密度行列繰り込み群法の二次元強相関系への応用

曽田　繁利

理研計算科学研究機構量子系物質科学研究チーム

共同研究者:
新城一矢 (京大基研)
遠山貴己 (東京理科大)
今村 穣、Shixun Zhang (理研AICS)
白川知功、柚木清司 (理研)

K computer

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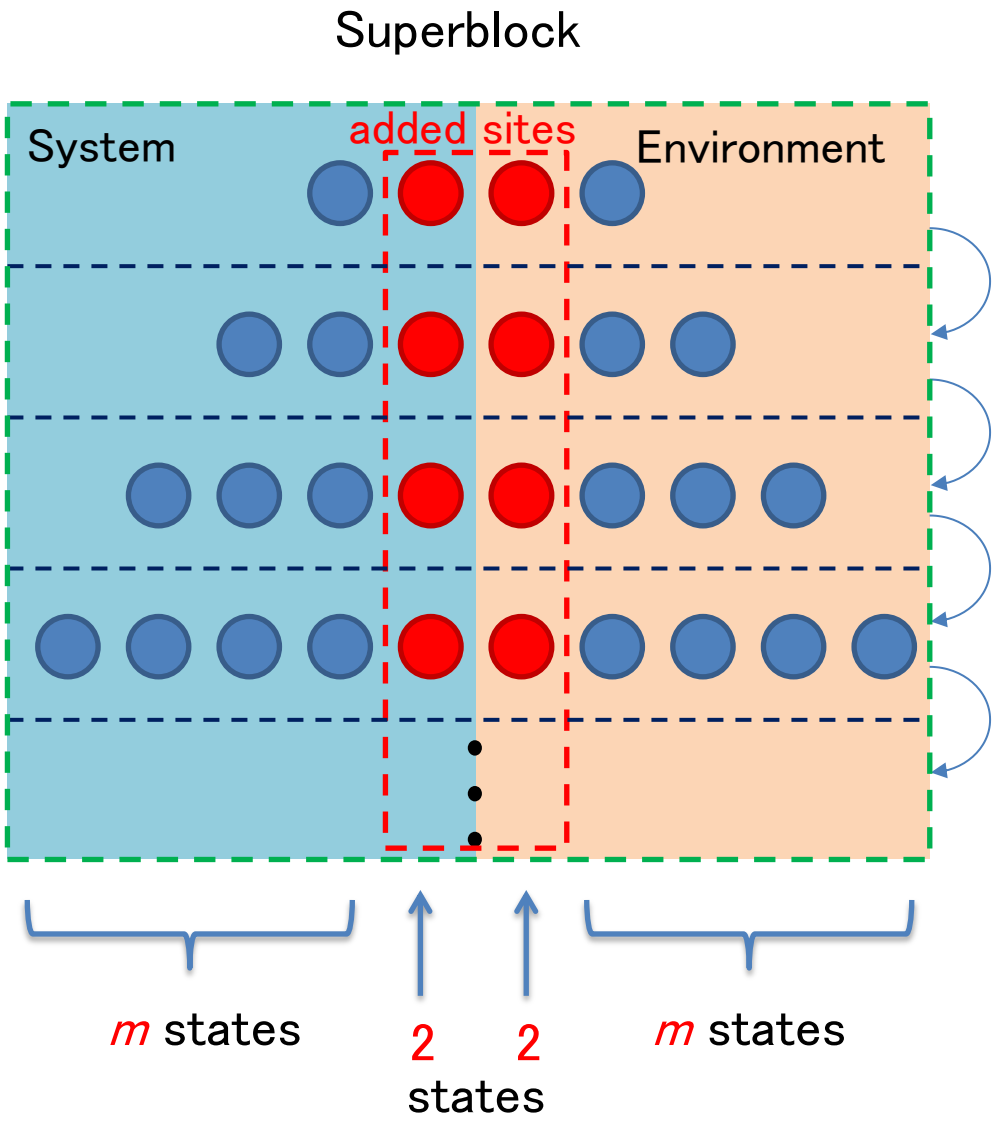
1. 密度行列繰り込み群法の二次元強相関系への応用の問題点

2. 密度行列繰り込み群法の大規模並列計算手法(並列化、メモリ節約)

3. Kernel polynomial methodを使った動的、有限温度、時間依存密度行列繰り込み群法の二次元系への応用について

4. まとめ

DMRG method (1)



- DMRG algorithm

1. Calculate the ground state of superblock

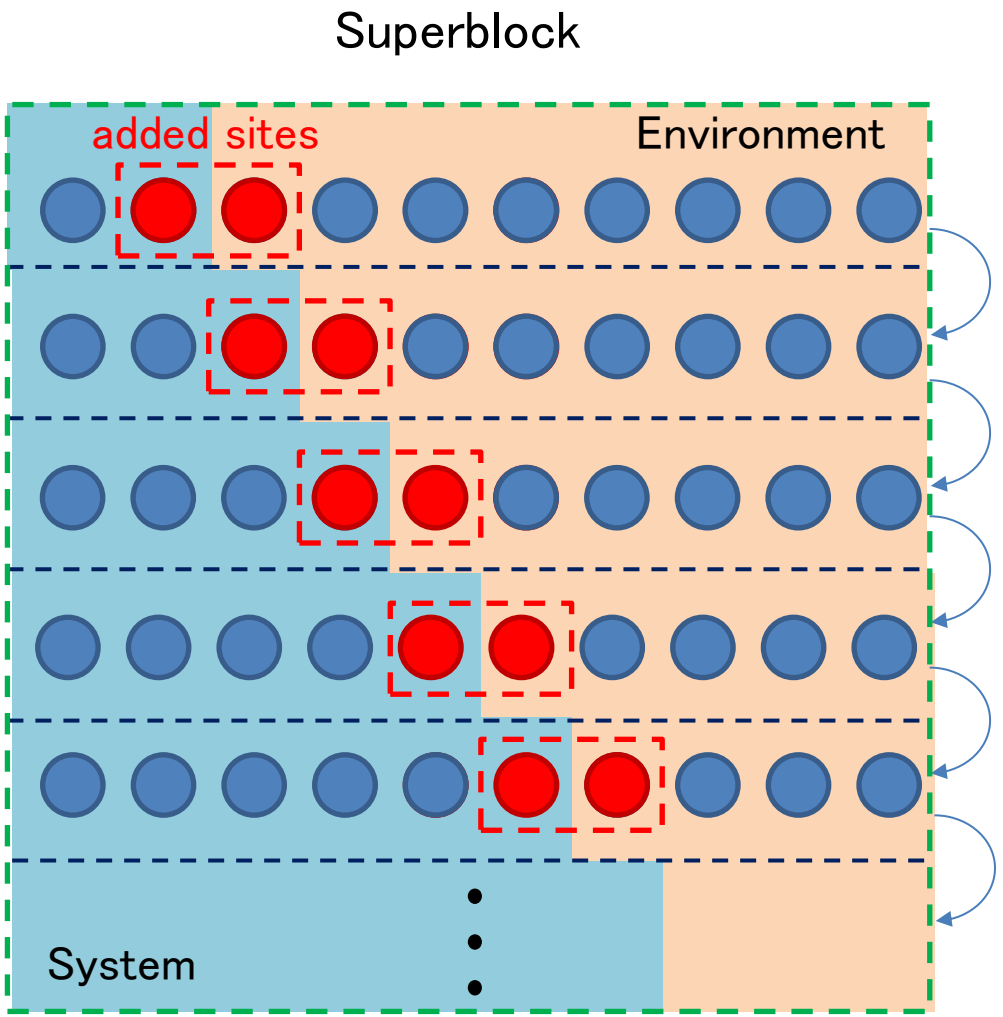
2. Make the reduced density matrix

3. Diagonalize the density matrix using Lanczos et al.

4. Keep only *m* basis states to describe the system

5. Go back to 1 until the system size reaches to *N*

DMRG method (2)



- DMRG algorithm

1. Calculate the ground state of superblock

2. Make the reduced density matrix

3. Diagonalize the density matrix using Lanczos et al.

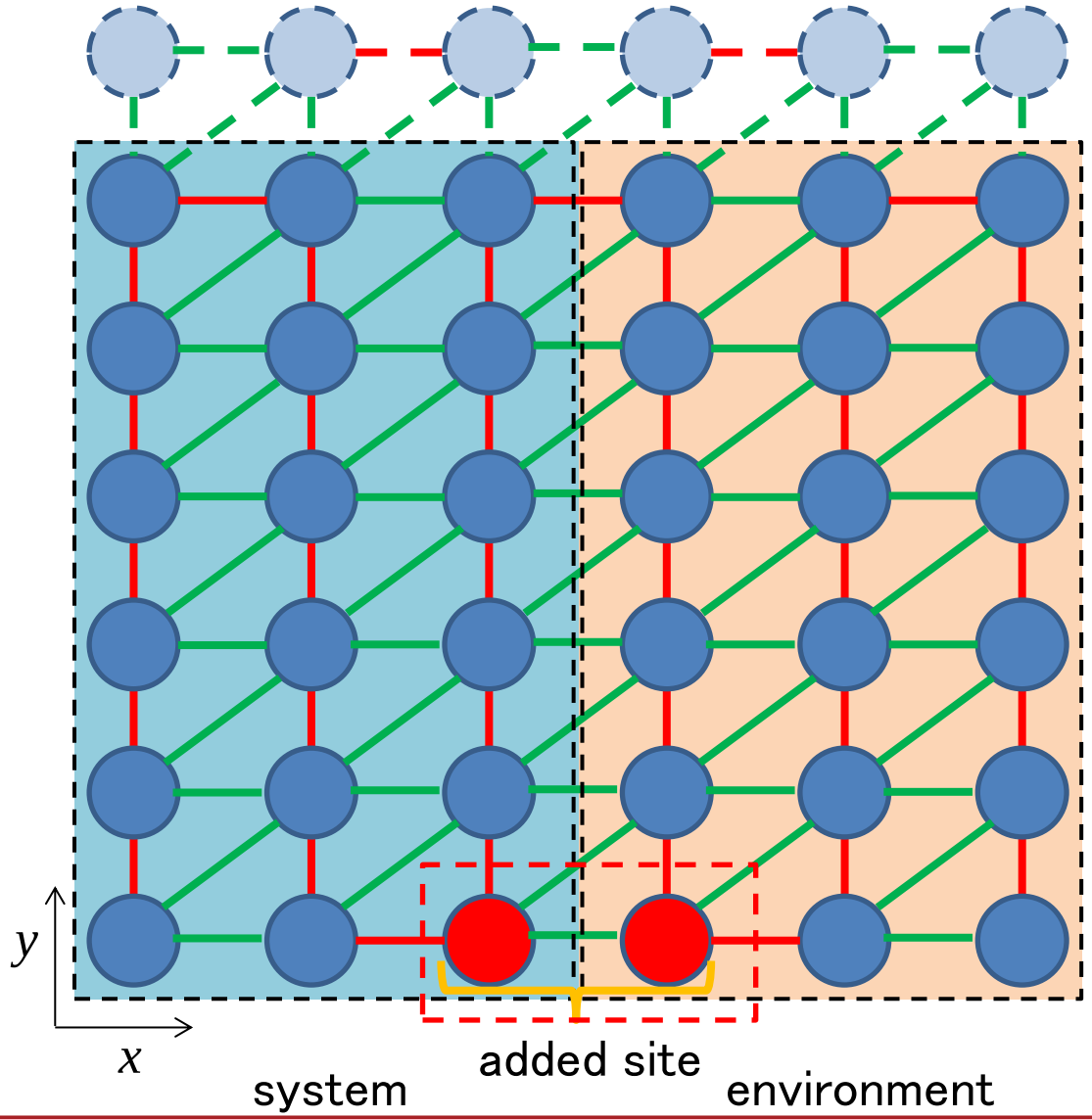
4. Keep only *m* basis states to describe the system

5. Go back to 1 until the convergence is achieved

DMRG procedure is suitable for 1D systems

DMRG in 2-D

DMRG method can be applied to 2-D systems



DMRG

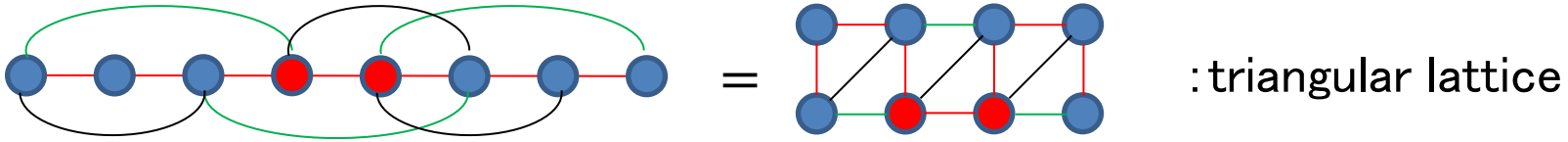
: 1D system

: long-range interactions

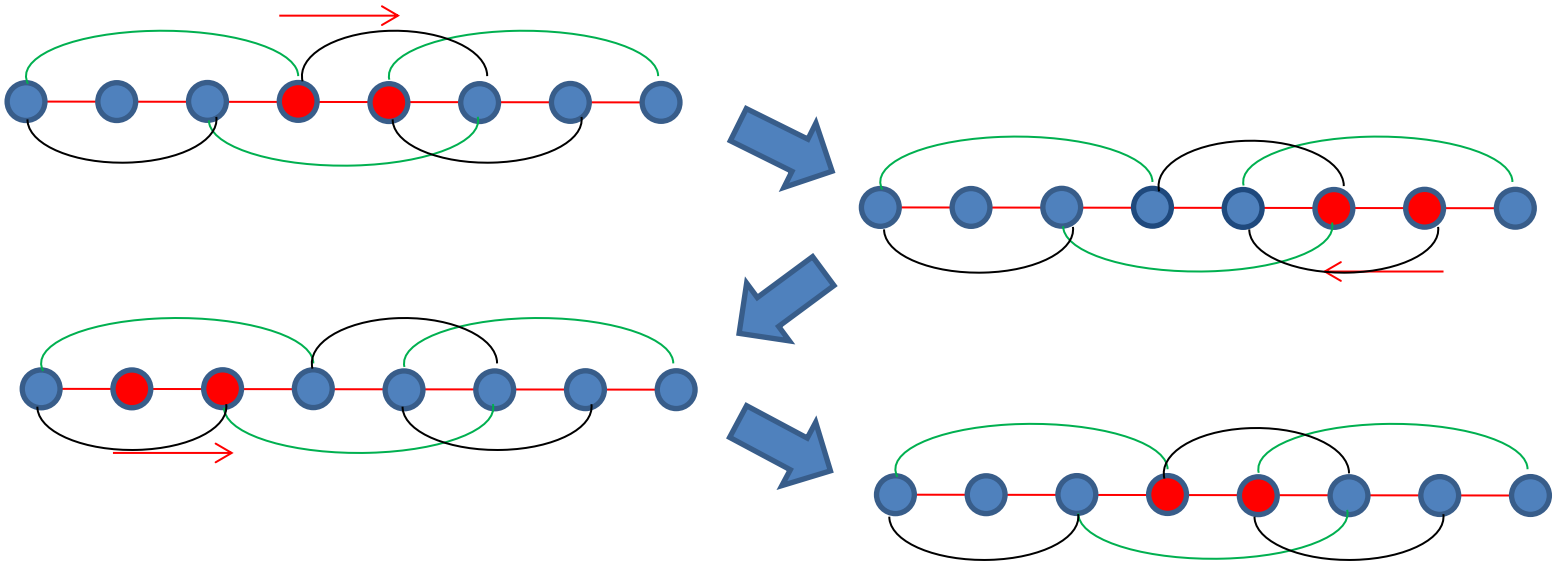
Introducing long-range interactions to an 1D system.

DMRG in 2-D

- Sweeping process



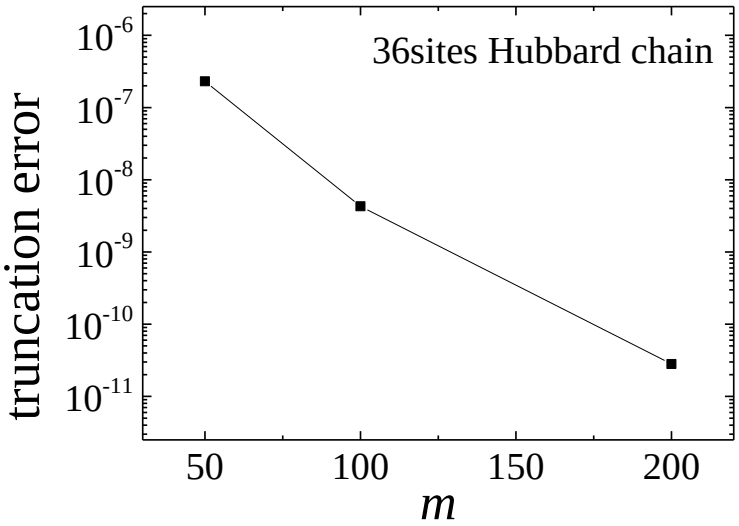
added sites (described by complete basis set)

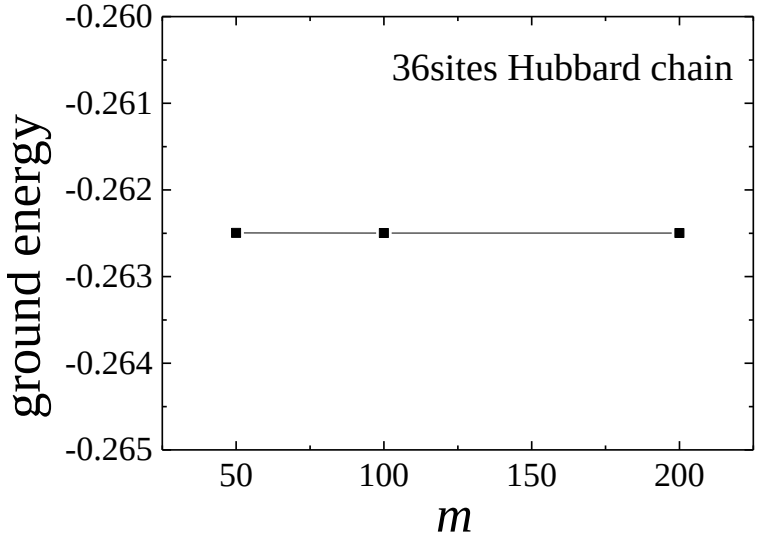


However, 2D DMRG method requires large *m* calculation.

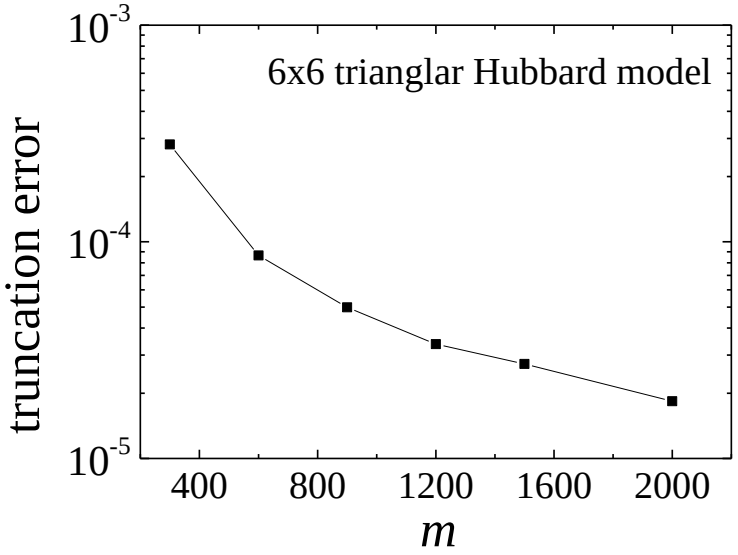
Why we need large *m* for 2-D ?

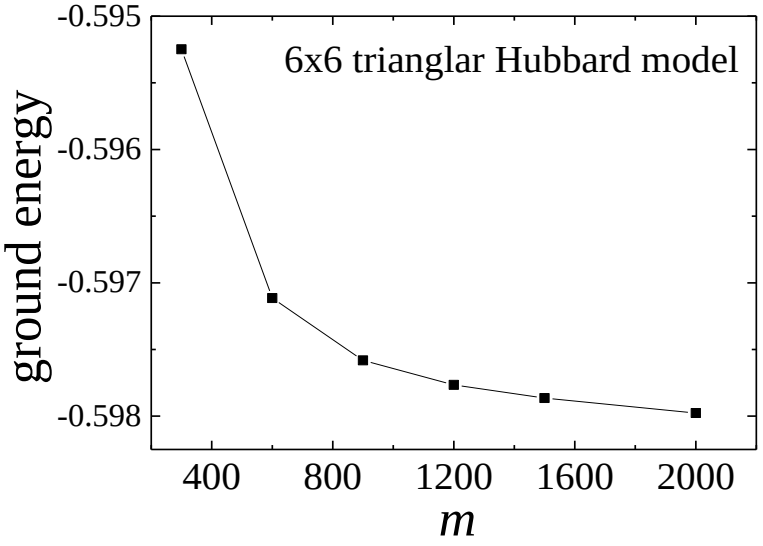
❖ 1D system (Hubbard model)





❖ 2D system (triangular Hubbard model)

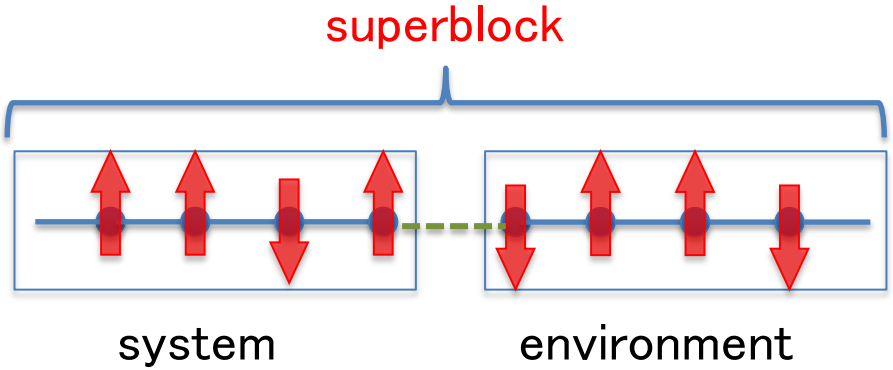




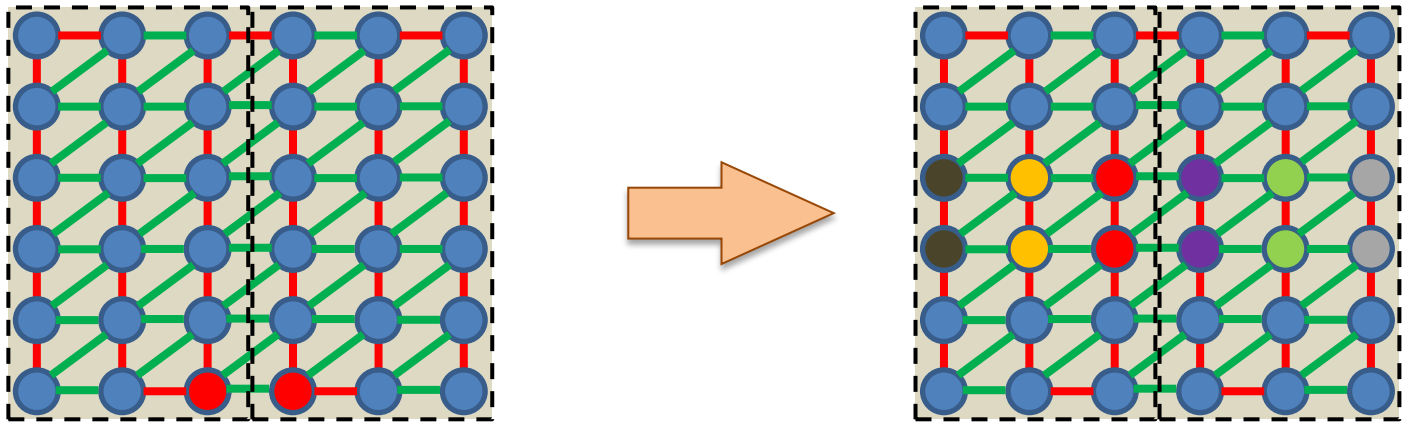
密度行列繰り込み群法の大規模並列化

- Parallelization of matrix・vector product in the ground state calculation of the superblock

$$|\Psi^{\mathrm{SB}}\rangle = \sum_{ij} \psi_{ij}^{\mathrm{SB}} |i^{(\mathrm{sys})}\rangle |j^{(\mathrm{env})}\rangle$$



- real-space parallelization for finite algorithm of DMRG



Ground state calculation

- matrix・vector product

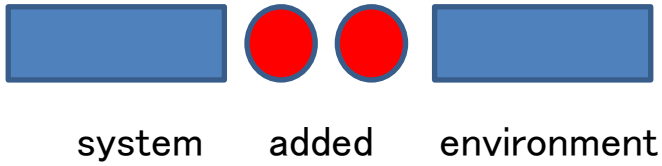
$$\mathbf{H}\cdot\mathbf{v} \rightarrow \mathbf{H}_{sys}\cdot\mathbf{v}_{sys}\ ,\ \mathbf{H}_{env}\cdot\mathbf{v}_{env}\ ,\ \mathbf{H}_{add}\cdot\mathbf{v}_{add}$$

$$\mathbf{v}\ \text{(vector)} \rightarrow \mathbf{v}_{sys}, \mathbf{v}_{env}, \mathbf{v}_{add}\ \text{(matrix)}$$

added sites + environment block

$$\mathbf{v}_{sys} = \begin{pmatrix} v_{1,1} & \cdots & \cdots & v_{1,am} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ v_{am,1} & \cdots & \cdots & v_{am,am} \end{pmatrix}$$

system block

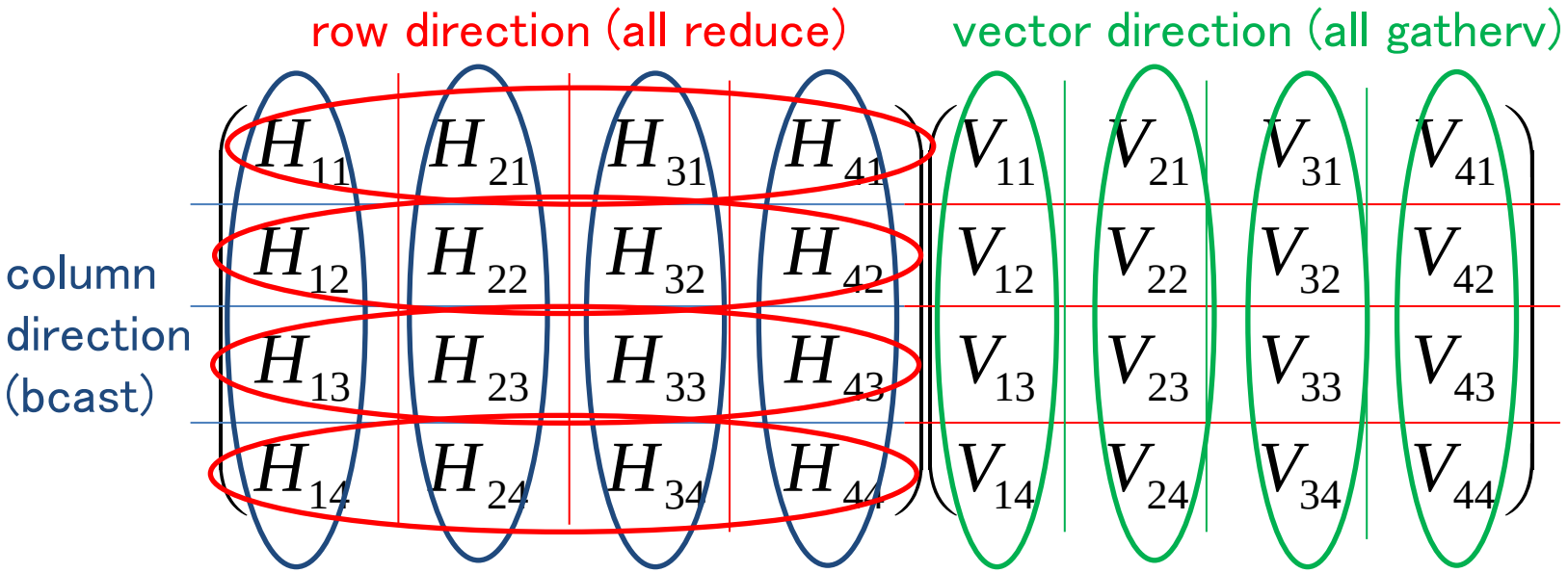


matrix ・vector product

matrix・matrix product

MPI communications

- matrix･matrix product （matrix･vector product)

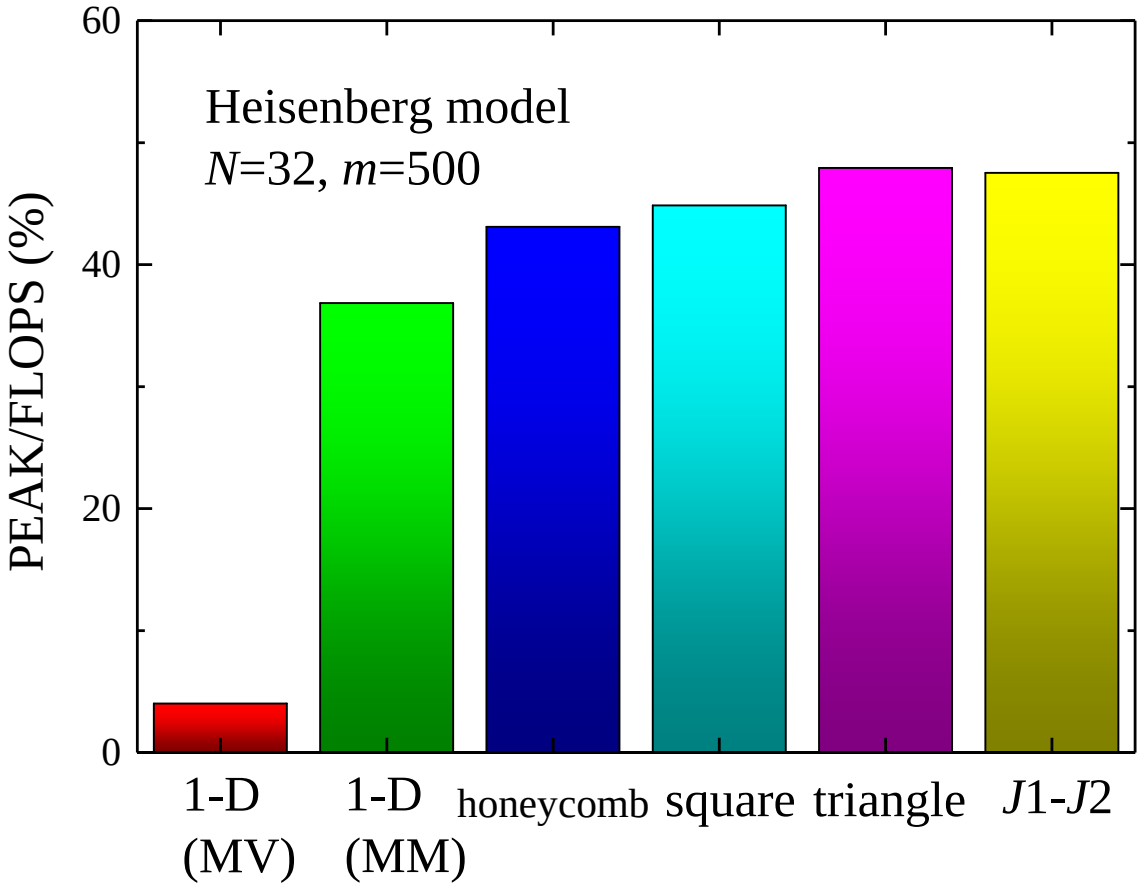


all to all communication → separated communication

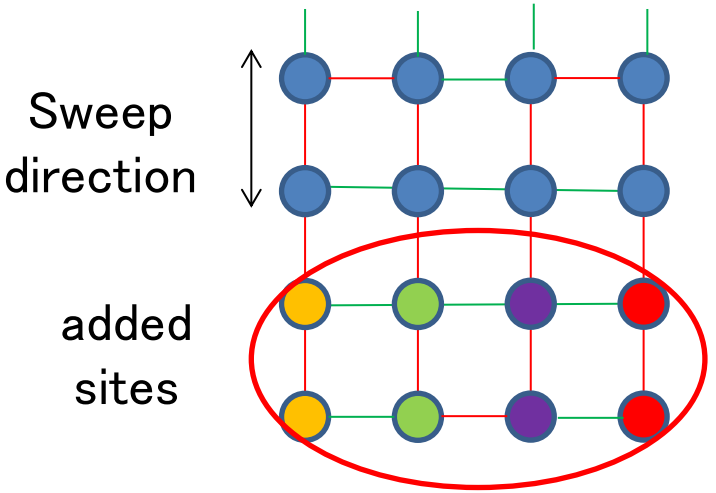
communication as local as possible

Performance

K computer

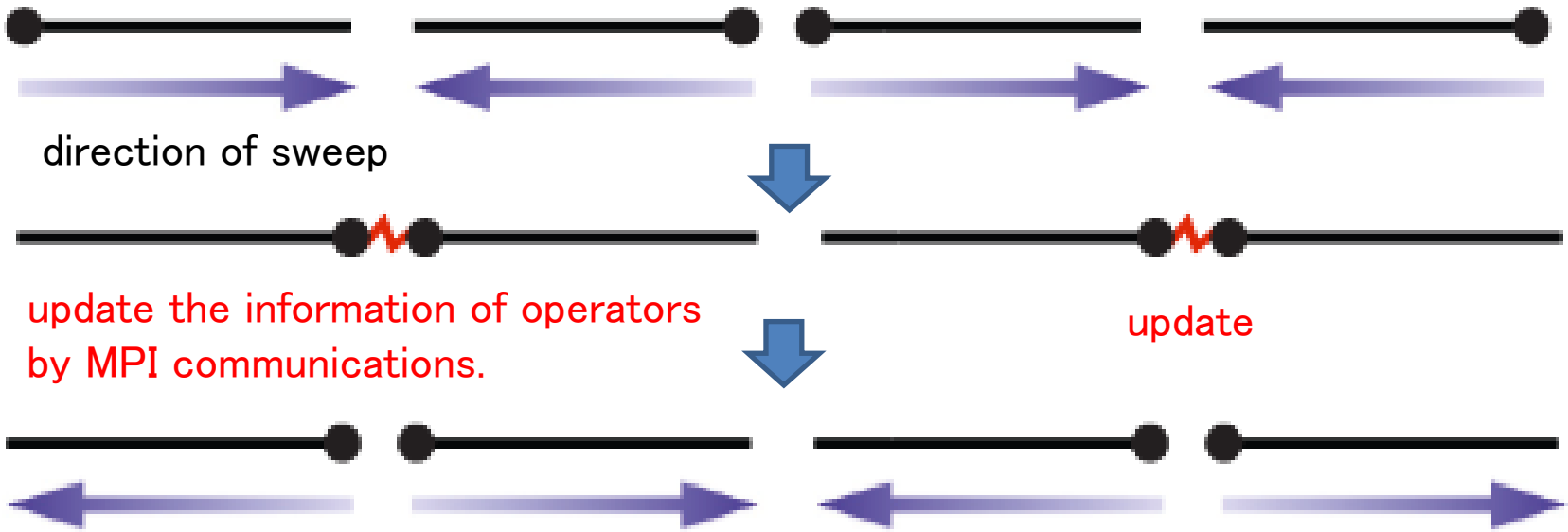


Real-space parallelization



E. M. Stoudenmire & S. R. White, PRB **87**, 155137 (2013)

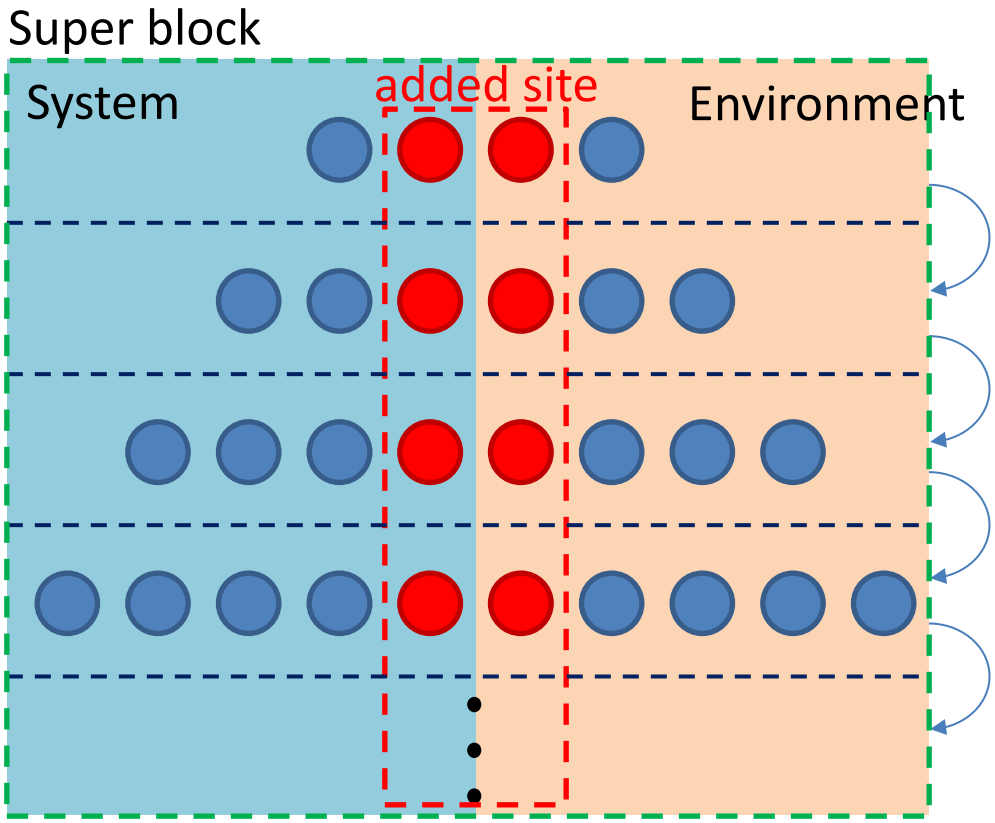
Many "*warms*" of a couple of added sites optimize simultaneously the separate parts of the system.



Skipping target state calculation

Most of elapsed time is for the ground state calculation for the superblock

Skipping the ground state calculation in the finite algorithm to expand the system size



- DMRG algorithm

1. Calculate the ground state of superblock

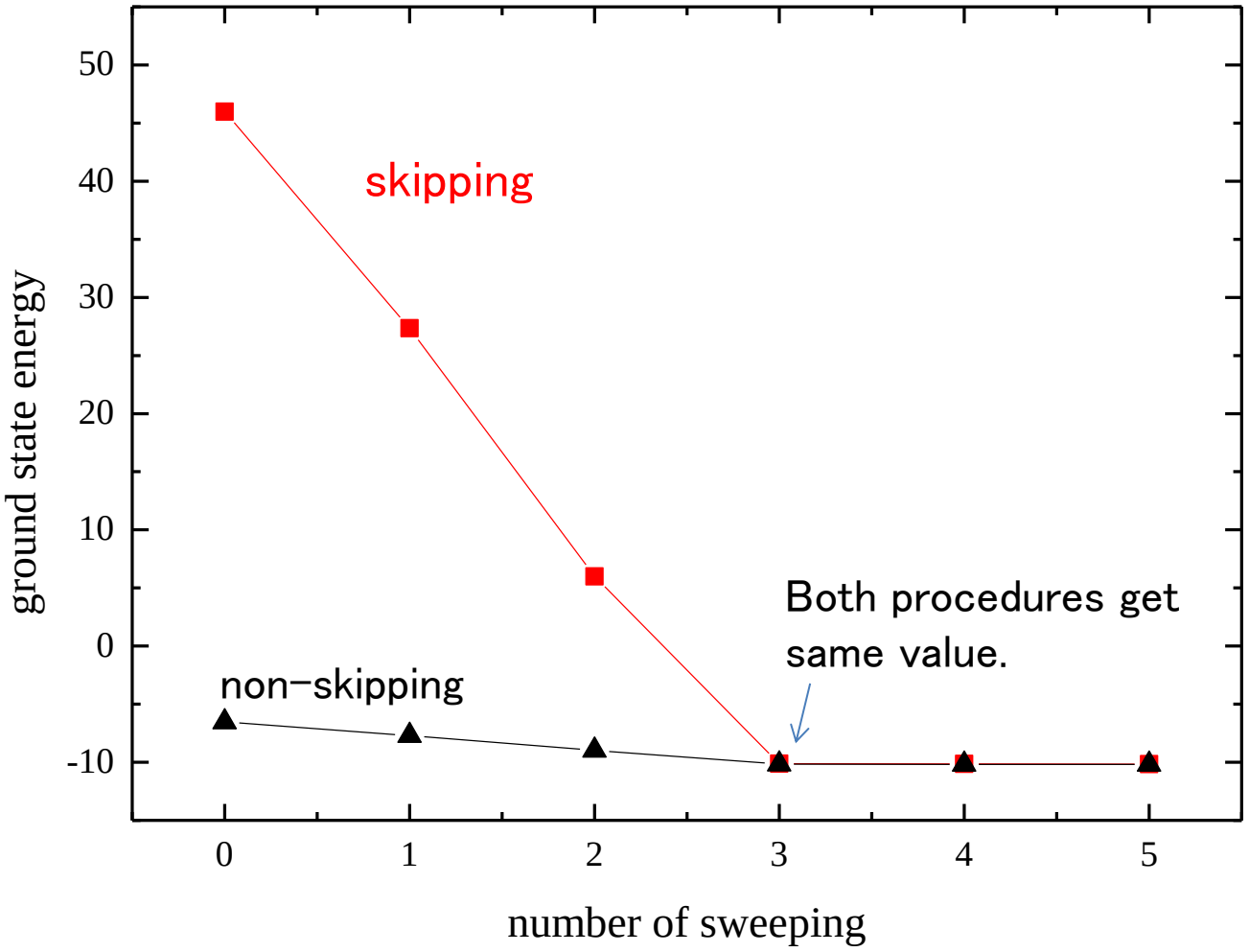
2. Make the reduced density matrix

3. Diagonalize the density matrix using Lanczos et al.

4. Keep only *m* basis states to describe the sysem

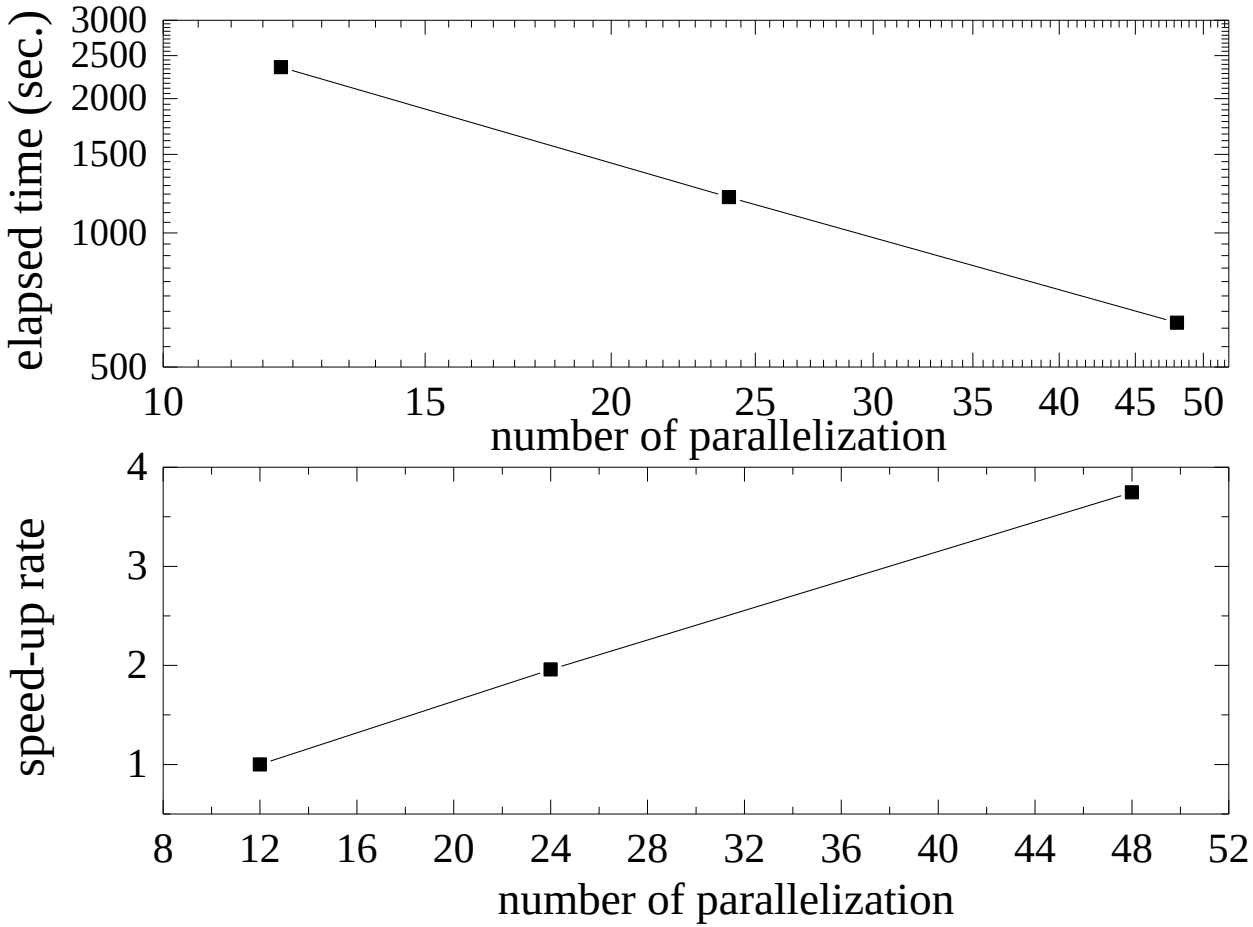
energy convergence

- triangular Hubbard model (3 x 8)



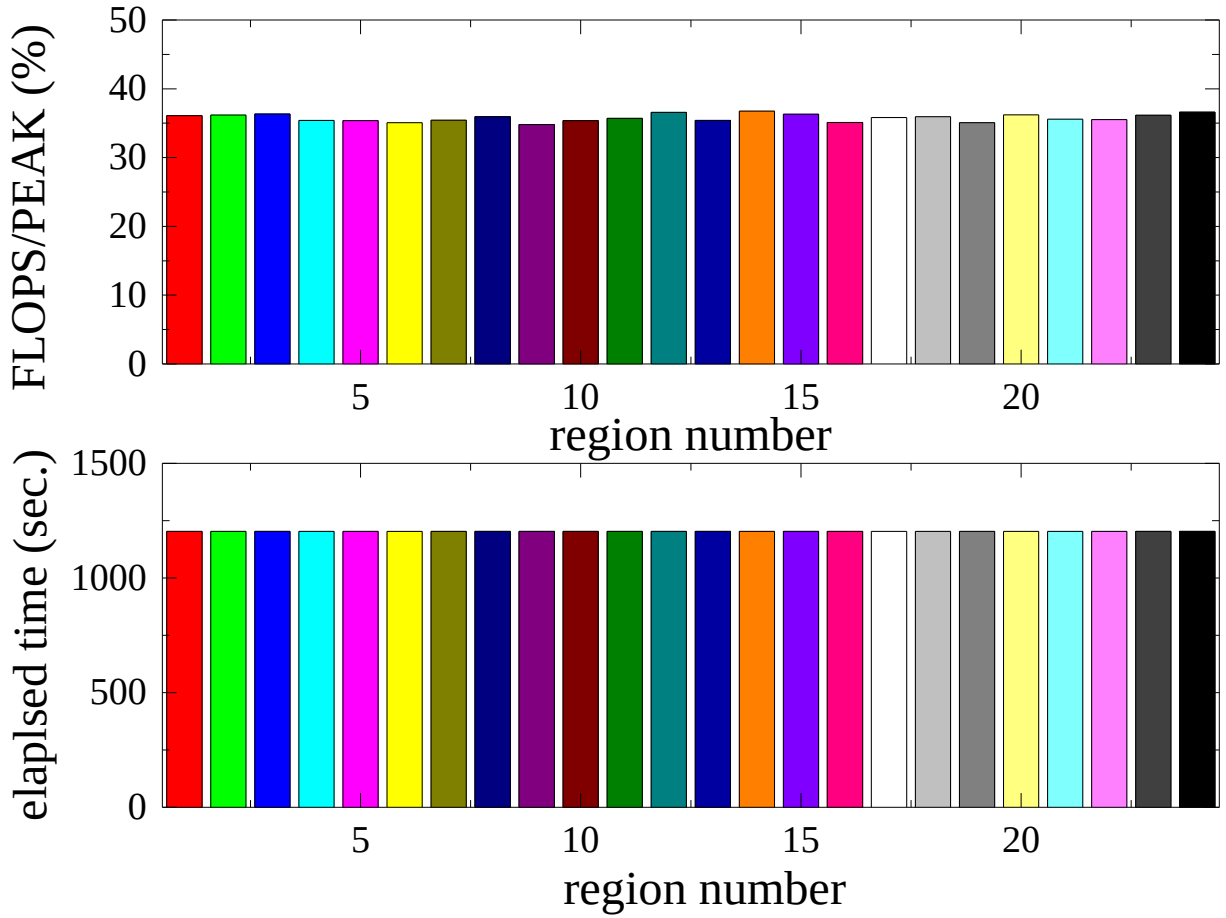
Performance

K computer, 3 × 8 triangular Hubbard model



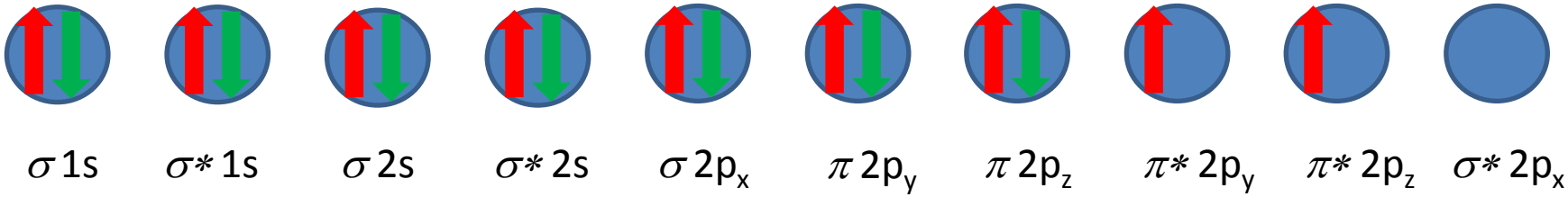
Performance

K computer, 3 × 8 triangular Hubbard model



All most perfect road balance

量子化学計算への応用



Hamiltonian: $$H = \sum_{p,q} h_{p,q} c_p^\dagger c_q + \frac{1}{2} \sum_{p,q,r,s} (pq|rs) c_p^\dagger c_r^\dagger c_s c_q$$

parameters

$$H|\psi\rangle = E|\psi\rangle$$

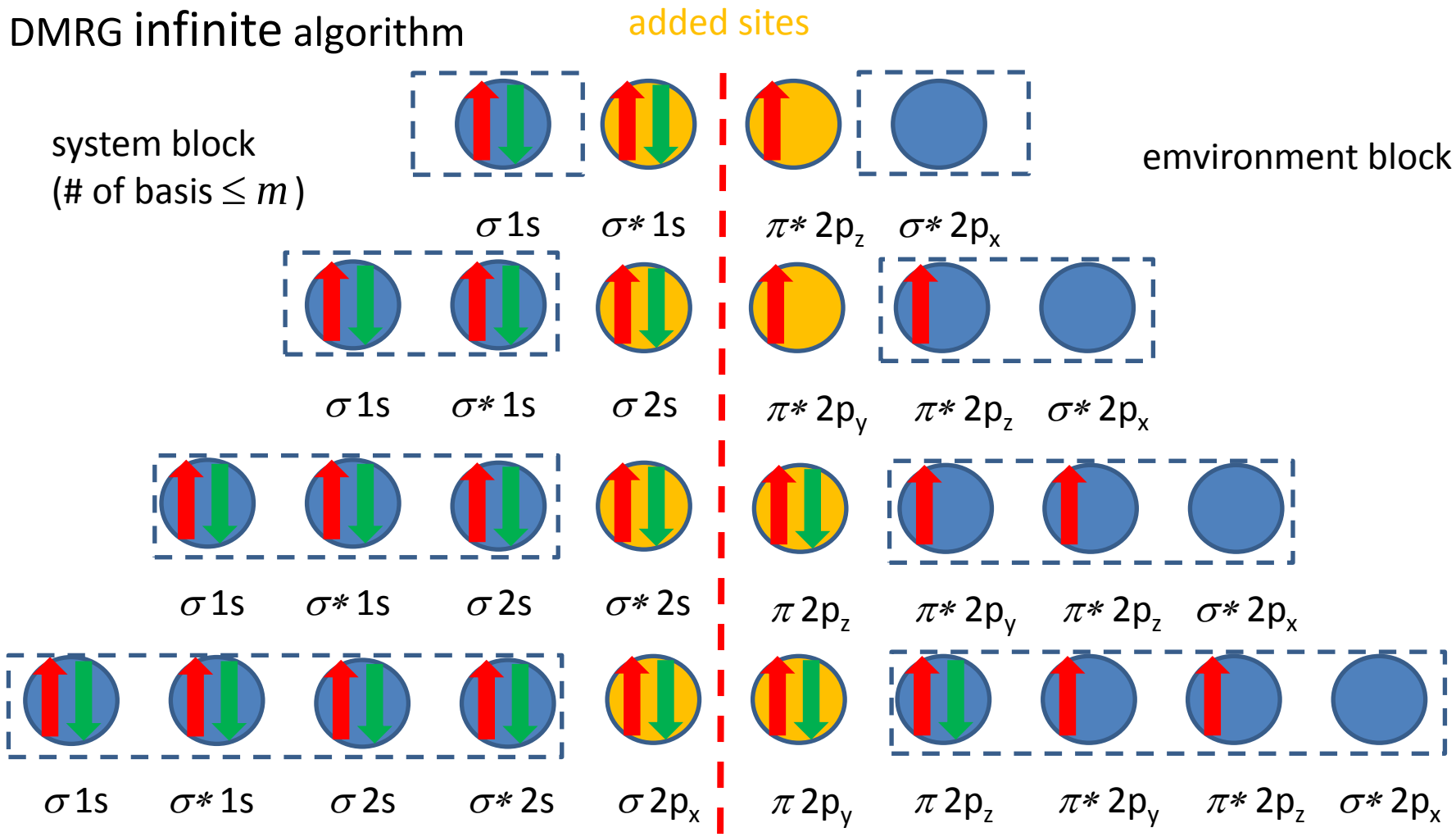
NTchem
(Nakajima team)

parameters of Hamiltonian

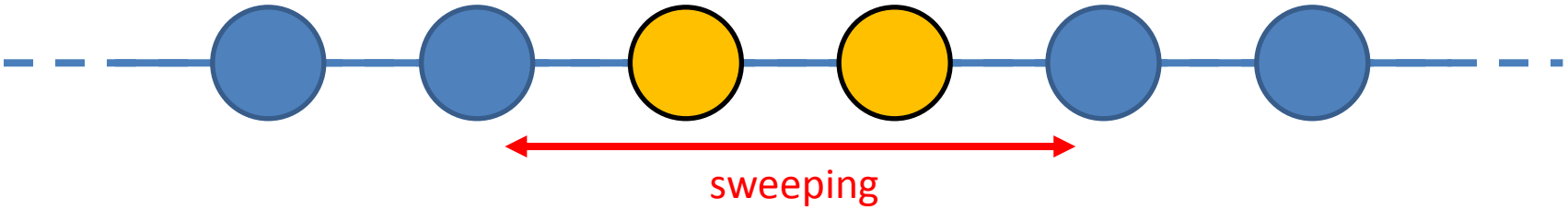
energy, density matrix ・・・

DMRG
(Yunoki team)

1. DMRG **infinite** algorithm



2. DMRG **finite** algorithm



Problem

How to preserve $c_p^\dagger c_r^\dagger c_s c_q$? (memory or HDD usage)

DMRG steps:

1. calculating target state
2. making reduced density matrix
3. diagonalization of reduced density matrix
4. transformation operators

We need to preserve all of operators during DMRG calculation.

For example, $c_p^\dagger c_q$

We cannot treat $c_p^\dagger$ and c_q independently in DMRG method.

(DRMG method cannot guarantee the accuracy $c_p^\dagger c_q$.)

Preservation of transformation matrix

(transformation matrix: eigenstates of reduced density matrix)

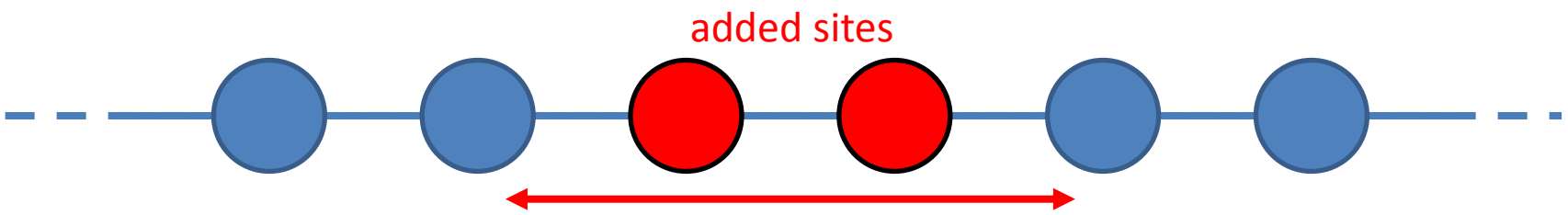
In the case of preserving operators,

$$(\text{memory usage}) \propto (\#\ \text{of sites})^5$$

$$\#\ \text{of indexes}\ (C_p^\dagger C_r^\dagger C_s C_q) + \#\ \text{of DMRG steps}$$

In the case of preserving transformation matrix,

$$(\text{memory usage}) \propto (\#\ \text{of sites})$$

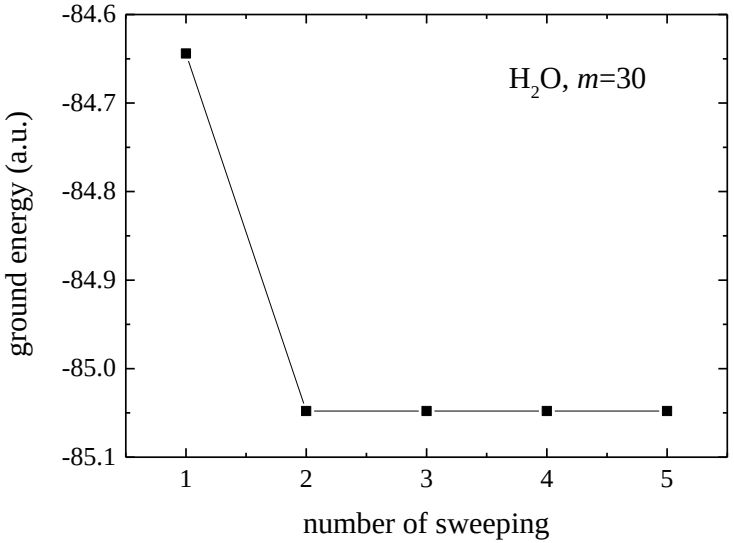


テスト計算(水分子)

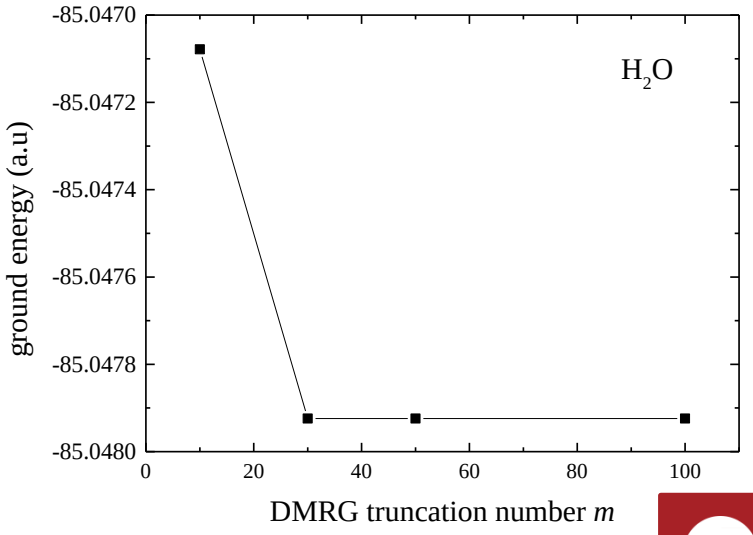
H_2O

	Ground energy(a.u.)
Exact diagonalization	-85.047924
DMRG(*m*=10)	-85.0470785
DMRG(*m*=30)	-85.0479241
DMRG(*m*=50)	-85.0479241
DMRG(*m*=100)	-85.0479241

- *m* dependence



- sweep dependence



直交多項式展開法によるDMRG

二次元強相関系に対する動的DMRG、有限温度DMRG、時間依存DMRG

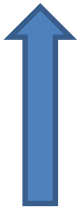
- 動的密度行列繰り込み群法

Arbitrary dynamical correlation function at zero temperature,

$$\chi_A(\omega) \equiv \frac{1}{2\pi N_s} \mathrm{Im} \langle 0 | \hat{A} \frac{1}{\omega - \hat{H} + \varepsilon_0 - i\gamma} \hat{A} | 0 \rangle$$

($\hat{A}$: arbitrary operator)

$$\hat{H}|0\rangle = \varepsilon_0 |0\rangle$$



In low-dimensional systems,

Dynamical DMRG method

Target states

$$|0\rangle, \quad \hat{A}|0\rangle, \quad \frac{1}{\omega - \hat{H} + \varepsilon_0 - i\gamma} \hat{A}|0\rangle$$

Multi target procedure

Kernel Polynomial Method (KPM)

$$\delta(x'-x) = w(x)\sum_{l=0}^{\infty} w_l^{-1}\varphi_l(x')\varphi_l(x)$$

$$G(\omega - i\gamma) \equiv \frac{1}{\omega - \hat{H} - i\gamma} = \sum_{l=0}^{\infty} w_l^{-1}\tilde{\varphi}_l(\omega - i\gamma)\varphi_l(\hat{H})$$

$$\tilde{\varphi}_l(\omega - i\gamma) \equiv \int_a^b dx \frac{w(x)}{\omega - x - i\gamma}\varphi_l(x)$$

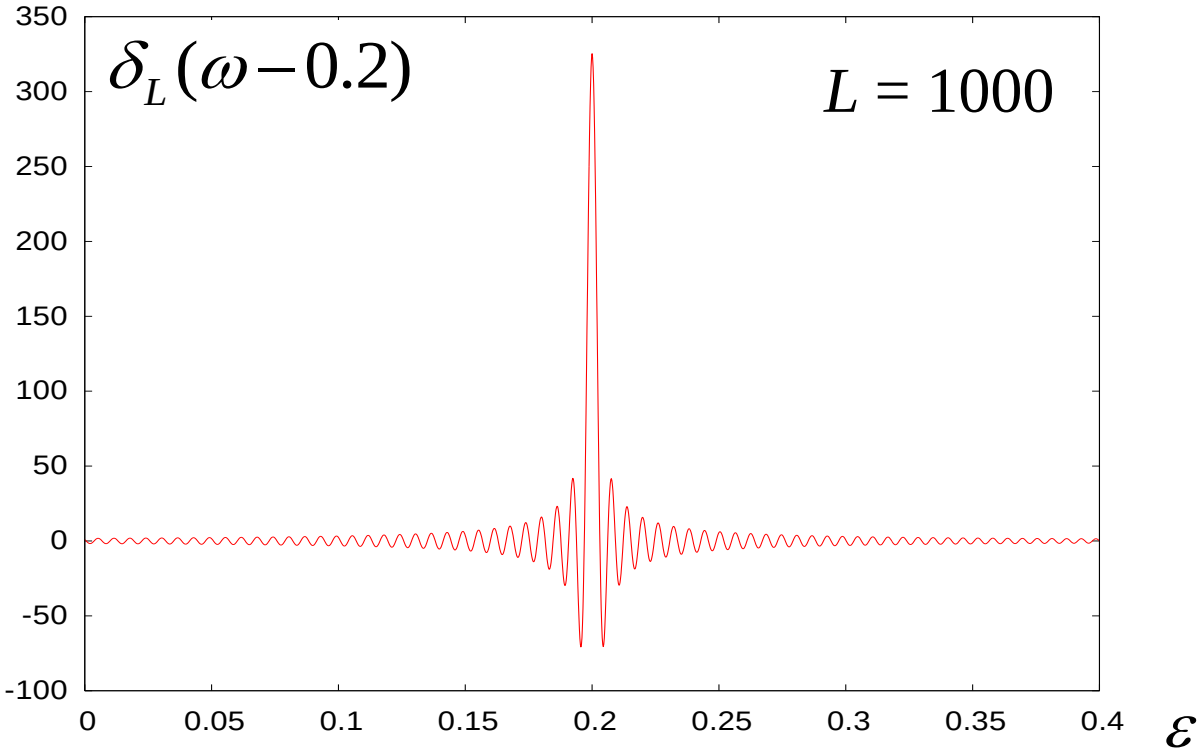
Legendre : $\tilde{P}_l(\omega \pm i\gamma) = 2Q_l(\omega) \mp i\pi P_l(\omega)$

$$\Rightarrow \quad \frac{1}{\omega - \hat{H} - i\gamma} = \sum_{l=0}^{\infty} w_l^{-1}\{2Q_l(\omega) + iP_l(\omega)\}P_l(\hat{H})$$

Kernel function

$$D(\omega)=\sum_{\mu}\delta(\omega-\varepsilon_{\mu}) \quad \text{(DOS)}$$

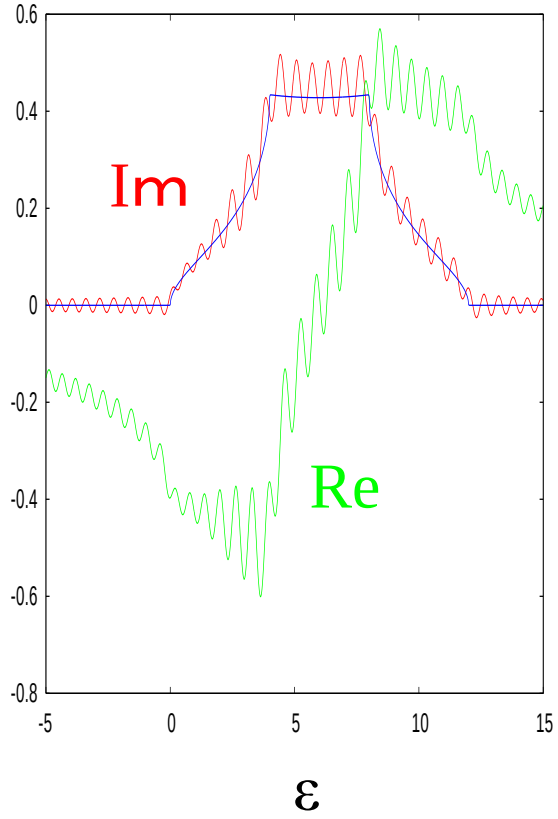
$$\delta_L(\omega-\varepsilon_{\mu})\equiv\sum_{l=0}^{L} w_l^{-1}P_l(\omega)P_l(\varepsilon_{\mu})$$



Ex.: Simple cubic lattice dynamics (19^3atoms)

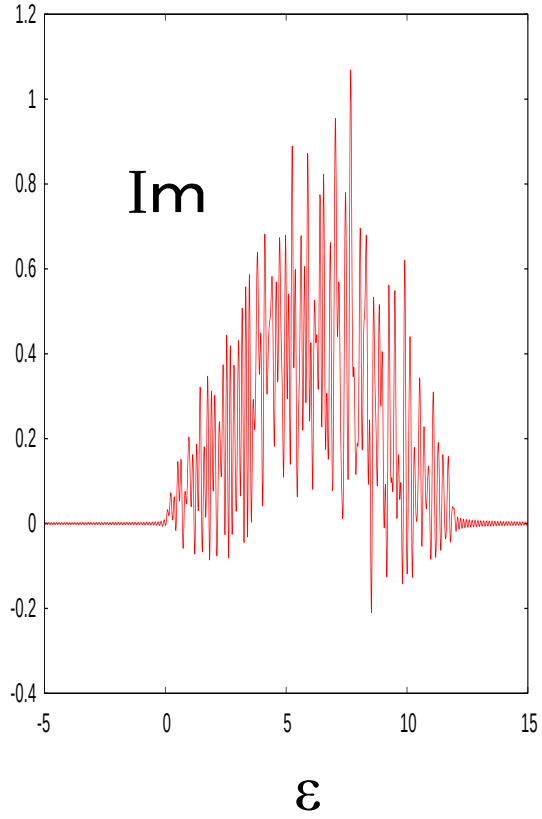
- N=200

$G_d(\varepsilon - i\delta)$



- N=1000

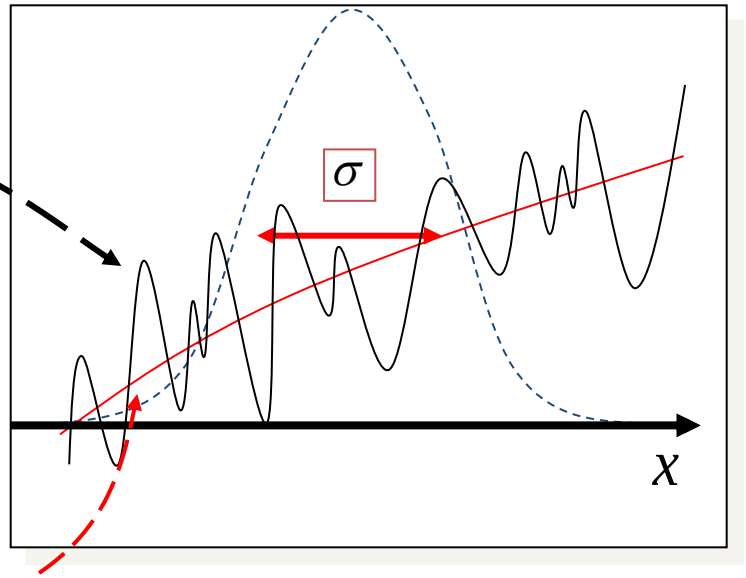
$G_d(\varepsilon - i\delta)$



Regulated Polynomial Expansion (RPE)

- Regulation ≡ Smearing an oscillating function by Gaussian distribution

$f(x)$



Regulated function

$$\langle f(x)\rangle_\sigma \equiv \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} e^{(x'-x)^2/2\sigma^2} \cdot f(x')dx' \quad (7)$$

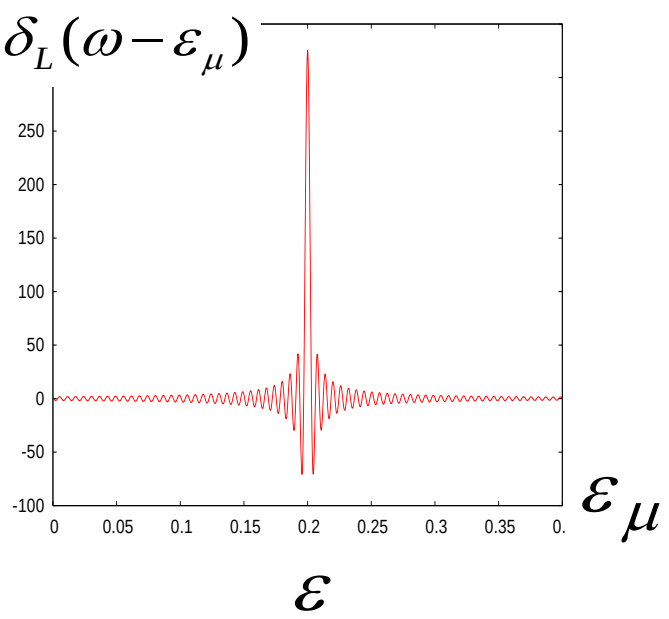
Smoothing Kernel polynomial

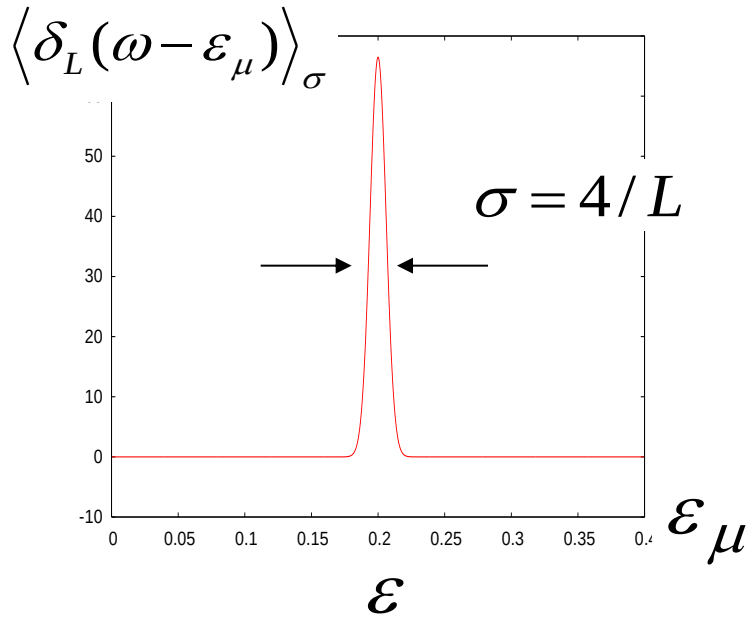
$$\delta_L(\omega-\varepsilon_\mu)=\sum_{l=0}^{L} w_l^{-1} P_l(\omega) P_l(\varepsilon_\mu)$$

Regulation

$$\left\langle \delta_L(\omega-\varepsilon_\mu)\right\rangle_\sigma = \sum_{l=0}^{L} w_l^{-1} P_l(\omega) \left\langle P_l(\varepsilon_\mu)\right\rangle_\sigma$$

Regulated Polynomial





Regulated Polynomial Expansion (RPE) of Green function

$$\hat{G}(z)=\sum_{l=0}^{L} w_l^{-1}\tilde{P}_l(z)\left\langle P_l(\hat{H})\right\rangle_\sigma \qquad \left\langle P_l(\hat{H})\right\rangle_\sigma \equiv \frac{1}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty} e^{(x'-\hat{H})^2/2\sigma^2}P_l(x')dx'$$

Coalitional 3-term recursive formula

$$\left\langle P_{l+1}(\hat{H})\right\rangle_\sigma = \frac{2l+1}{l+1}\hat{H}\left\langle P_l(\hat{H})\right\rangle_\sigma - \frac{l}{l-1}\left\langle P_{l-1}(\hat{H})\right\rangle_\sigma + \frac{2l+1}{l+1}\sigma^2\left\langle P_l'(\hat{H})\right\rangle_\sigma$$

$$\left\langle P'_{l+1}(\hat{H})\right\rangle_\sigma = (2n+1)\left\langle P_l(\hat{H})\right\rangle_\sigma + \left\langle P'_{l-1}(\hat{H})\right\rangle_\sigma$$

$$\left.\begin{aligned} P_{l+1}(\hat{H}) &= \frac{2l+1}{l+1}\hat{H}P_l(\hat{H}) - \frac{l}{l-1}P_{l-1}(\hat{H}) \\ P'_{l+1}(\hat{H}) &= (2l+1)P_l(\hat{H}) + P'_{l-1}(\hat{H}) \end{aligned}\right\}$$

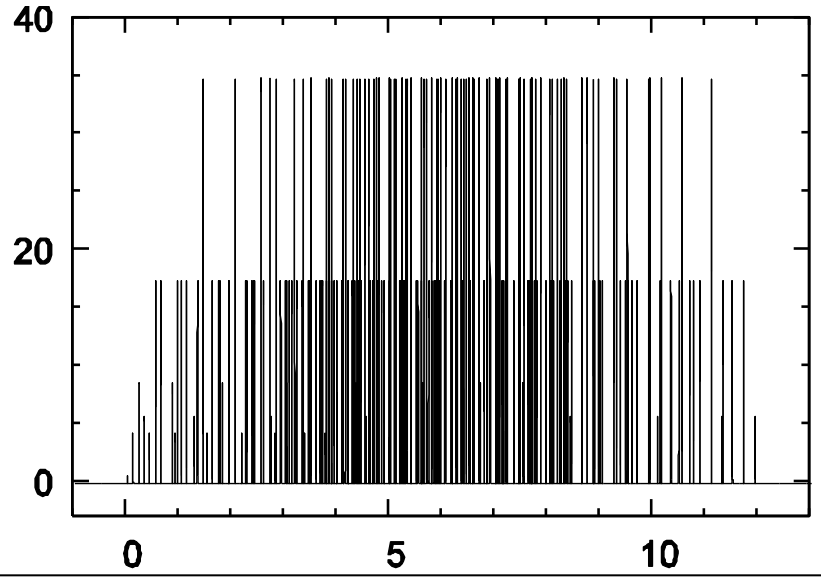
Simultaneous recursive equations of Legendre polynomial

For an arbitrary vector $|\xi\rangle$, $\left\langle P_l(\hat{H})\right\rangle_\sigma |\xi\rangle$ can be calculated recursively!

CPU time practically unchanged!

Example 1. Eigenvalue spectrum of simple cubic lattice dynamics

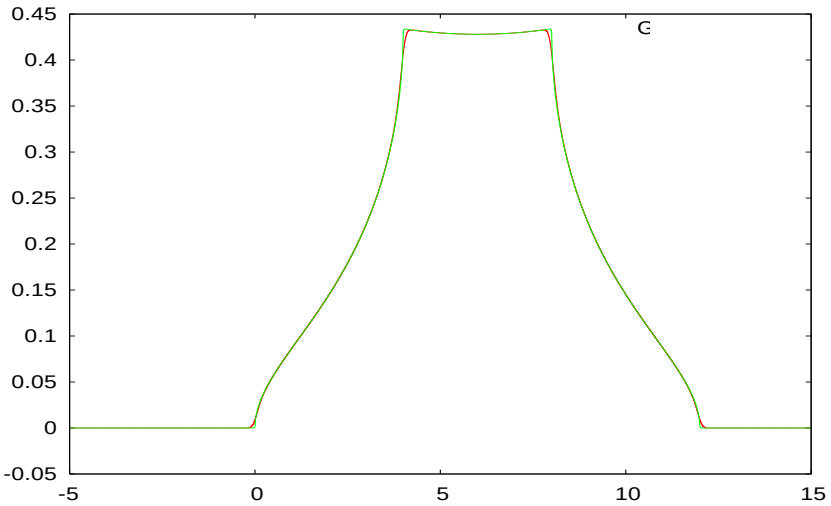
Convergence result（$N=5\times10^5$, 19^3atoms）



- 220 eigenvalues
- height ∝ degeneracy

Accuracy comparable to diagonalization
(up to six digits)

Comparison to bulk spectrum with a larger matrix（151^3 atoms）



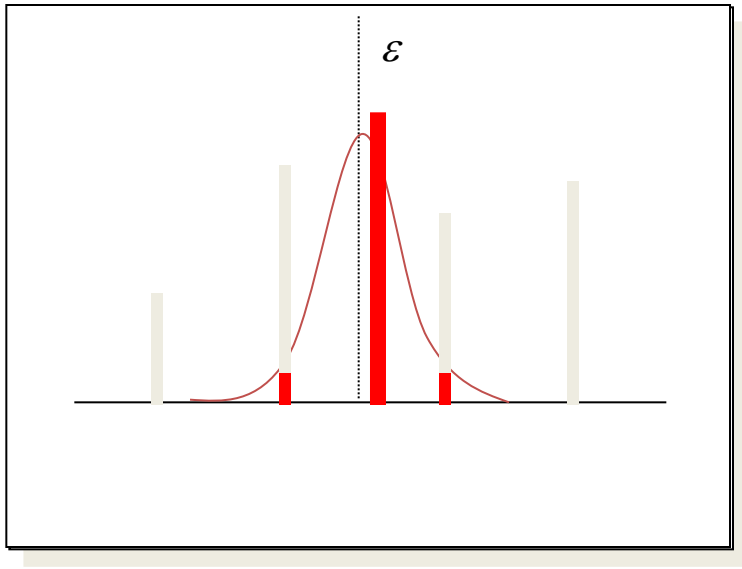
Eigenvector calculation

Arbitrary vector $\xi = \sum_\mu C_\mu \xi_\mu \quad \left(\mathbf{H}\xi_\mu = \varepsilon_\mu \xi_\mu\right)$

$$\left\langle \delta_N(\varepsilon - \mathbf{H}) \right\rangle_\sigma = \sum_{n=0}^{N} w_n^{-1} P_n(\varepsilon) \left\langle P_n(\mathbf{H}) \right\rangle_\sigma$$

Serving as a filter,

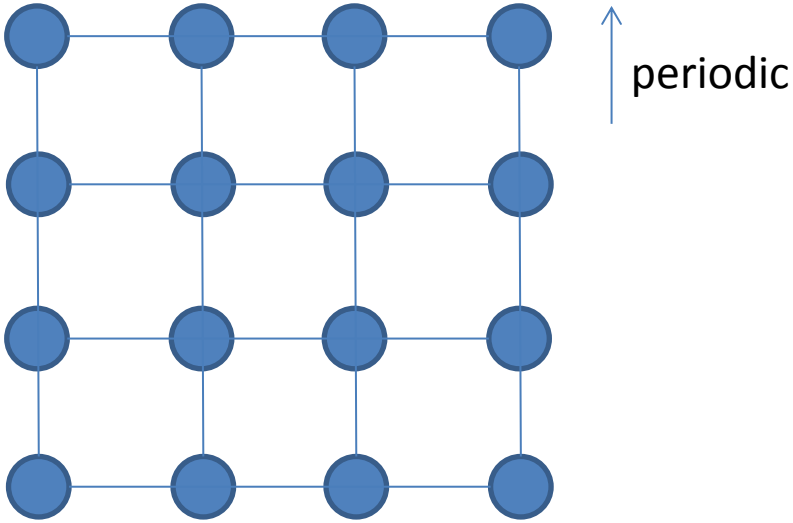
nearest eigenvector picked up!



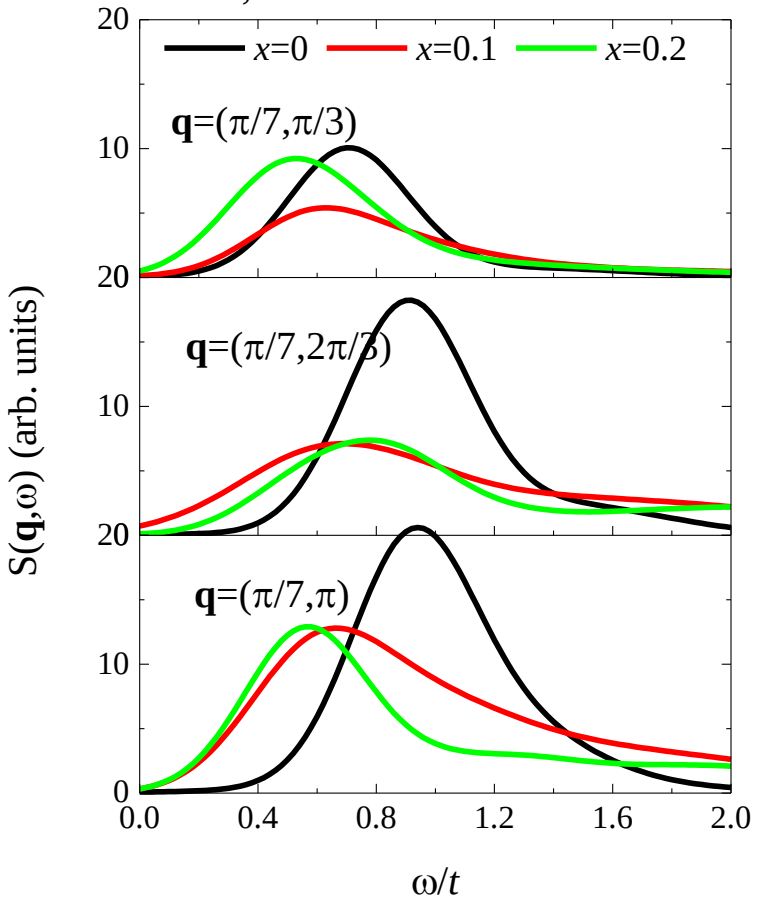
$$\left\langle \delta_N(\varepsilon - \mathbf{H}) \right\rangle_\sigma \xi = \sum_\mu \left\langle \delta_N(\varepsilon - \varepsilon_\mu) \right\rangle_\sigma C_\mu \xi_\mu$$

例：動的スピン-スピン相関関数

正方格子ハバード模型



6x6 hole-doped Hubbard cylinder
U/t=8, t'/t=-0.3



動的スピン-スピン相関関数

$$S(\mathbf{q},\omega) \propto \frac{1}{N}\mathrm{Im}\langle 0|S(\mathbf{q})\frac{1}{\omega-\hat{H}+\varepsilon_0-i\gamma}S(\mathbf{q})|0\rangle$$

有限温度DMRG

$$\left| \tilde{\xi} \right\rangle \equiv \sum_{n=1}^{N} e^{-\beta \hat{H}/2} \left| \xi \right\rangle = \sum_{n} e^{-\beta \varepsilon_n / 2} a_n \left| n \right\rangle$$

: Target state

$$\left| \xi \right\rangle \equiv \sum_{n=1}^{N} a_n \left| n \right\rangle$$

: Arbitrary vector

$$\hat{H} \left| n \right\rangle = \varepsilon_n \left| n \right\rangle$$

$$a_n \equiv \left\langle n \middle| \xi \right\rangle$$

: coefficient

In the case of $a_1^{\,2} = a_2^{\,2} = a_3^{\,2} = \cdots = a_N^{\,2} = 1$,

the linear product of $\left| \tilde{\xi} \right\rangle$ gives

$$\left\langle \tilde{\xi} \middle| \tilde{\xi} \right\rangle = \sum_{n} e^{-\beta \varepsilon_n} = Z(\beta)$$

: Partition function

Kernel polynomial method

$$\left| \tilde{\xi} \right\rangle = \sum_{n=1}^{N} e^{-\beta\varepsilon_n/2} a_n \left| n \right\rangle \qquad \text{(definition)}$$

$$= \int_{-\infty}^{\infty} d\varepsilon' \, e^{-\beta\varepsilon'/2} \sum_{n=1}^{N} \delta(\varepsilon' - \varepsilon_n) a_n \left| n \right\rangle$$

$$= \int_{-\infty}^{\infty} d\varepsilon' \, e^{-\beta\varepsilon'/2} \delta(\varepsilon' - \hat{H}) \left| \xi \right\rangle$$

$$= \int_{-1}^{1} d\varepsilon \, e^{-\beta\varepsilon/2} \lim_{L\to\infty} \sum_{l=0}^{L} w_l^{-1} P_l(\varepsilon) P_l(\hat{H}_s) \left| \xi \right\rangle$$

$\hat{H}\left|n\right\rangle = \varepsilon_n \left|n\right\rangle, \ \left|\xi\right\rangle \equiv \sum_{n=1}^{N} a_n \left|n\right\rangle$

Kernel polynomial method

$P_l(\varepsilon)$: Legendre polynomial, $\hat{H}_s \equiv (\hat{H} - b)/d$ (d, b: rescaling parametar)

$$\left| \tilde{\xi} \right\rangle \propto \lim_{L\to\infty} \sum_{l=0}^{L} w_l^{-1} i_l(-\beta/2) \left\langle P_l(\hat{H}_s) \right\rangle_{\sigma} \left| \xi \right\rangle$$

← Recursive calculation

時間依存DMRG

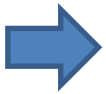
Two-dimensional density matrix renormalization group method

+

Adaptive time-dependent density matrix renormalization group method

+

Kernel polynomial method



2D time dependent DMRG

Kernel polynomial method

- Calculation of target states

$$e^{-iH\Delta\tau}\left|t\right\rangle = \int d\omega\, e^{-i\omega\Delta\tau}\delta(\omega - H)\left|t\right\rangle$$

$$= \int d\omega\, e^{-i\omega\Delta\tau} \lim_{N\to\infty}\sum_{n=0}^{N} w_n^{-1} P_n(\omega)P_n(H)\left|t\right\rangle$$

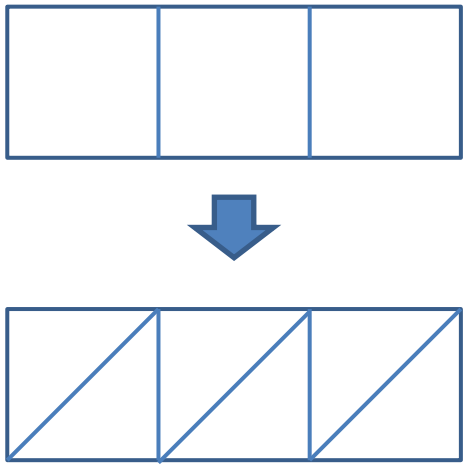
$$= \lim_{N\to\infty}\sum_{n=0}^{N} (-i)^n(2n+1)\, j_n(\Delta\tau)P_n(H)\left|t\right\rangle$$

$P_n(x)$: Legendre polynomial, $j_n(x)$: spherical Bessel function

3-term recursive formula

Demonstration

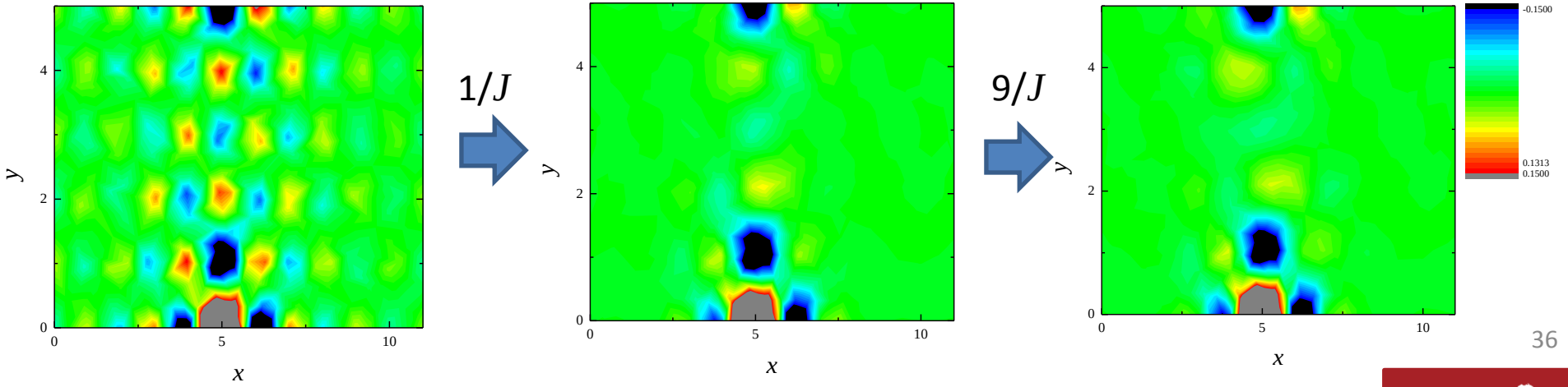
Heisenberg model: $\hat{H} = J \sum_{<i,j>} \hat{S}_i \cdot \hat{S}_j$



Initial state : ground state of square lattice

triangular lattice

- 6x12 Heisenberg model (cylinder boundary condition)



Summary

- 密度行列繰り込み群法の二次元系への適用には巨大な計算資源を必要とする。
- 密度行列繰り込み群法の大規模計算として、実空間並列化等の並列計算手法とメモリ使用量の削減について紹介した。
- 密度行列繰り込み群法の二次元系への応用の今後の発展として、動的、有限温度、時間依存密度行列繰り込み群法の応用について紹介した。