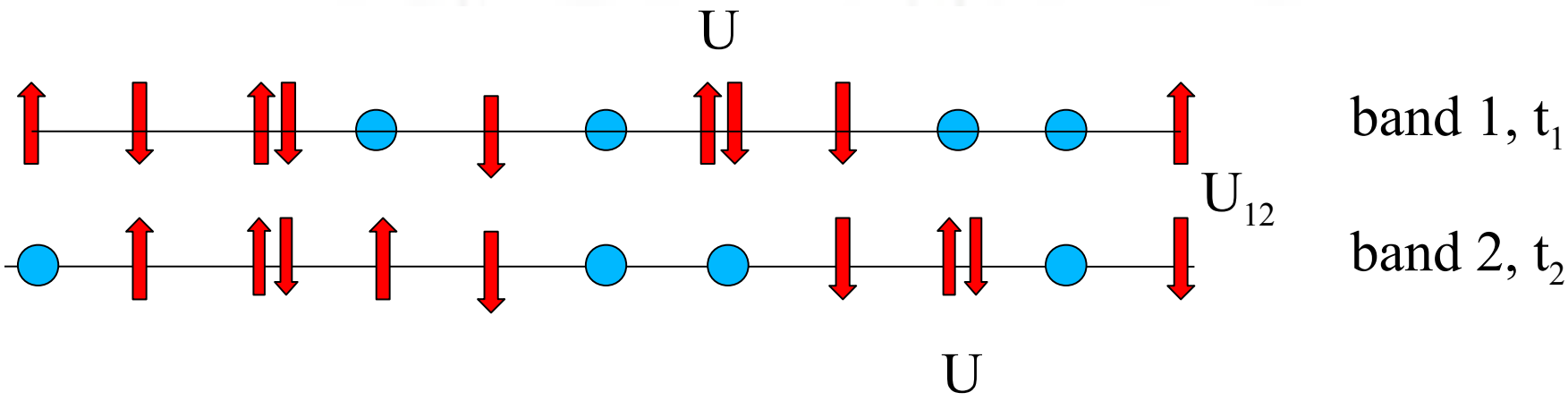
Real ω axis
All ω scales
Arbitrary interactions
No sign problem
Large baths
Several orbitals
Several sites (k-dependence)
Finite T (?)

- García, KH, Rozenberg, PRL. 2004 and PRB(RC) 2005
- F. Wolf, I. McCulloch and U. Schollwoeck, Phys. Rev. B 2014
- KH, García, Cornaglia, Facio, Núñez Fernández, EPL Perspectives 2015
- *Solving the multi-site and multi-orbital Dynamical Mean Field Theory using Density Matrix Renormalization*, Y. Núñez-Fernández and K.H., Front. Phys. 6:13 (2018)

Example: Two band Hubbard model

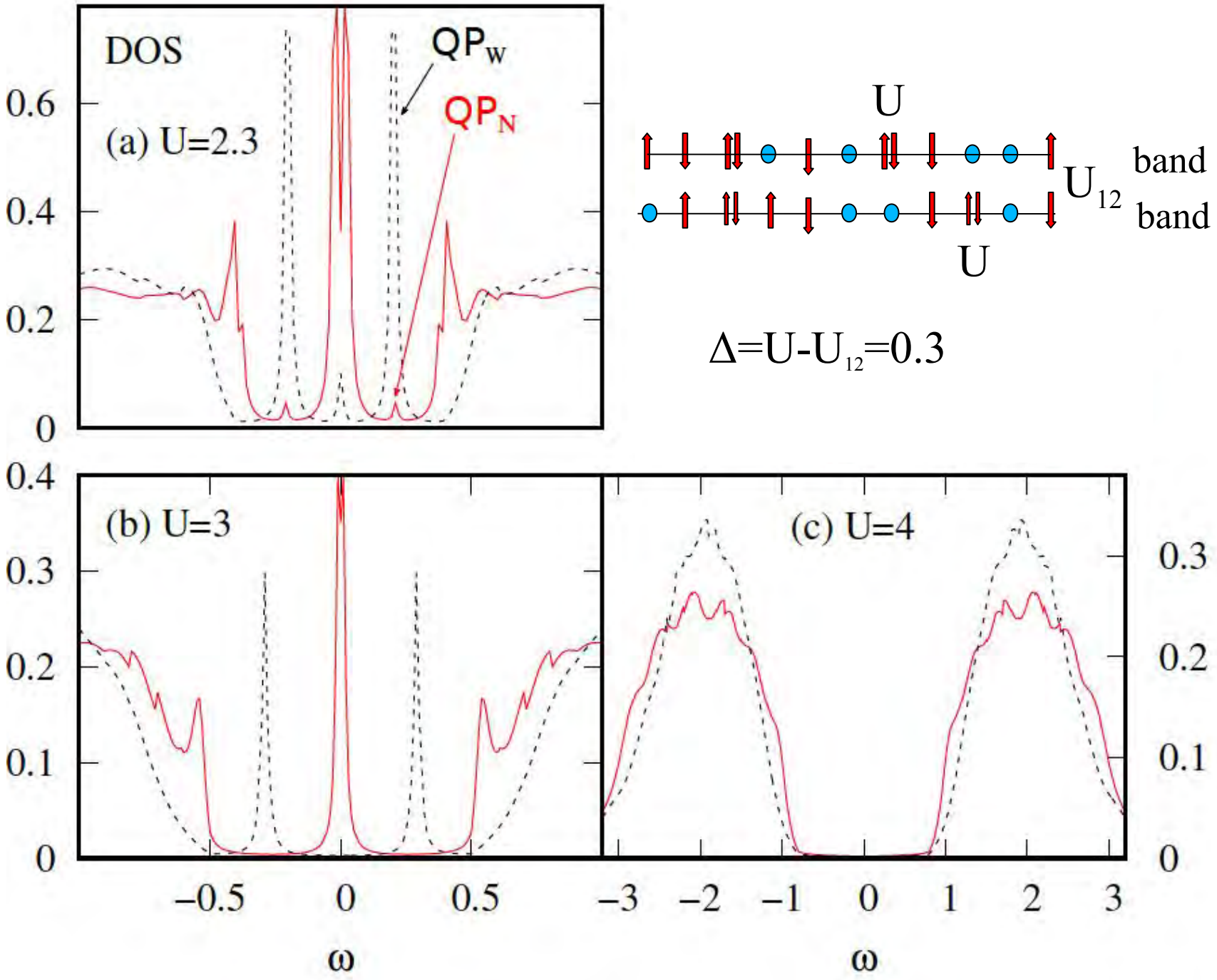
$$H = \sum_{\langle ij\rangle\alpha\sigma} t_\alpha c^\dagger_{i\alpha\sigma} c_{j\alpha\sigma} +$$

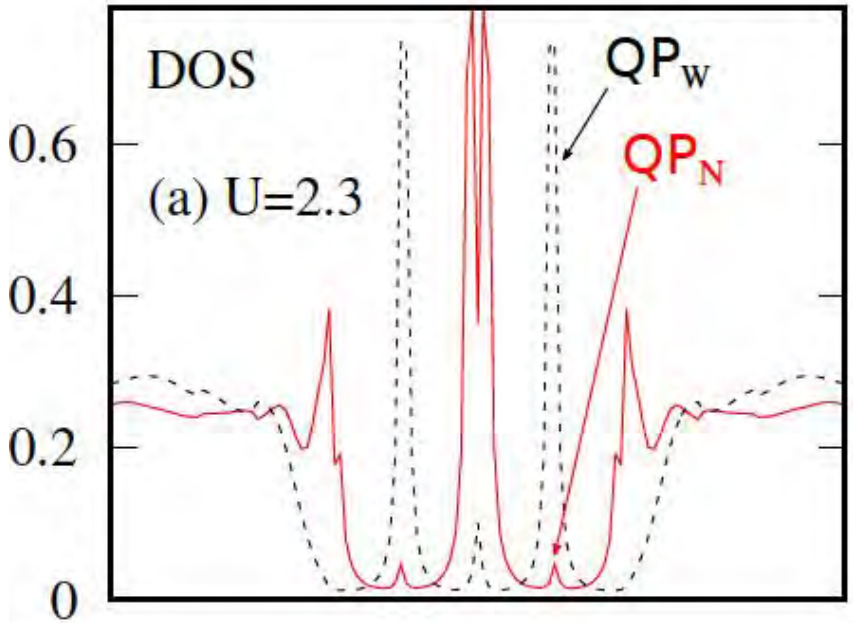
$$+ U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + \sum_{i\sigma\sigma'} U_{12} n_{i1\sigma} n_{i2\sigma'}$$



Half-filled and doped T=0 t'=0 $t_1 \geq t_2$ $U_{12} \leq U$ $\Delta = U - U_{12}$

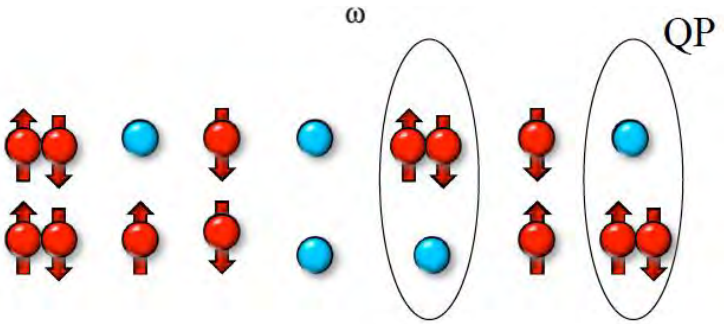
square lattice (2D)!

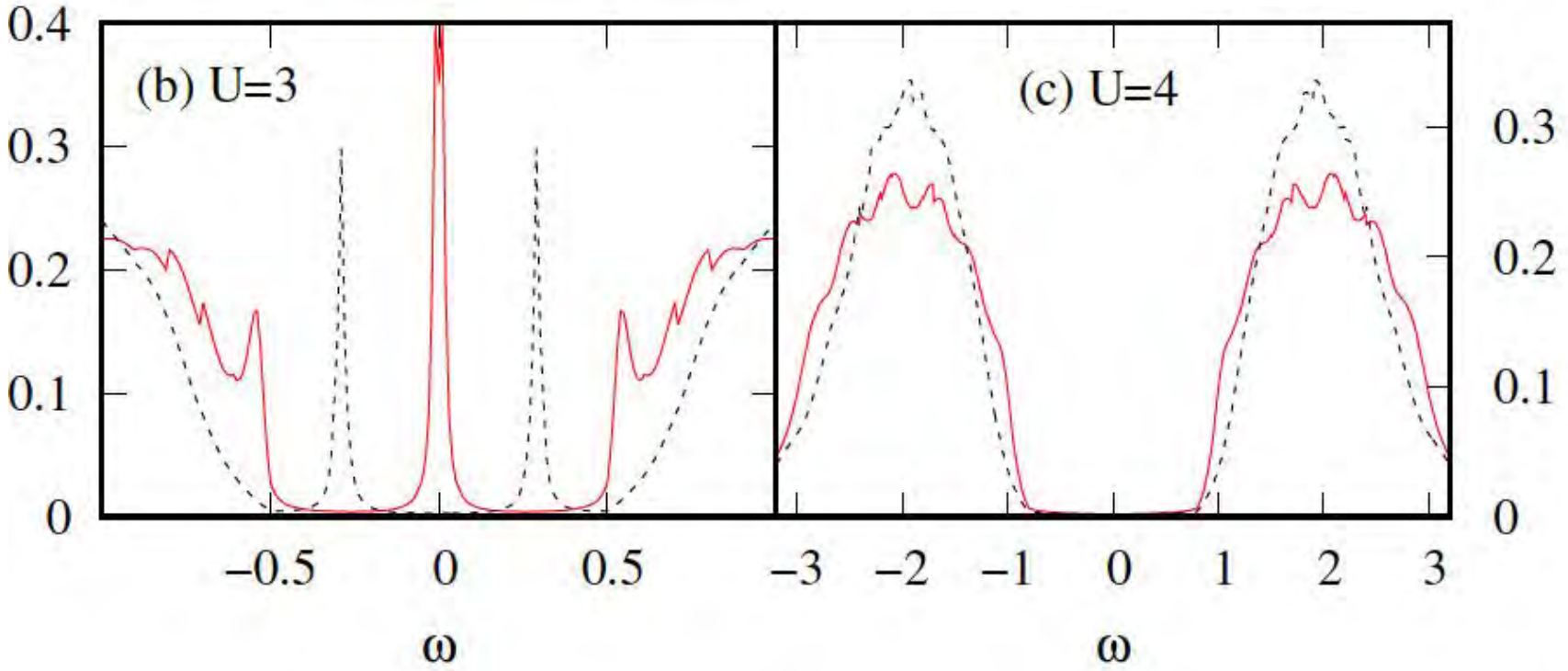

DOS
(a) U=2.3
QP_W
QP_N
0.6
0.4
0.2
0
U
U_12
band 1, t_1
band 2, t_2
U
Δ=U-U_12=0.3
0.4
0.3
0.2
0.1
0
(b) U=3
(c) U=4
0.3
0.2
0.1
0
−0.5
0
0.5
−3
−2
−1
0
1
2
3
ω
ω



Looking closer: quasiparticles!

$\Delta = U - U_{12} = 0.3$






Thank you for your attention!