Controlled Bond Expansion (CBE) for DMRG Ground State Search and TDVP Time Evolution

Benasque, 02.03.2022

Andreas Gleis, Jheng-Wei Li, Jan von Delft

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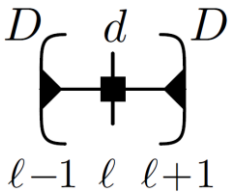

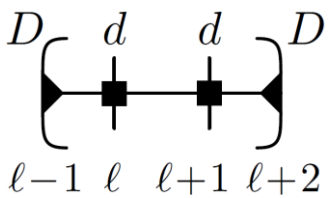

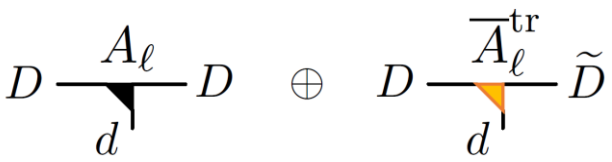

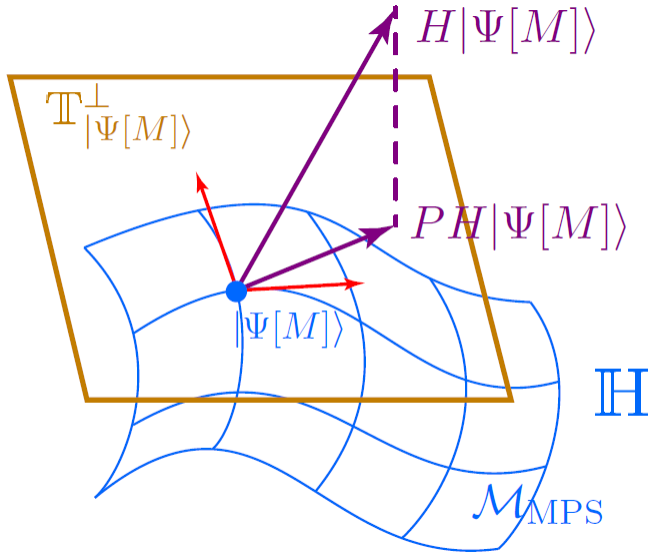

Andreas Gleis

Jheng-Wei Li

Controlled bond expansion into truncated orthogonal subspace achieves 2-site accuracy at 1-site costs!

LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

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CeNS Center for NanoScience

MUNICH QUANTUM CENTER

MCQST

Munich Quantum Valley

DMRG / methods for 1D ground state search & time evolution

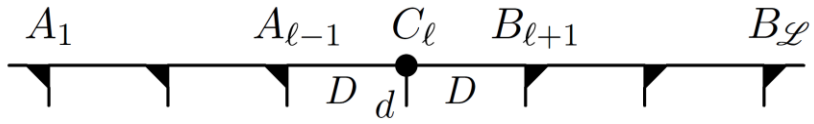
DMRG / MPS methods are gold standards for 1D ground state searches and time evolution

Google Scholar 28.02.2022

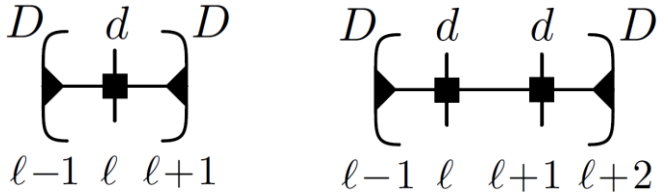
1992	Steve White, ***Invention*** *of DMRG*	> 7100 citations
1993		> 3100 citations
2004	Frank Verstraete, Diego Porras, Ignacio Cirac, *Reinvention of DMRG in MPS language*	> 700 citations
2004	Steve White, Adrian Feiguin, ***Time-dependent*** *DMRG*	> 1300 citations
2004	Andrew Daley, Corinna Kollath, Ulrich Schollwöck, Guiffre Vidal, ***Time-dependent*** *DMRG*	> 1000 citations
2005	Ulrich Schollwöck, *DMRG* ***review*** (RMP)	> 3200 citations
2011	Ulrich Schollwöck, *DMRG review* in **MPS language** (Annals Phys.)	> 3200 citations
2011	Jhuto Haegeman, Ignacio Cirac, Tobias Osborne, Iztok Pižorn, Henri Verschelde, Frank Verstraete **Tangent space** methods – Time-dependent variational principle (TDVP)	> 460 citations
2016	Jutho Haegeman, Christian Lubich, Ivan Oseledets, Bart Vandereycken, Frank Verstraete **Unifying** time evolution and optimization with MPS	> 370 citations
2019	Sebastian Paeckel, Thomas Köhler, Andreas Swoboda, Salvatore Manmana, Ulrich Schollwöck, Claudius Hubig, ***Review*** *of MPS methods for time evolution*	> 290 citations

Outline

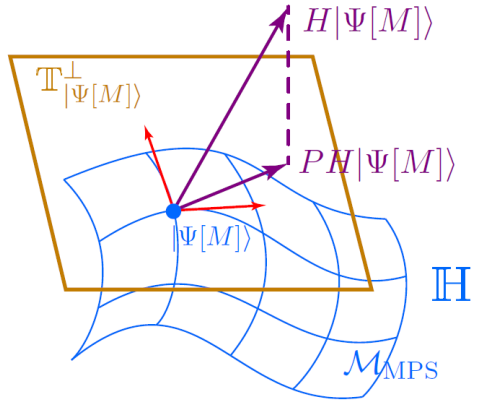
- Review of MPS basics



- DMRG ground state search: 1-site vs. 2-site algorithms



- Tangent space



- Controlled bond expansion

- CBE-DMRG for ground state search – results [slides by Andreas Gleis]

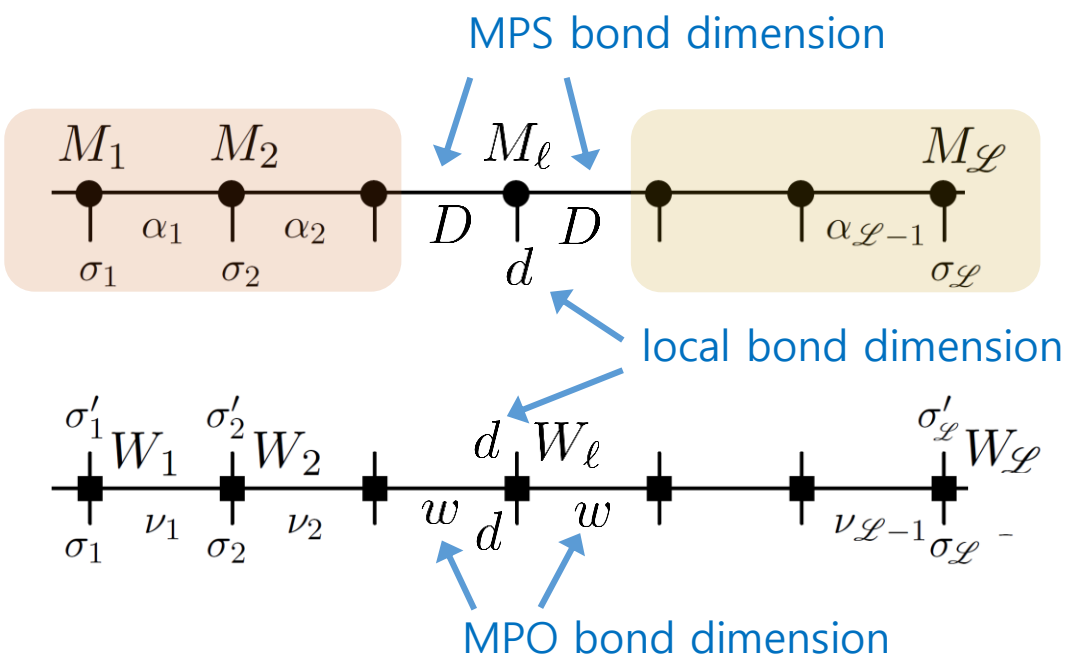
- CBE-TDVP for time evolution – results [slides by Jheng-Wei Li]

Basis: $|\boldsymbol{\sigma}\rangle = |\sigma_1\rangle|\sigma_2\rangle\cdots|\sigma_{\mathscr{L}}\rangle$

MPS: $|\Psi\rangle = |\boldsymbol{\sigma}\rangle [M_1]^{\sigma_1}_{1\alpha_1}[M_2]^{\sigma_2}_{\alpha_1\alpha_2}\cdots[M_{\mathscr{L}}]^{\sigma_{\mathscr{L}}}_{\alpha_{\mathscr{L}-1}1}$

$= |\Psi_{\ell-1,\alpha}\rangle|\sigma_\ell\rangle|\Phi_{\ell+1,\alpha'}\rangle[M^{\sigma_\ell}]_{\alpha\alpha'}$

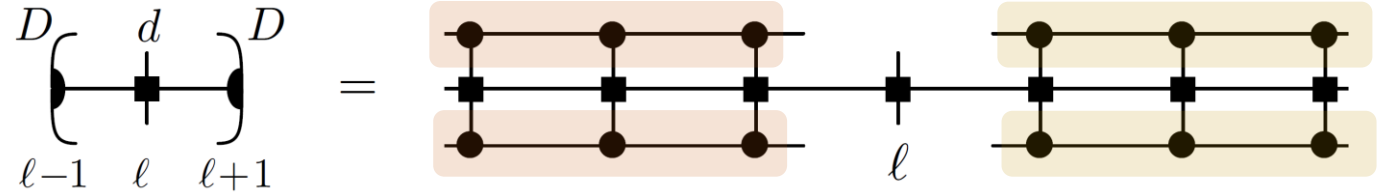
MPO: $H^{\boldsymbol{\sigma}\boldsymbol{\sigma}'} = [W_1]^{\sigma_1\sigma_1'}_{1\nu_1}[W_2]^{\sigma_2\sigma_2'}_{\nu_1\nu_2}\cdots[W_{\mathscr{L}}]^{\sigma_{\mathscr{L}}\sigma_{\mathscr{L}}'}_{\nu_{\mathscr{L}-1}1}$



Projection of Hamiltonian into local subspace:

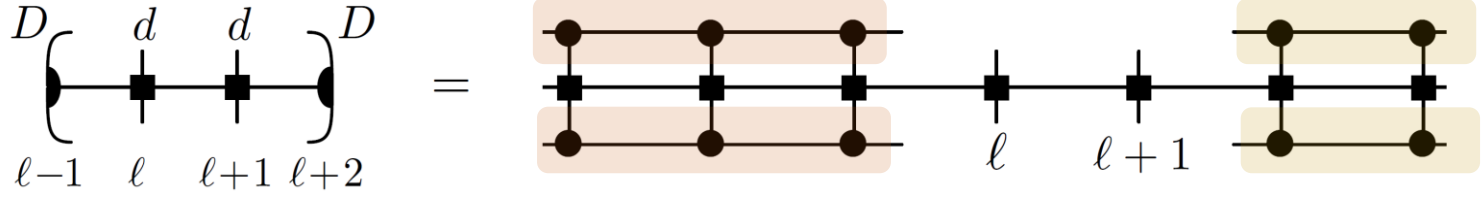
One-site Hamiltonian: $D^2d \times D^2d$

$H^{(1)}_\ell =$



Two-site Hamiltonian: $D^2d^2 \times D^2d^2$

$H^{(2)}_\ell =$

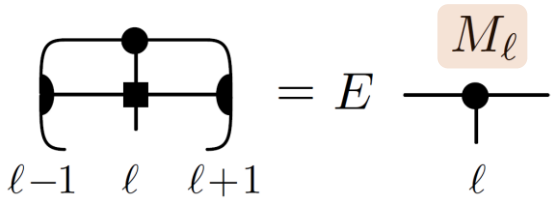


MPS basics: minimize energy by local optimization of MPS

Update MPS locally, by finding ground state of local Schrödinger equation (e.g. by Krylov methods):

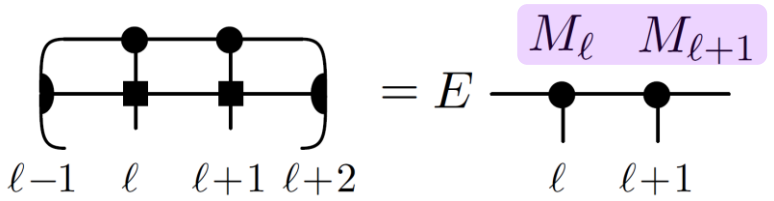
1-site:

$|\Psi_{\ell-1,\alpha}\rangle|\sigma_\ell\rangle|\Phi_{\ell+1,\alpha'}\rangle[M^{\sigma_\ell}]_{\alpha\alpha'}$



2-site:

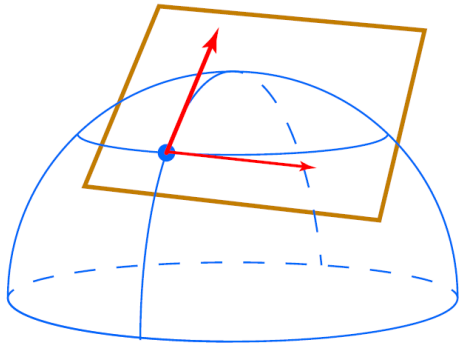
$|\Psi_{\ell-1,\alpha}\rangle|\sigma_\ell\rangle|\sigma_{\ell+1}\rangle|\Phi_{\ell+2,\alpha'}\rangle[M^{\sigma_\ell}M^{\sigma_{\ell+1}}]_{\alpha\alpha'}$



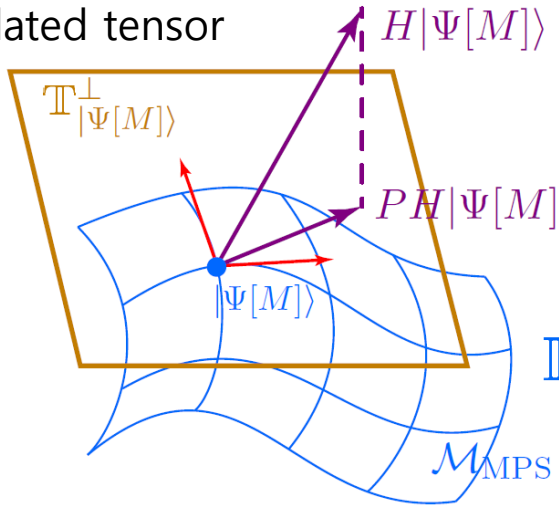
cost	convergence
$\mathcal{O}(D^3\, d\, w)$	bad
$\mathcal{O}(D^3\, d^2\, w)$	good

[Haegemann *et al.*, PRL 2011]

tangent space: spanned by vectors tangent to curves running within a smooth geometric structure



tangent space of MPSs having one updated tensor



2-site explores orthogonal space: larger bond dimensions, new quantum numbers

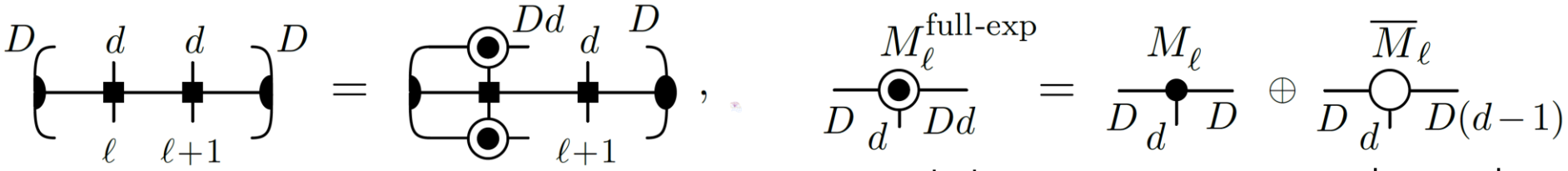
1-site confined to tangent space

$\mathbb{H}$ full Hilbert space of dimension $d^{\mathscr{L}}$

$\mathcal{M}_{\mathrm{MPS}}$ space of MPS with specified dimensions

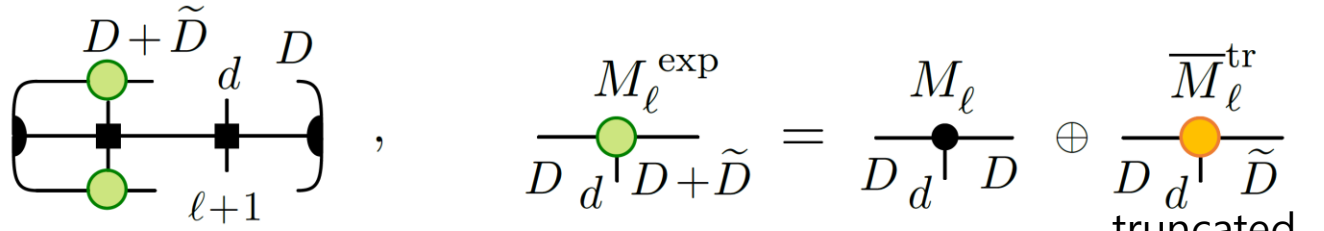
Bond expansion

2-site can be formulated as 1-site, with expanded bond:



expanded bond | tangent space | orthogonal complement

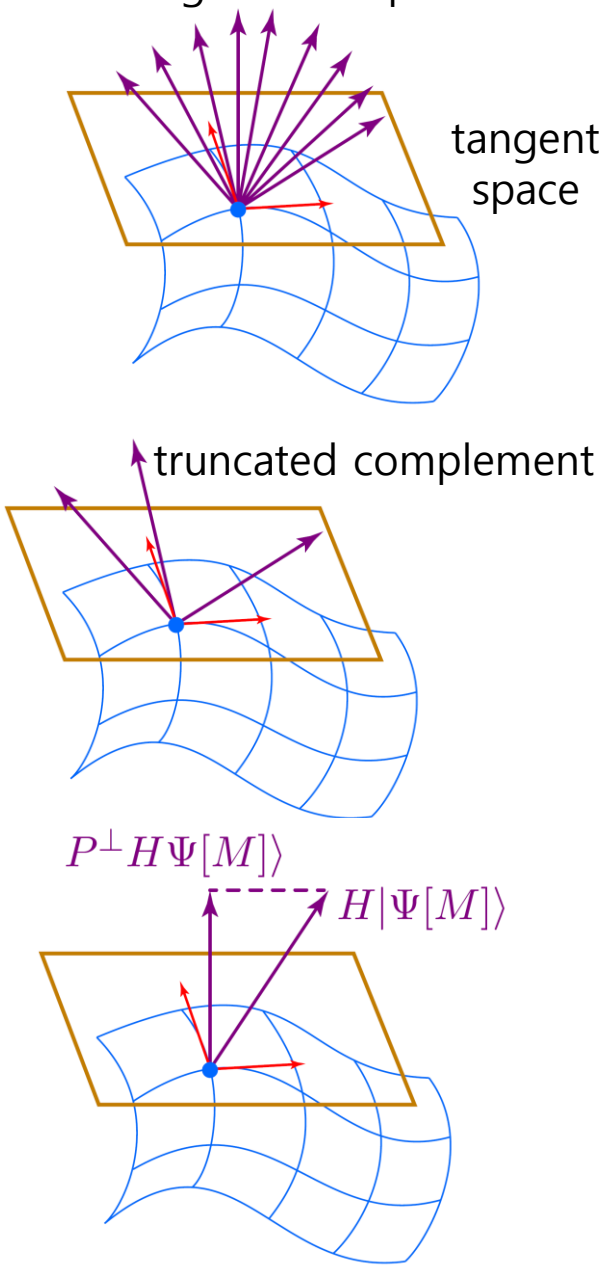
instead, truncate!



truncated complement

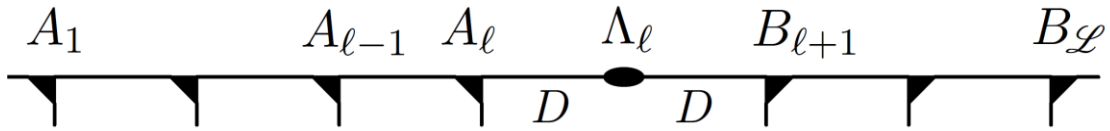
How should we truncate the complement?

- White [PRB 2005]: density matrix perturbation (add noise)
- Hubig, McCulloch, Schollwöck, Wolf [PRB 2015]: apply H on only one of two sites, "add zeros" for other site
- Gleis, Li, von Delft [2022]: apply H on both sites, retain maximal weight parts

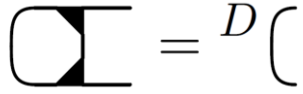
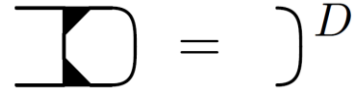


Identify orthogonal complement

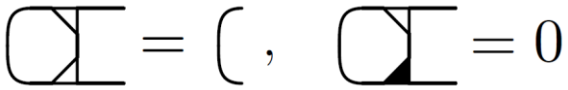
Bond-canonical form:

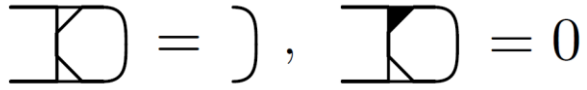


Isometry conditions:

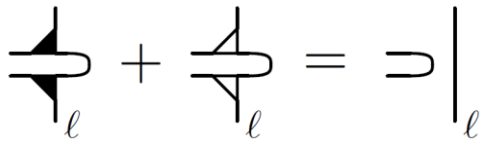
$A_\ell^\dagger A_\ell = \mathbb{1}_\ell$  $B_\ell B_\ell^\dagger = \mathbb{1}_{\ell-1}$ 

Orthonormality:

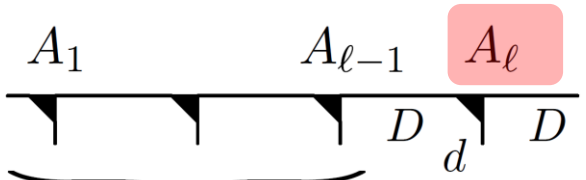




Completeness:

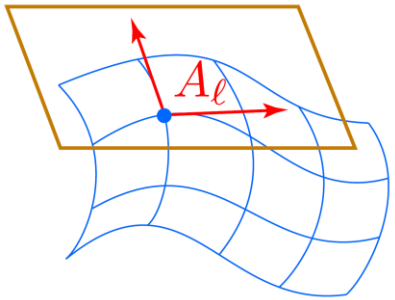


A_ℓ is an isometric map into tangent space of MPS defined on sites $1, \ldots, \ell-1$

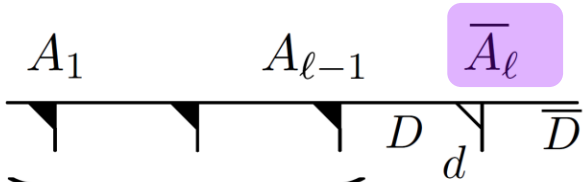


$$|\Psi_{\ell-1,\alpha}\rangle \otimes |\sigma_\ell\rangle [A_\ell]^{\sigma_\ell}_{\alpha\alpha'} = |\Psi_{\ell,\alpha'}\rangle$$

varying A_ℓ explores tangent space of MPS defined on sites $1, \ldots, \ell-1$

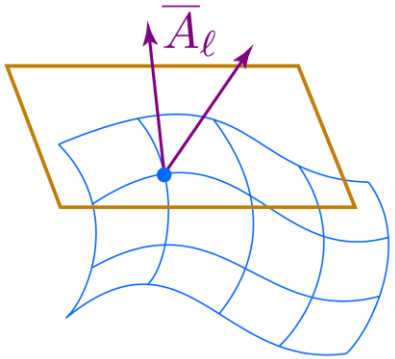


$\overline{A}_\ell$ is an isometric map into orthogonal complement of that tangent space

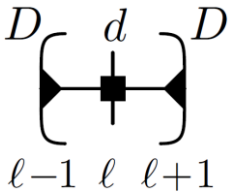
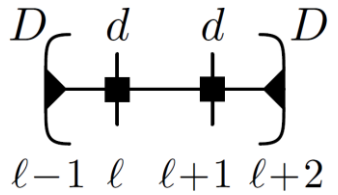


$$|\Psi_{\ell-1,\alpha}\rangle \otimes |\sigma_\ell\rangle [\overline{A}_\ell]^{\sigma_\ell}_{\alpha\alpha'} = |\overline{\Psi}_{\ell,\alpha'}\rangle$$

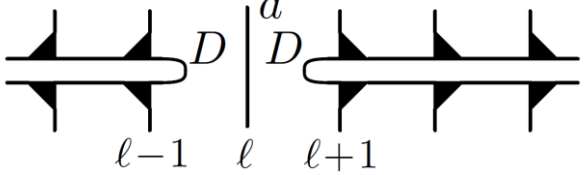
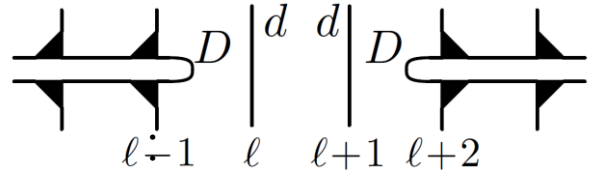
varying $\overline{A}_\ell$ explores orthogonal complement

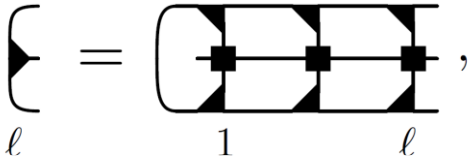
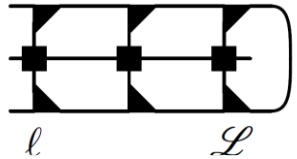


Which part of 2-site Hamiltonian is missing from 1-site Hamiltonian?

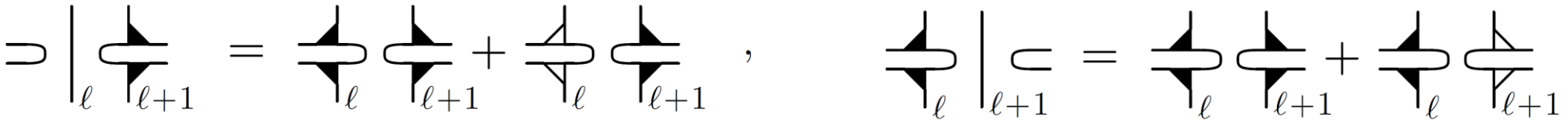
Local Hamiltonians, $H_\ell^{(1)} =$  and $H_\ell^{(2)} =$ 

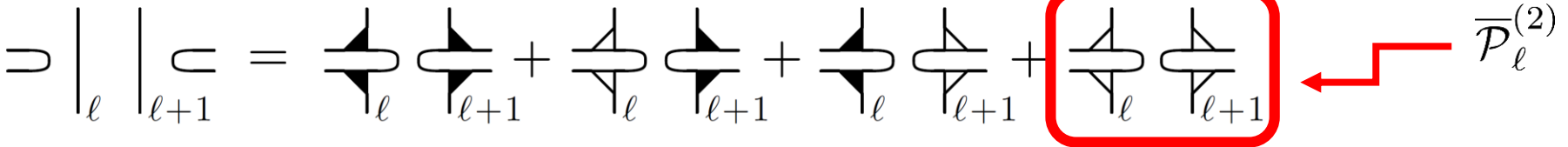
are matrix elements of $\mathcal{P}_\ell^{(1)} H \mathcal{P}_\ell^{(1)}$ and $\mathcal{P}_\ell^{(2)} H \mathcal{P}_\ell^{(2)}$

with $\mathcal{P}_\ell^{(1)} =$  $\mathcal{P}_\ell^{(2)} =$ 

with left an right environments L_ℓ  R_ℓ 

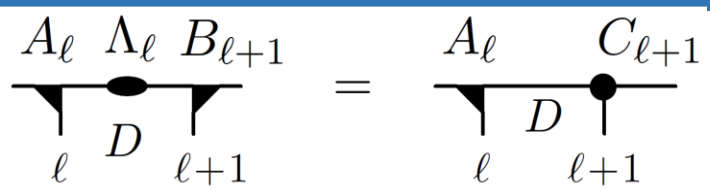
Projector identities reveal essential difference between 1-site and 2-site Hamiltonians:

1-site: 

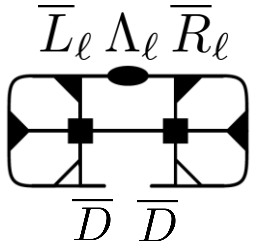
2-site: 

Controlled bond expansion (CBE) algorithm (sweeping right to left)

Wavefunction of $|\Psi\rangle$:

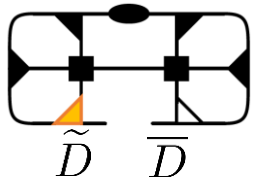


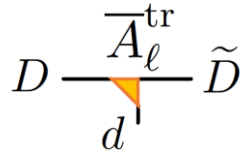
Wavefunction of $\overline{\mathcal{P}}_\ell^{(2)} H|\Psi\rangle$:



full computation requires 2-site costs, since orthogonal complement is huge: $\overline{D} = D(d+1)$

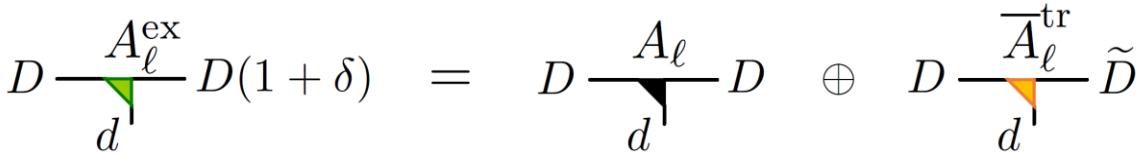
(i) Truncate this to



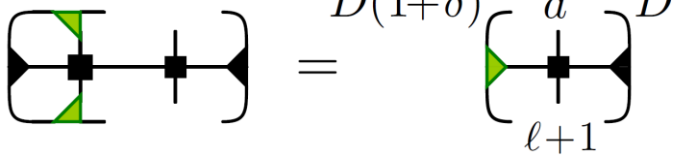
involving truncated complement 

with $\widetilde{D} = D\delta, \quad \delta < 1$

(ii) Do bond expansion:

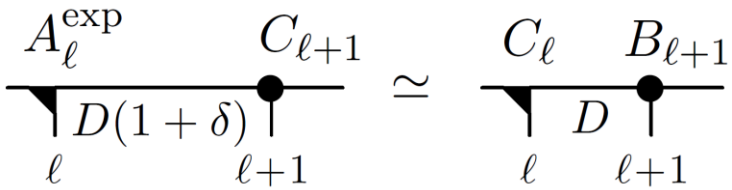


(iii) Construct expanded 1-site $H_{\ell+1}^{(1,\mathrm{exp})}$ =



compute its ground state and use it to update $C_{\ell+1}$

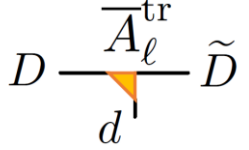
(iv) Shift orthogonality center by SVD



truncate bond back to D

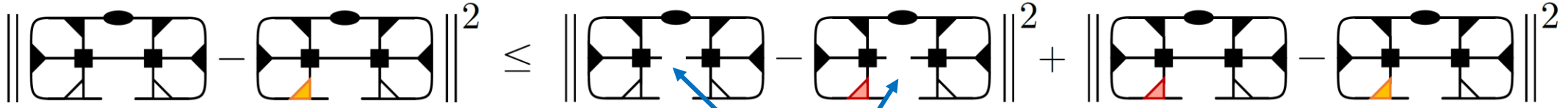
error measure: discarded weight ξ

Computing truncated complement



When computing truncated complement, try to minimize truncation error, while maintaining 1-site costs!

Cost function:



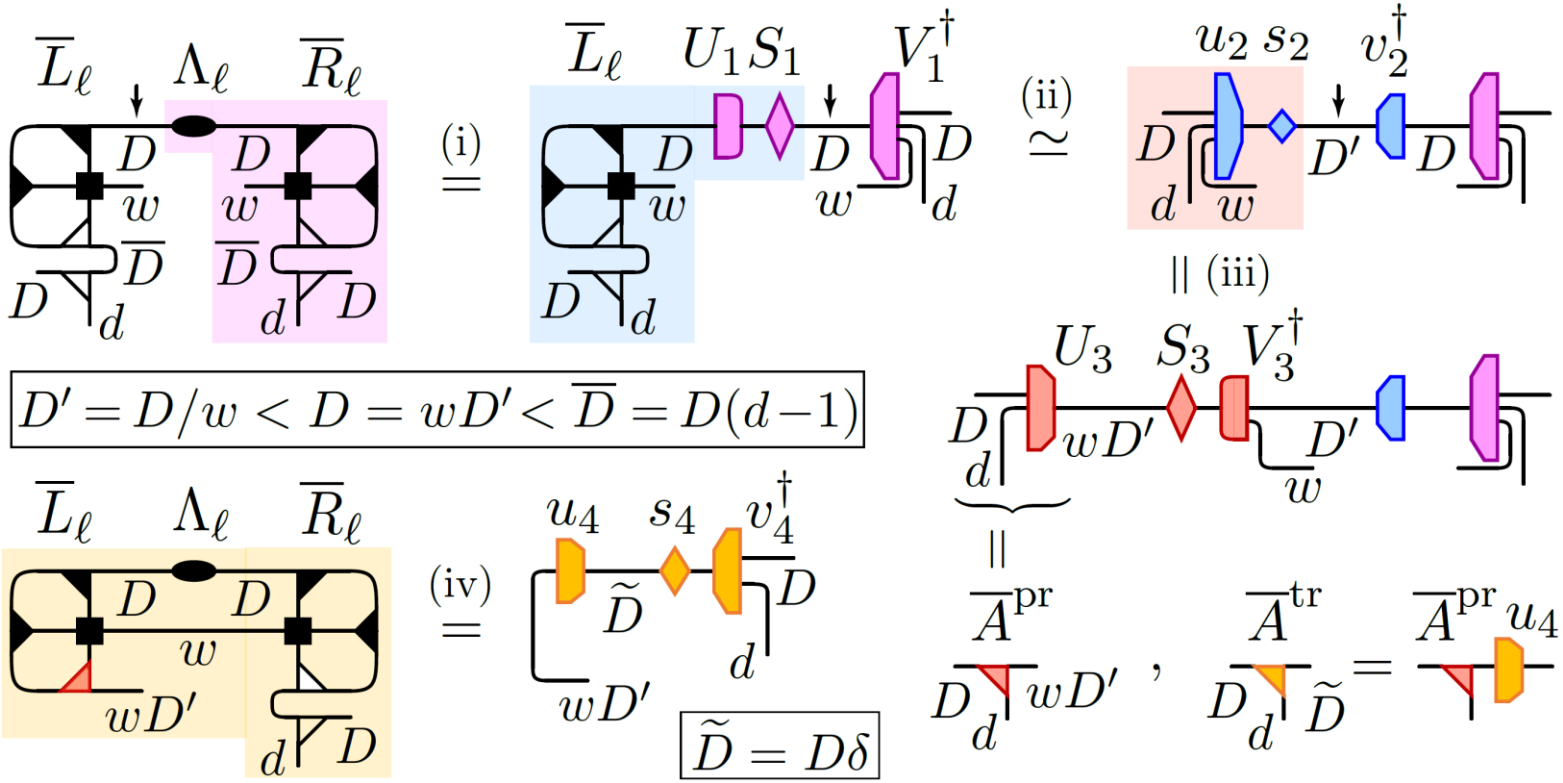
To keep numerical costs low: cut MPO bond; prune central MPS bond

(i) incorporate weights from $\overline{R}_\ell$

(ii) prune central bond from D to $D' = D/w$

(iii) redirect MPO bond to obtain pruned complement, A_ℓ^{pr}

(iv) truncate pruned complement to obtain truncated complement A_ℓ^{tr}



Free fermions in one dimension: singular values spectra

$$H_{\rm ff} = -\sum_{i=1}^{L-1}\sum_{\sigma=\uparrow,\downarrow}\left(c^\dagger_{i\sigma}c_{i+1\sigma} + h.c.\right)$$

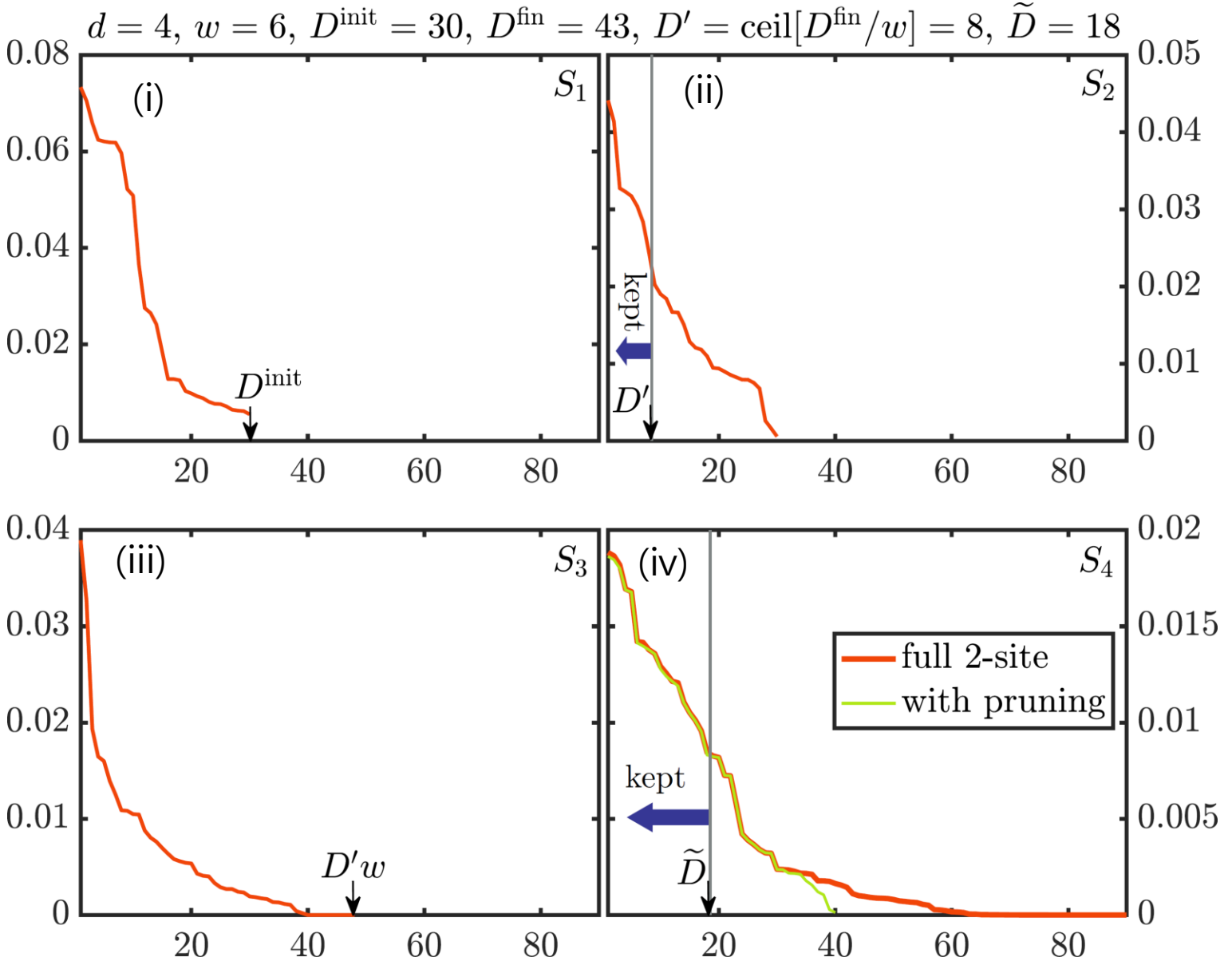
$$L = N = 100\,,\; S = 0$$

(i) incorporate weights from $\overline{R}_\ell$

(ii) prune central bond
from D to $D' = D/w$

(iii) redirect MPO bond to obtain
pruned complement, $A^{\rm pr}_\ell$

(iv) truncate pruned complement to
obtain truncated complement $A^{\rm tr}_\ell$



Free fermions in one dimension

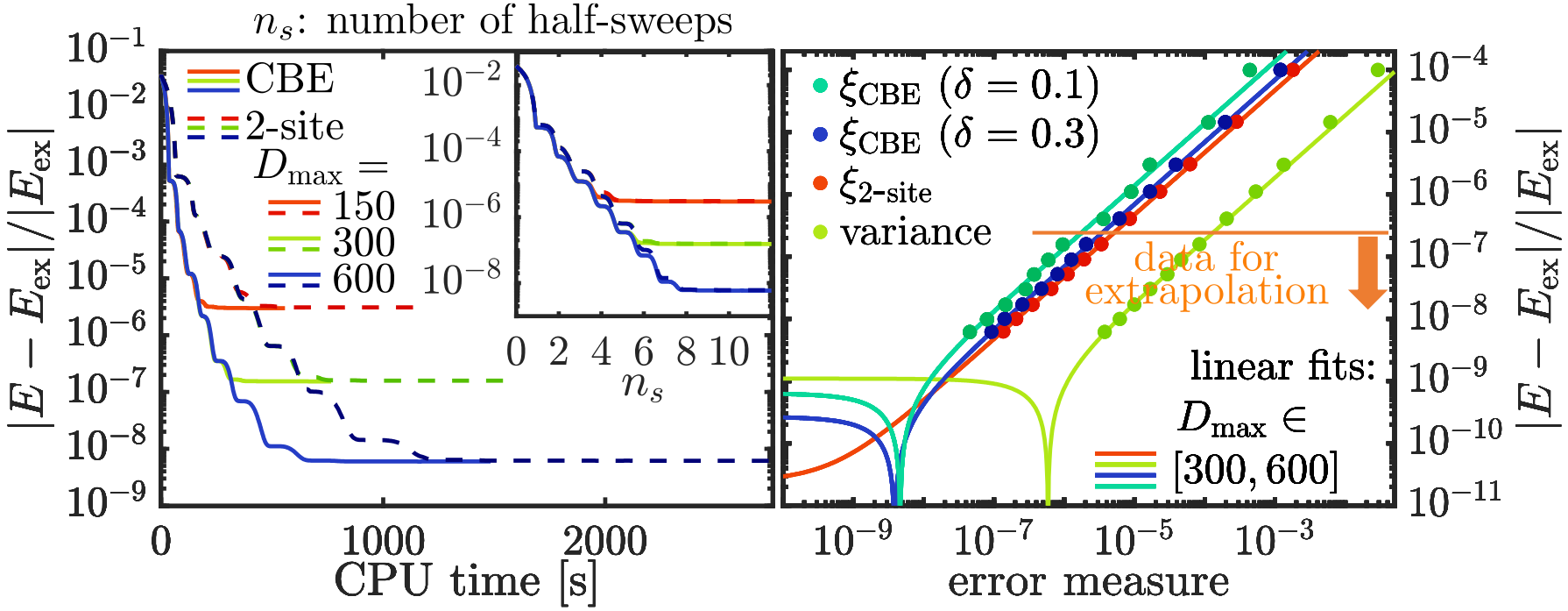
$$H_{\mathrm{ff}} = -\sum_{i=1}^{L-1} \sum_{\sigma=\uparrow,\downarrow} \left(c_{i\sigma}^{\dagger} c_{i+1\sigma} + h.c. \right)$$

$L = N = 100\,,\ S = 0$

$E_{\mathrm{ex}} = -126.6023783108...$

$N_{\mathrm{Lanczos}} = 3$

$\mathrm{SU}(2)_{\mathrm{sp}} \otimes \mathrm{U}(1)_{\mathrm{ch}}$



- CBE faster than 2-site!
- similar convergence with n_s!

- ξ_{CBE}: error measure suitable for extrapolation!

Hubbard-Holstein model in one dimension

$$H_{\mathrm{HH}} = -\sum_{i,\sigma}\left(c^{\dagger}_{i\sigma}c_{i+1\sigma} + h.c.\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$
$$+\omega_0\sum_i b^{\dagger}_i b_i + g\sum_i (n_{i\uparrow}+n_{i\downarrow}-1)\left(b^{\dagger}_i + b_i\right)$$

$U = 0.8,\ \omega_0 = 0.5,\ g = \sqrt{0.2}$

$N = L = 50,\ S = 0$ $\quad \mathrm{SU}(2)_{\mathrm{sp}} \otimes \mathrm{U}(1)_{\mathrm{ch}}$

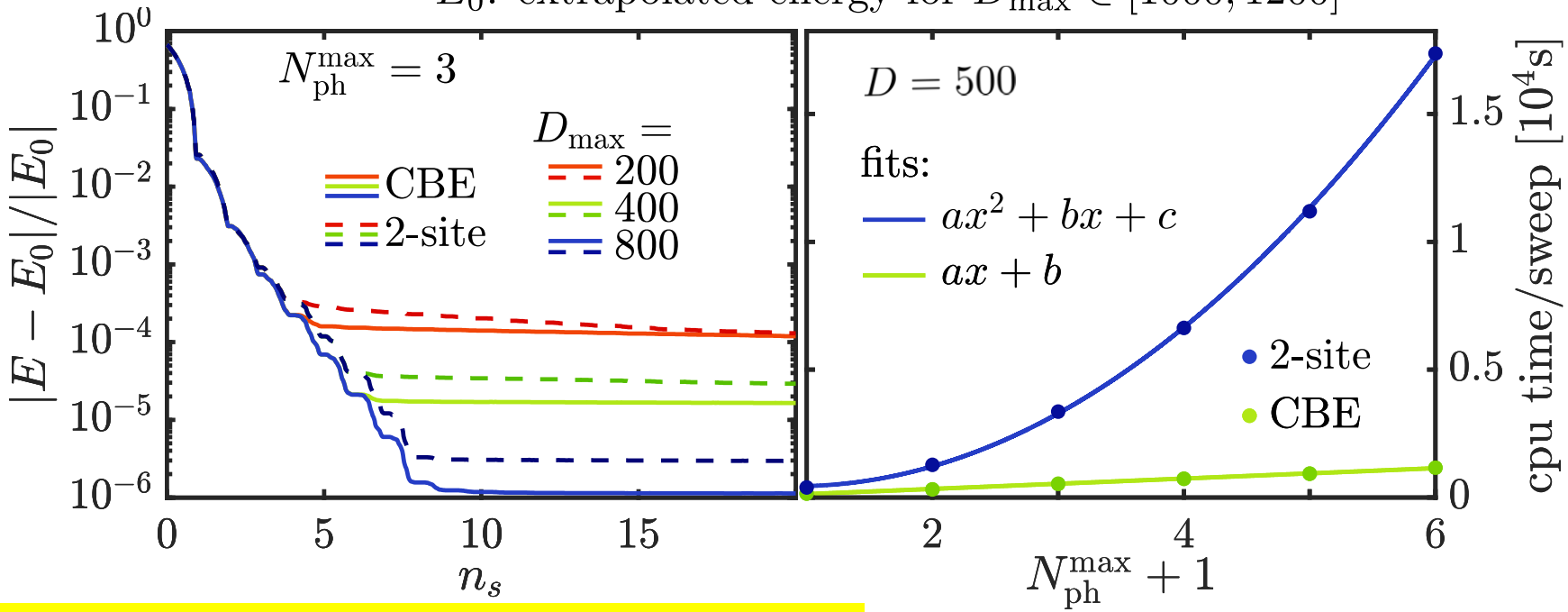
maximum allowed local phonon occupation: $N_{\mathrm{ph}}^{\max} \longrightarrow d = 4(N_{\mathrm{ph}}^{\max}+1)$

E_0: extrapolated energy for $D_{\max} \in [1000, 1200]$

$w = 6$

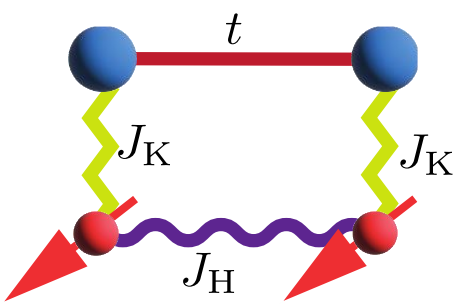
$\delta = 0.1$

$N_{\mathrm{Lanczos}} = 3$



- CBE converges even faster with n_s than 2-site!
- Possibly due to much larger variational space in 2-site, $N_{\mathrm{Lanczos}} > 3$should be used.
- d vs d^2 scaling!

Kondo-Heisenberg (KH) lattice model on a 10x4 cylinder



$$H_{\mathrm{KH}} = -\sum_{\sigma}\sum_{y=1}^{L_y}\sum_{x=1}^{L_x-1}\left(c^{\dagger}_{xy\sigma}c_{x+1y\sigma}+h.c.\right) - \sum_{\sigma}\sum_{y=1}^{L_y}\sum_{x=1}^{L_x}\left(c^{\dagger}_{xy\sigma}c_{xy+1\sigma}+h.c.\right)$$

electrons hopping

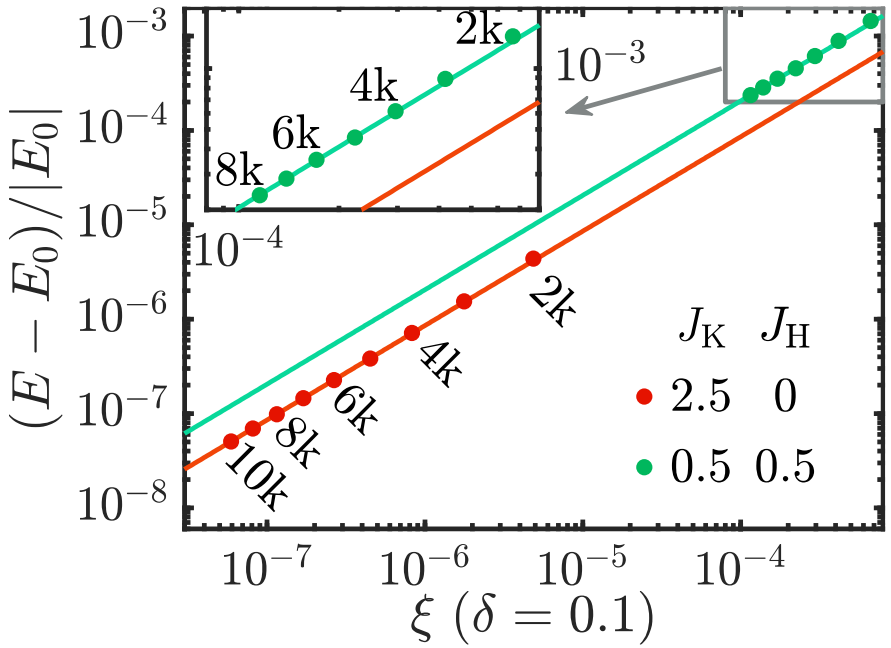
$$+ 2J_{\mathrm{K}}\sum_{x,y}\boldsymbol{S}_{xy}\cdot\boldsymbol{s}_{xy} + J_{\mathrm{H}}\sum_{\langle x,x'\rangle}\sum_{\langle y,y'\rangle}\boldsymbol{S}_{xy}\cdot\boldsymbol{S}_{x'y'}$$

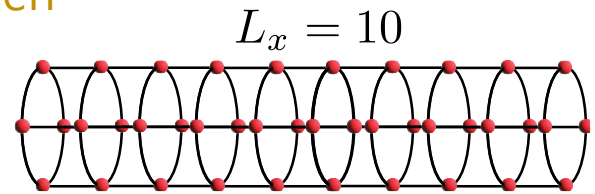
Kondo interaction between electrons and spins

Heisenberg interaction between spins

$N_{\mathrm{Lanczos}} = 3$

$\mathrm{SU}(2)_{\mathrm{sp}} \otimes \mathrm{U}(1)_{\mathrm{ch}}$





$N = 1.25 \cdot L_x \cdot L_y = 50,\ S = 0$

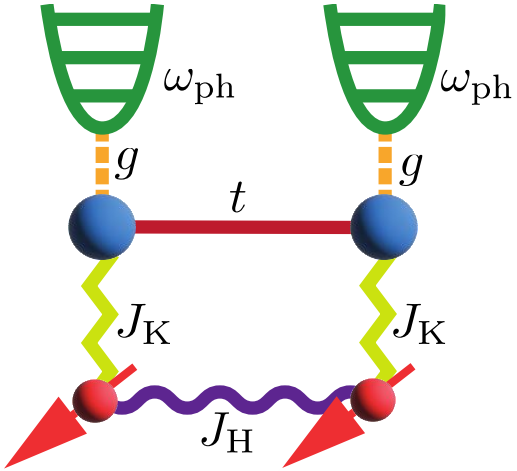
$w = 6$

relevance: heavy-fermion materials (Coleman 2007)

	local dimension d	MPO dimension w
$J_{\mathrm{H}} = 0$	8 (4 multiplets)	18 (10 multiplets)
$J_{\mathrm{H}} \neq 0$	8 (4 multiplets)	30 (14 multiplets)

- possible to keep 10000/8000 multiplets!
- ξ_{CBE}: reliable and cheap error measure!

Kondo-Heisenberg-Holstein (KHH) lattice model on a 10x4 cylinder



$$H_{\rm KHH} = H_{\rm KH} + \omega_{\rm ph} \sum_{x,y} b^\dagger_{xy} b_{xy} + g \sum_{x,y} \left(n_{xy\uparrow} + n_{xy\downarrow} - 1\right)\left(b^\dagger_{xy} + b_{xy}\right)$$

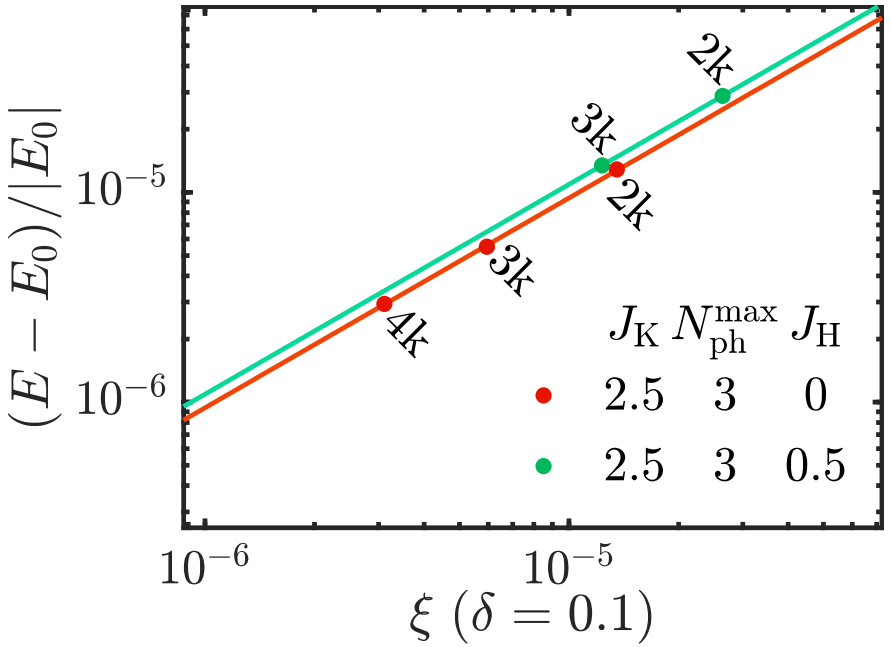
optical phonons

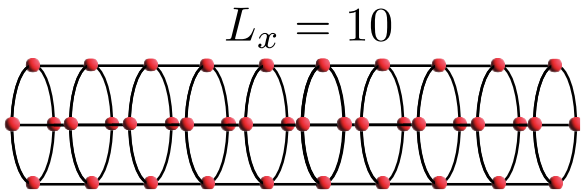
Holstein interaction between electrons and phonons

$N_{\rm Lanczos} = 3$

$\mathrm{SU}(2)_{\rm sp} \otimes \mathrm{U}(1)_{\rm ch}$

$N_{\rm ph}^{\rm max} = 3$





$N = 1.25 \cdot L_x \cdot L_y = 50,\ S = 0$

$\omega_{\rm ph} = 0.5,\ g = 0.5$

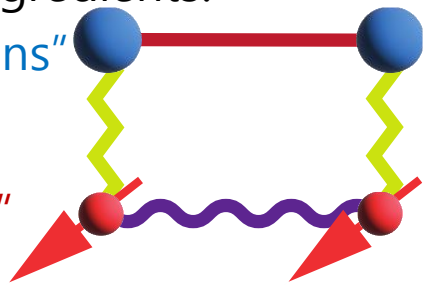
	local dimension d	MPO dimension w
$J_{\rm H} = 0$	32 (16 multiplets)	18 (10 multiplets)
$J_{\rm H} \neq 0$	32 (16 multiplets)	30 (14 multiplets)

- possible to keep 4000/3000 multiplets despite huge d and w!
- $\xi_{\rm CBE}$: only computable error meassure!
  Even the 2-site variance is too expensive!

What are heavy fermion materials?

Basic ingredients:

"c-electrons" itinerant conduction electrons



c-f hybridization leads to Kondo coupling between f-spin and c-electrons

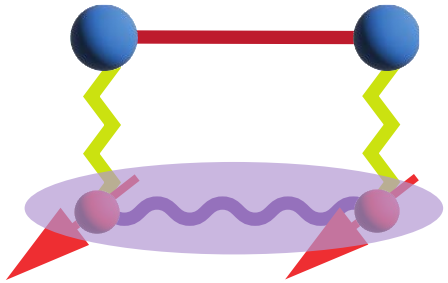
"f-spins" localized f-orbitals, strong local repulsion prevents double occupation
→ only spin degree of freedom left at low energies

f-f hopping leads to Heisenberg coupling between f-spins

Kondo-Heisenberg lattice model

Rudermann-Kittel-Kasuya-Yosida (RKKY) correlations

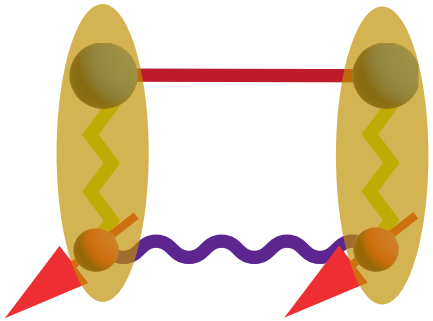
small Kondo coupling: f-f entanglement dominates



competing correlations

Kondo correlations

large Kondo coupling: c-f entanglement dominates



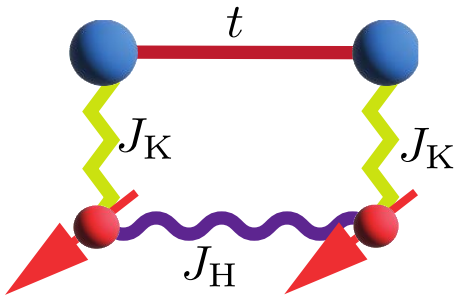
f-spins "remember" their electronic origin
and behave like itinerant charge carriers

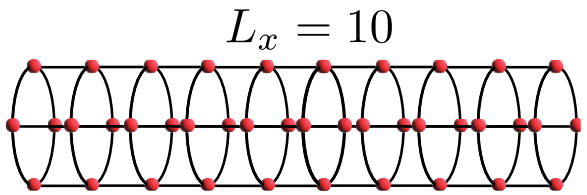
FS volume of the c-electrons: "small" FS — QCP — f-spins are included in Fermi surface (FS) volume: "large" FS

Ruderman, Kittel, PR **96** (1954) ; Kasuya, PTP **16** (1956) ; Yosida, PR **106** (1957)

Coleman, "Heavy Fermions: Electrons at the Edge of Magnetism" (

Fermi surface reconstruction in the Kondo-Heisenberg model





$N = 1.25 \cdot L_x \cdot L_y = 50,\ S = 0$

to detect FS reconstruction: compute $(\rho_{1\mathrm{p}})_{\alpha\beta} = \sum_\sigma \langle c^\dagger_{\alpha\sigma} c_{\beta\sigma} \rangle$ with $\alpha, \beta = (x, y)$

RKKY

expectation: $N/2 = 25$ filled orbitals

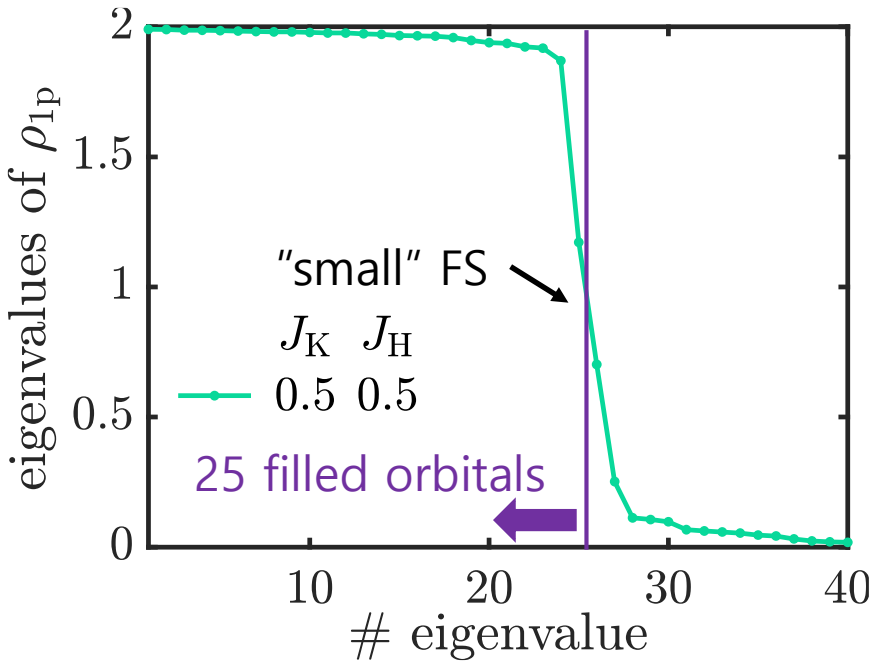
due to spin degree of freedom

Kondo

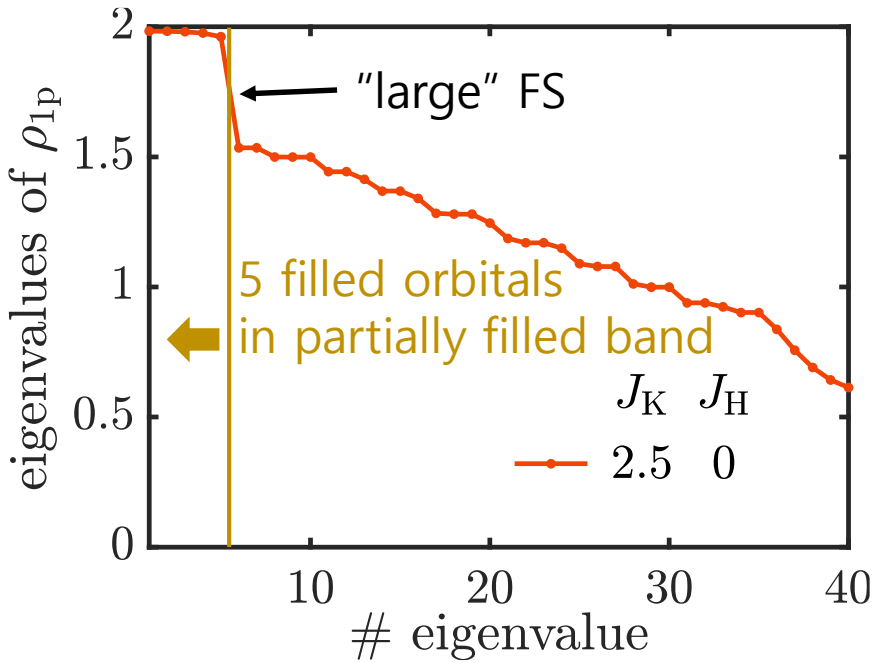
expectation: $(N + L_x \cdot L_y)/2 = 45 = 40 + 5$ filled orbitals

completely filled hybrid c-f band

partially filled hybrid c-f band



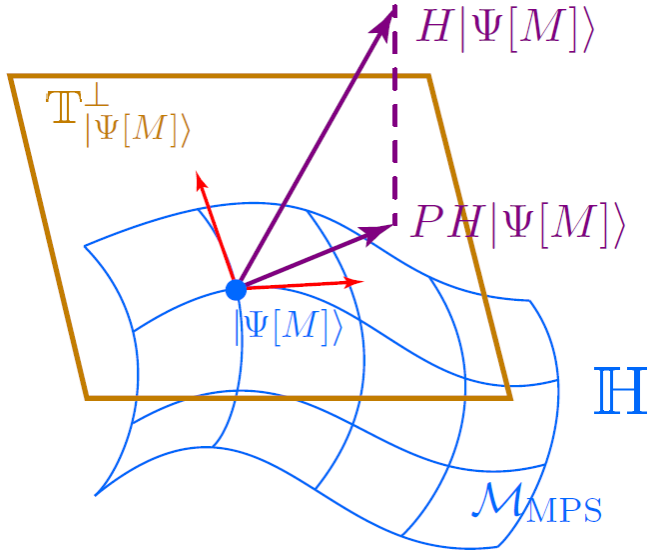
FS reconstruction captured on cylinder



One-Site TDVP

Time dependent variational principle:

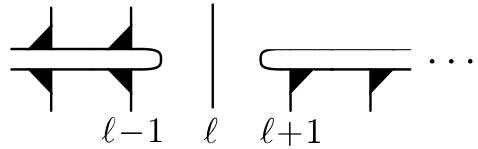
$$\frac{d|\Psi\rangle}{dt} = P_\Psi H\,|\Psi\rangle$$



Projector-splitting integrator:

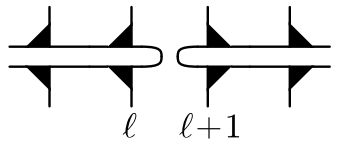
$$P_\Psi = \sum_{\ell=1}^{L} P_\ell^{(1)} - \sum_{\ell=1}^{L-1} P_\ell^{(0)}$$

$$P_i^{(1)} = P_{\ell-1}^{L} \otimes \mathbb{I}_\ell \otimes P_{\ell+1}^{R} = \cdots$$



$$\cdots$$

$$P_i^{(0)} = P_\ell^{L} \otimes P_{\ell+1}^{R} = \cdots$$



$$\cdots$$

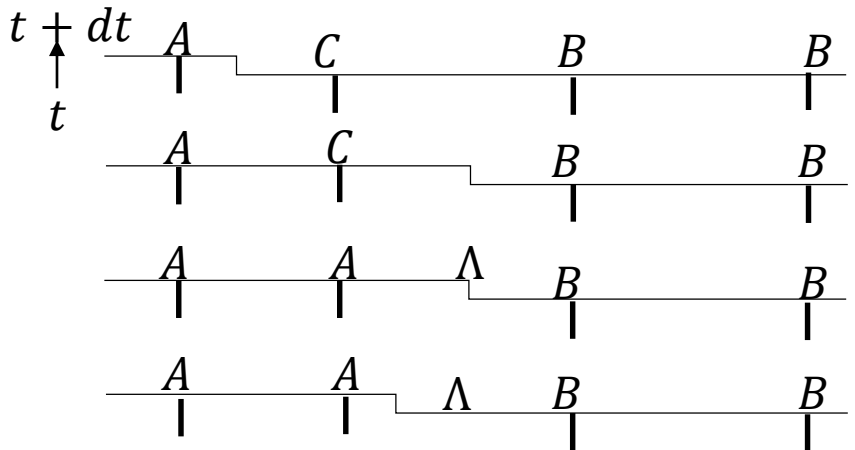
Sweeping (Lie-Trotter scheme):

$$C_\ell(t)B_{\ell+1}(t)$$

$$\xrightarrow{H_\ell^{(1)}} C_\ell(t+dt)B_{\ell+1}(t)$$

$$= A_\ell(t+dt)\Lambda_\ell(t+dt)B_{\ell+1}(t)$$

$$\xrightarrow{H_\ell^{(0)}} A_\ell(t+dt)\Lambda_\ell(t)B_{\ell+1}(t)$$



- sweeping error

  1st order

  $L_{dt} \to R_{dt} \to \ldots$

  2nd order

  $L_{dt/2} \to R_{dt/2} \to \ldots$

  3rd order

  $L_{dt/4} \to R_{dt/2} \to L_{dt/4} \to \ldots$

- projection error $(\mathbb{I} - P_\Psi)H\,|\Psi\rangle$

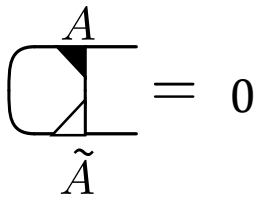
  global subspace expansion (Yang & White 2020)

  rank-adaptive robust integrator (Ceruti, Kusch, and Lubich 2021)

  controlled bond expansion (CBE)

Bond expansion:

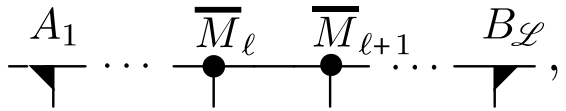
$$|\Psi\rangle = A_1 \dots A_{\ell-1} \begin{pmatrix} A_\ell & \tilde{A}_\ell \end{pmatrix} \begin{pmatrix} B_{\ell+1} \\ 0 \end{pmatrix} B_{\ell+2} \dots B_L.$$



$= 0$

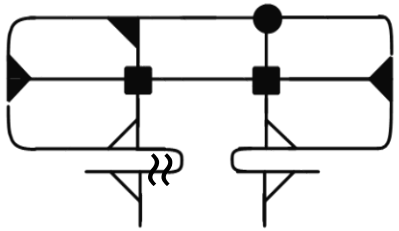
How to find the $\overline{B}$?

$$P_\ell^{(2)} \underbrace{(\mathbb{I} - P_\Psi) H |\Psi\rangle}_{\text{global projection error}} =$$



,

- Obvious choice :
  do SVD to find the right singular vector $\overline{B}$
  with non-zero singular values ($s > 10^{-6}$)



- Memory saving choice:
  pruning ($s > 10^{-2}$) prior doing SVD
  consider this for large d

Example 1: XX model — domain wall motion

$$H = \sum_{\ell} S^x_\ell S^x_{\ell+1} + S^y_\ell S^y_{\ell+1}$$

$$|\Psi_{t=0}\rangle = |\uparrow \ldots \uparrow\downarrow \ldots \downarrow\rangle$$

$L = 100, dt = 0.05,$
U(1) symmetry

- Ballistic diffusion :
  (T. Antal, etal. 1999)

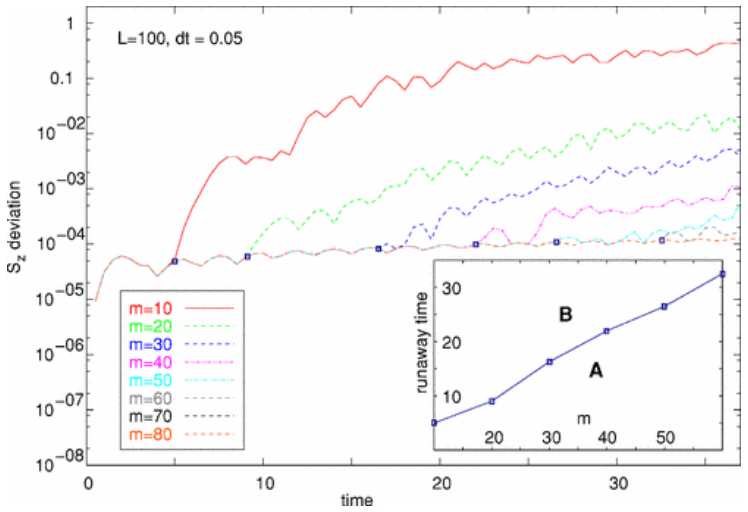
$$S^z_\ell(t) = -1/2 \sum_{n=1-\ell}^{\ell-1} J_n(t)^2$$

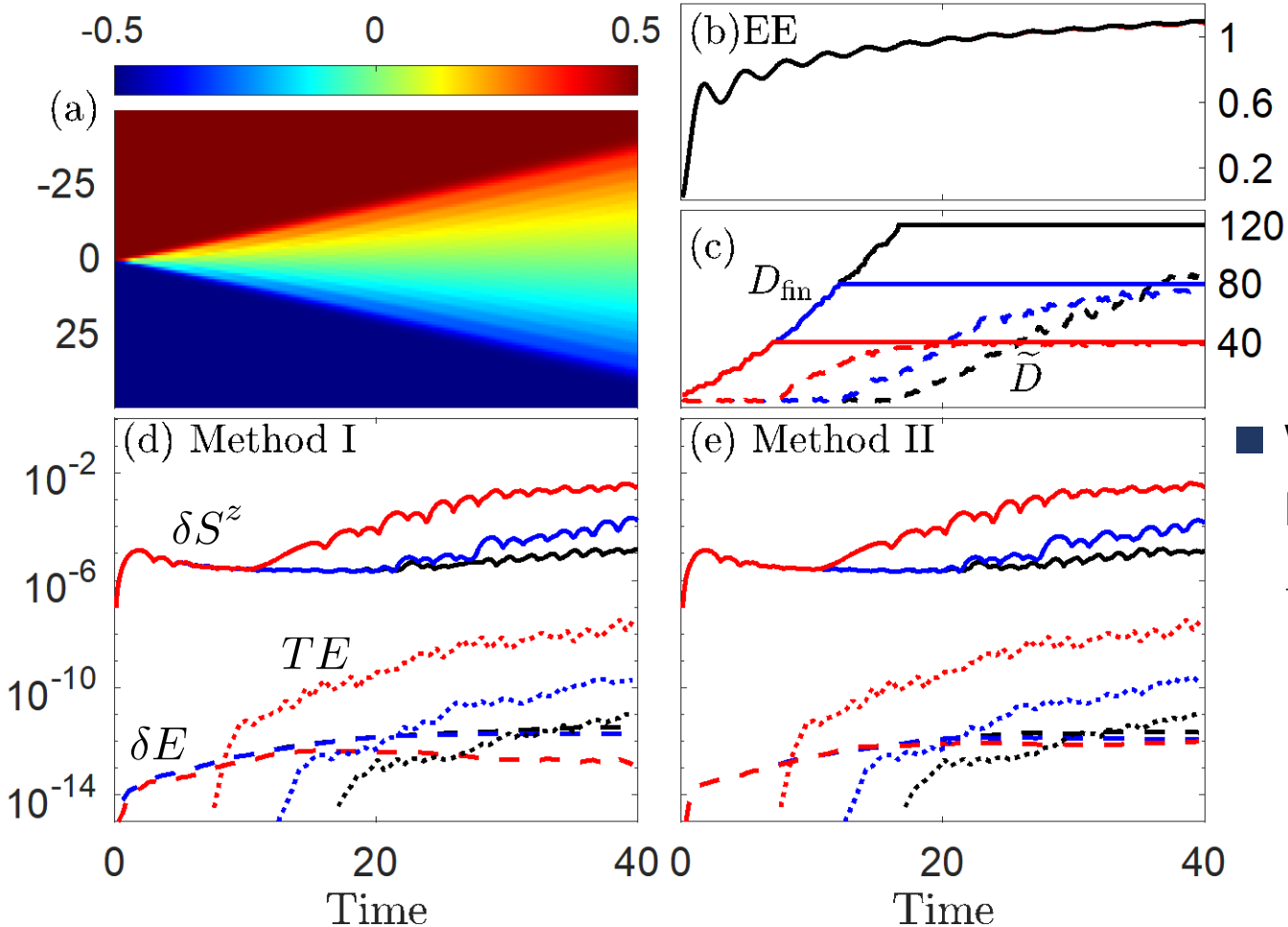
- Rank-adaptive :

$$D_{\text{fin}} = D_{\text{init}} + \widetilde{D}$$

slow increase from $D = 1$

- Finite $D_{\max}$ effect :
  accuracy ∝ tDMRG
  (D. Gobert *et al.* 2005)





- Why CBE-TDVP?
  linear increase of D
  $\widetilde{D} \le (d-1)D$

Example 2: One-axis twisting model — quantum revival

$$H = (\sum_{\ell} s_{\ell}^{z})^2/2$$

$$|\Psi_{t=0}\rangle = |\rightarrow\rightarrow \ldots \rightarrow\rangle$$

- Numerical stability?

$$S_x^{\mathrm{tot}}(t) = (L/2)\cos^{L-1}(t/2)$$

- Why CBE-TDVP?

  long-ranged interactions

  $\widetilde{D} < (d-1)D$

$L = 100, dt = 0.01,$
Z_2 symmetry

- Finite Δt errors

  large but don't accu-

  mulate

  Can we improve?

  Yes, time-adaptive C

  BE-TDVP

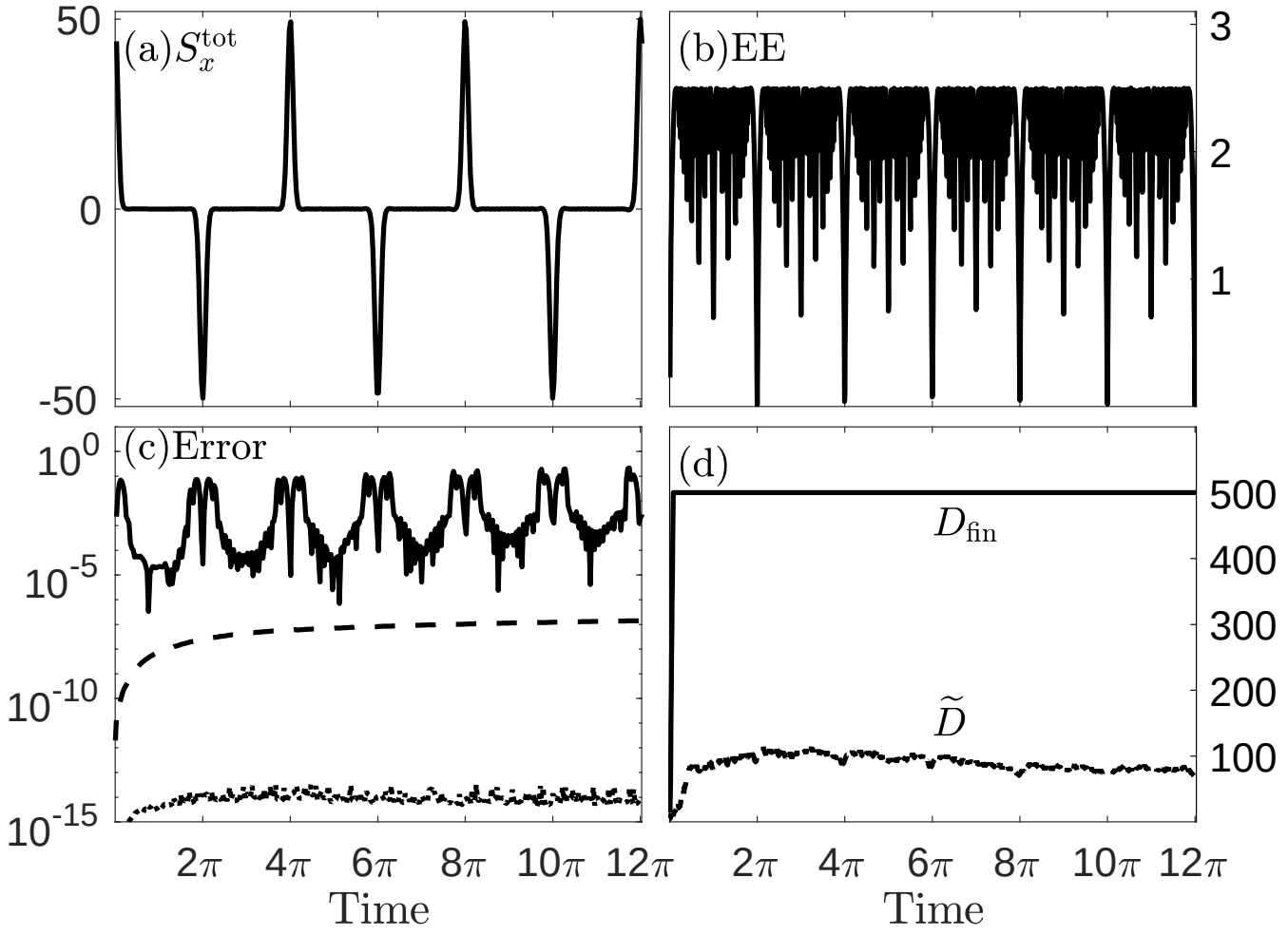
- Symplectic:

  $L_{-\Delta t} \circ R_{\Delta t} \approx \mathbb{I}$

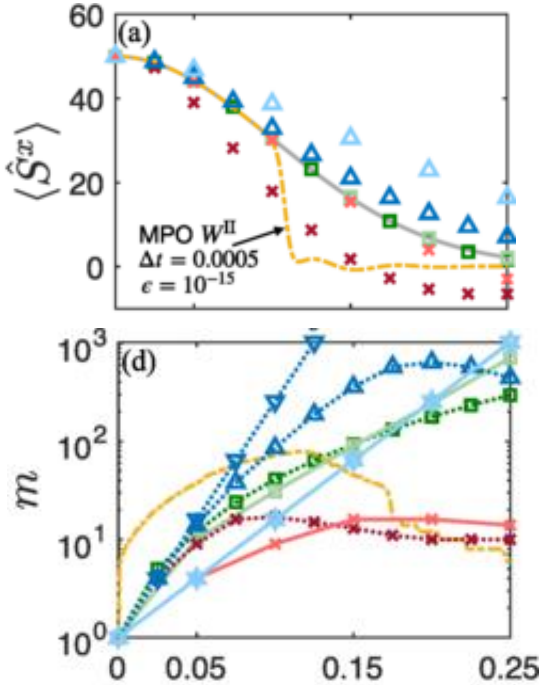
  $\delta E \approx 0$

  up to truncation error

  (G. Ceruti *etal.* 2021)



Yang and White (2020)



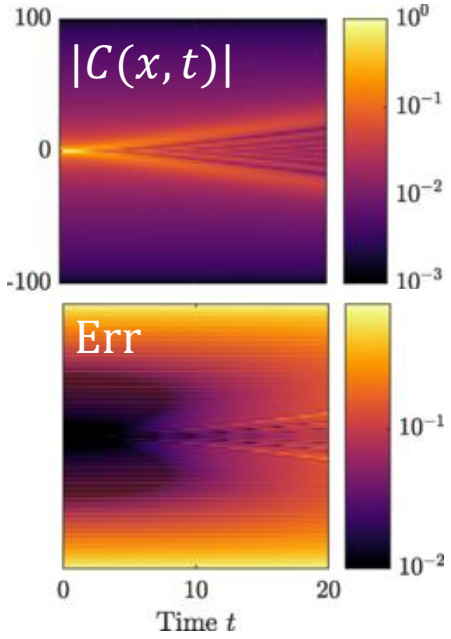
Example 3: SU(2) Haldane-Shastry model --- spectral function

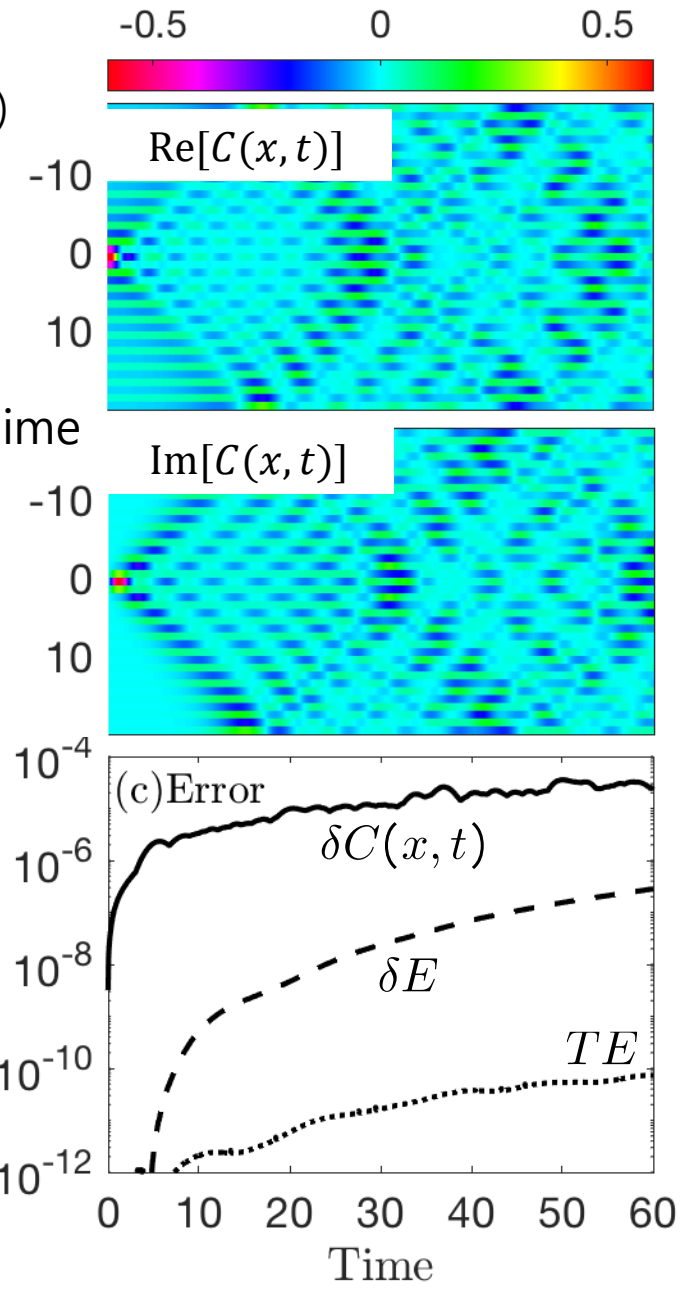
$$H = J \sum_{\ell<\ell'\le L} \frac{\pi^2 \mathbf{S}_\ell \cdot \mathbf{S}_{\ell'}}{L^2 \sin^2 \frac{\pi}{L}(\ell-\ell')} \quad \text{(PBC)}$$

$$C(x,t) = \langle \psi_0 | e^{iHt} \mathbf{S}_x e^{-iHt} \mathbf{S}_0 | \psi_0 \rangle$$

$L = 40, dt = 0.05,$
SU(2) symmetry

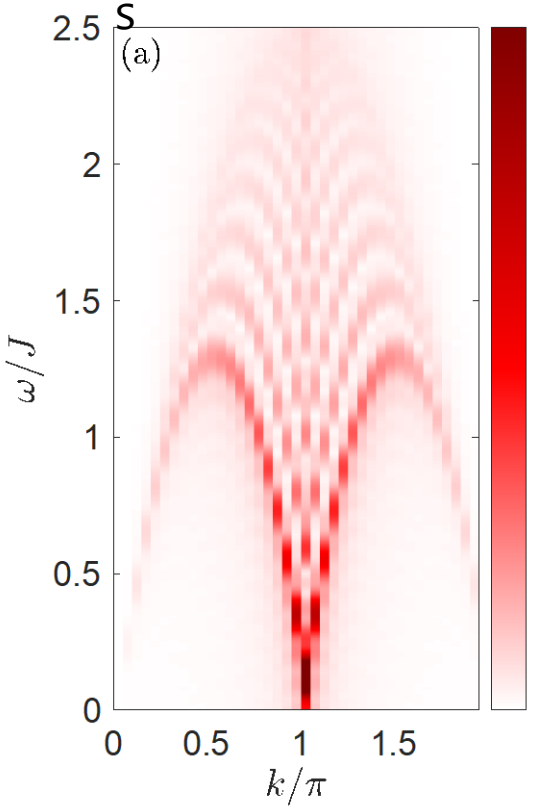
Previous works at light-cone regime
M. P. Zaletel *et al.* 2015
P. Secular *et al.* 2020

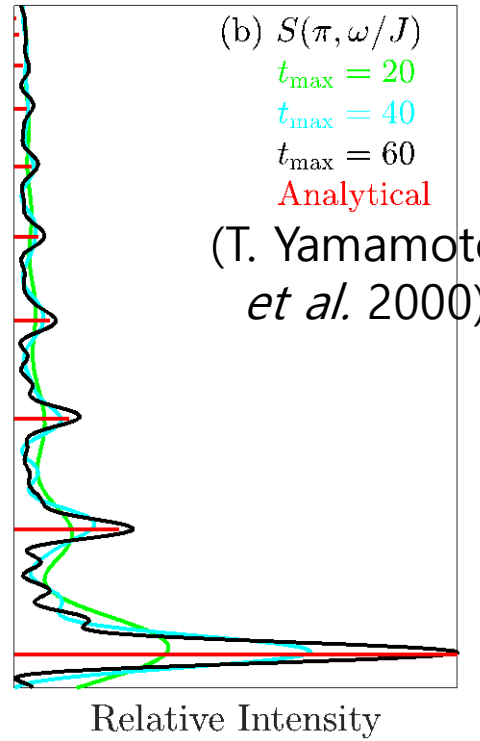




D* = 500 multiplets

No linear prediction!

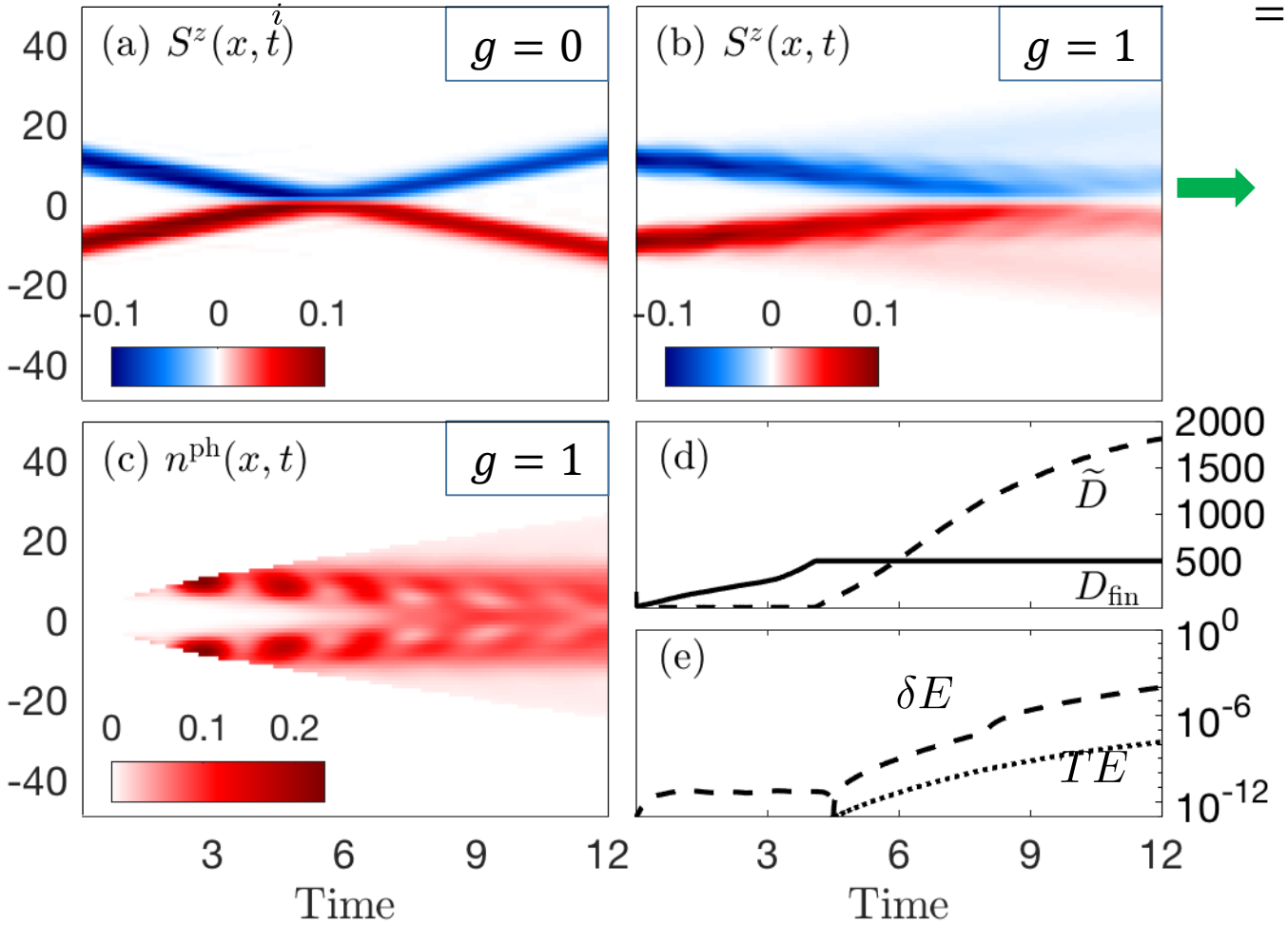




(T. Yamamoto *et al.* 2000)

Example 4: Peierls--Hubbard model --- scattering dynamics

$$H = -\sum_{i,\sigma}(c^\dagger_{i,\sigma}c_{i+1,\sigma} + h.c.) + U\sum_i n_{i\uparrow}n_{i,\downarrow} + \omega\sum_i b^\dagger_i b_i$$
$$+ g\sum_{i\sigma}(c^\dagger_{i,\sigma}c_{i+1,\sigma} + h.c.)(b^\dagger_i + b_i - b^\dagger_{i+1} - b_{i+1})$$
$$|\Psi_{\text{Gaussian}}\rangle = A\sum_i e^{(x_\ell - x_0)^2/W^2} e^{ikx_i} c^\dagger_\ell |0\rangle$$



- Non-perturbative
  $U = 10, \omega = 3, g = 1$
- Large local dim. d
  $= 36, n^{\text{ph}}_{\text{max}} = 8$

$L = 100, dt = 0.05,$
$\text{U(1)}_{\text{fermion}}$ symmetry

Elastic scattering
vs
Bi-polaron formation
(J. Sous *et al.* 2018)

$\overline{D} \ll (d-1)D$

- Speedup after reaching D_{max}?
  limit complementary space → finite $\widetilde{D}$ effect
  if $\widetilde{D} = 0$ → one-site TDVP
  speed vs. accuracy **[user's discretion]**