The Lanczos Method

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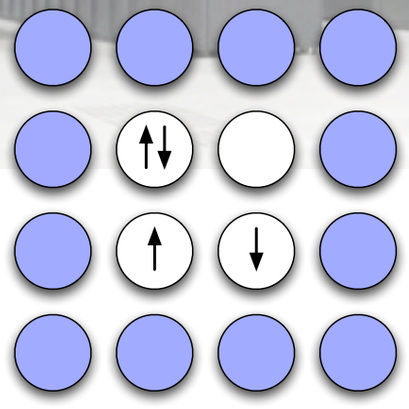
$$\frac{\delta E[\psi]}{\delta\langle\psi|} = \frac{H|\psi\rangle - E[\psi]|\psi\rangle}{\langle\psi|\psi\rangle} = |\psi_a\rangle$$

$$\mathcal{K}^L(|v_0\rangle) = \text{span}\left(|v_0\rangle, H|v_0\rangle, H^2|v_0\rangle, \ldots, H^N|v_0\rangle\right)$$

$$H = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{j,\sigma}\, c_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

$$G_k(\omega) = \cfrac{b_0^2}{\omega - a_0 - \cfrac{b_1^2}{\omega - a_1 - \cfrac{b_2^2}{\omega - a_2 - \cfrac{b_3^2}{\omega - a_3 - \cdots}}}}$$



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finite difference methods

example: 1-dim harmonic oscillator

$$\underbrace{\left(-\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2}+\frac{m_e\omega_0}{2}x^2\right)}_{=:H}\phi(x)=E\,\phi(x)$$

represent wavefunction on equidistant mesh:

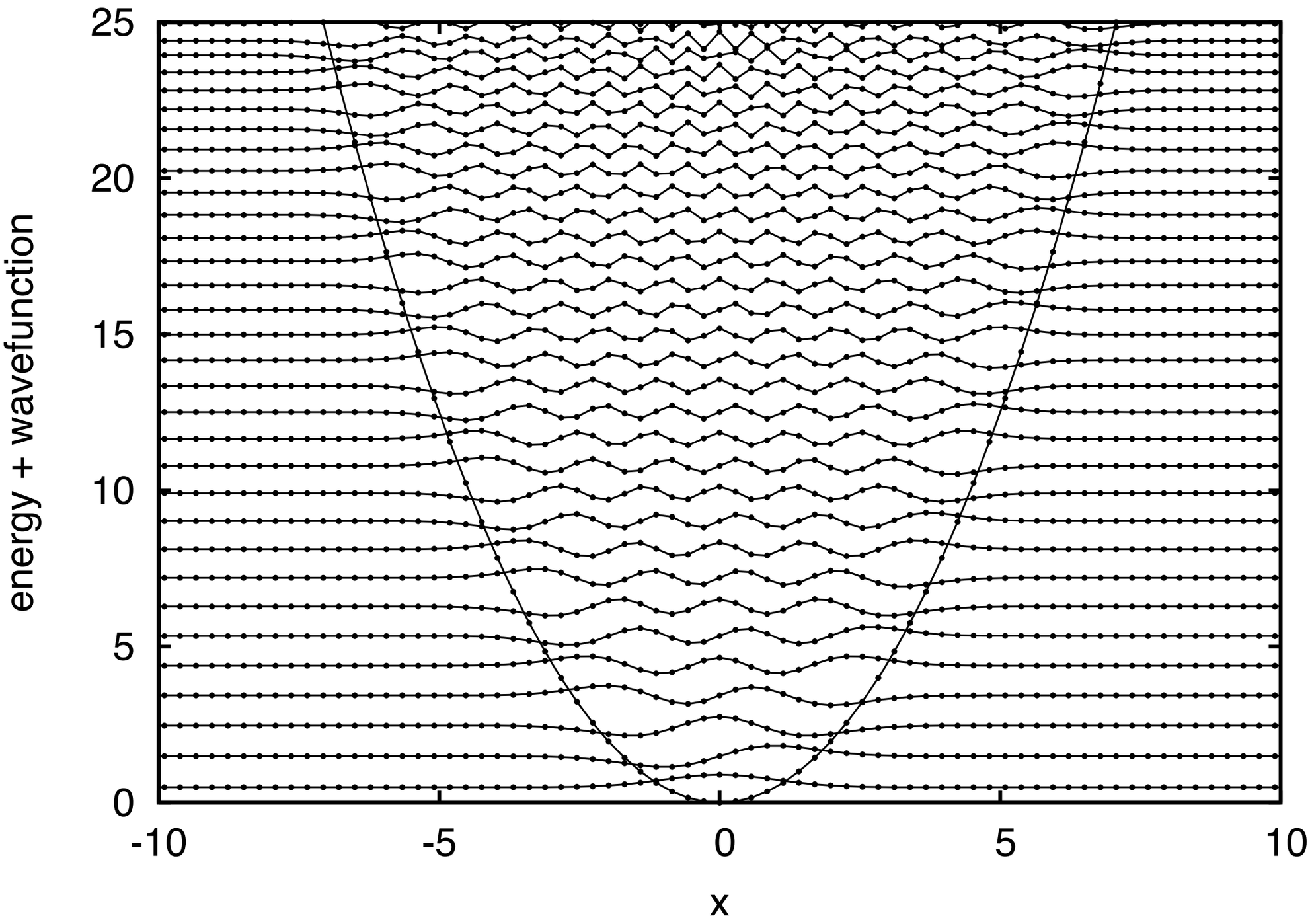
$$\frac{d^2\phi(x_i)}{dx^2}\approx\frac{\phi(x_{i-1})-2\phi(x_i)+\phi(x_{i+1})}{h^2}$$

sparse symmetric matrix

$$H_{\text{mesh}}=\begin{pmatrix} 1/h^2+V(x_0) & -1/2h^2 & 0 & 0 & \cdots & 0 & 0 \\ -1/2h^2 & 1/h^2+V(x_1) & -1/2h^2 & 0 & \cdots & 0 & 0 \\ 0 & -1/2h^2 & 1/h^2+V(x_2) & -1/2h^2 & \cdots & 0 & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1/2h^2 & 1/h^2+V(x_N) \end{pmatrix}$$

finite difference methods

discretization: only lower eigenstates are correct



Why Lanczos?

- ☑ numerically exact solution
- ☑ efficient for sparse Hamiltonians
- ☑ ground state (T=0) or finite (but low) temperature
- ☑ spectral function on real axis

- ☐ only finite (actually quite small) systems
  - ○ efficient parallelization to use shared memory
  - ○ optimal bath parametrization

minimal eigenvalue: steepest descent

energy functional

$$E[\psi] = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

direction (in Hilbert space) of steepest ascent

$$\frac{\delta E[\psi]}{\delta\langle\psi|} = \frac{H|\psi\rangle - E[\psi]|\psi\rangle}{\langle\psi|\psi\rangle} = |\psi_a\rangle \in \text{span}\left(|\psi\rangle, H|\psi\rangle\right)$$

minimize energy in $\text{span}\left(|\psi\rangle, H|\psi\rangle\right)$

minimal eigenvalue: steepest descent

minimize energy in $\mathrm{span}\left(|\psi\rangle, H|\psi\rangle\right)$

construct orthonormal basis

$$\begin{aligned} |v_0\rangle &= |\psi\rangle / \sqrt{\langle\psi|\psi\rangle} \\ b_1 |v_1\rangle &= |\tilde{v}_1\rangle = H|v_0\rangle - |v_0\rangle\langle v_0|H|v_0\rangle \end{aligned}$$

define: $a_n := \langle v_n|H|v_n\rangle \qquad b_1 := \sqrt{\langle\tilde{v}_1|\tilde{v}_1\rangle}$

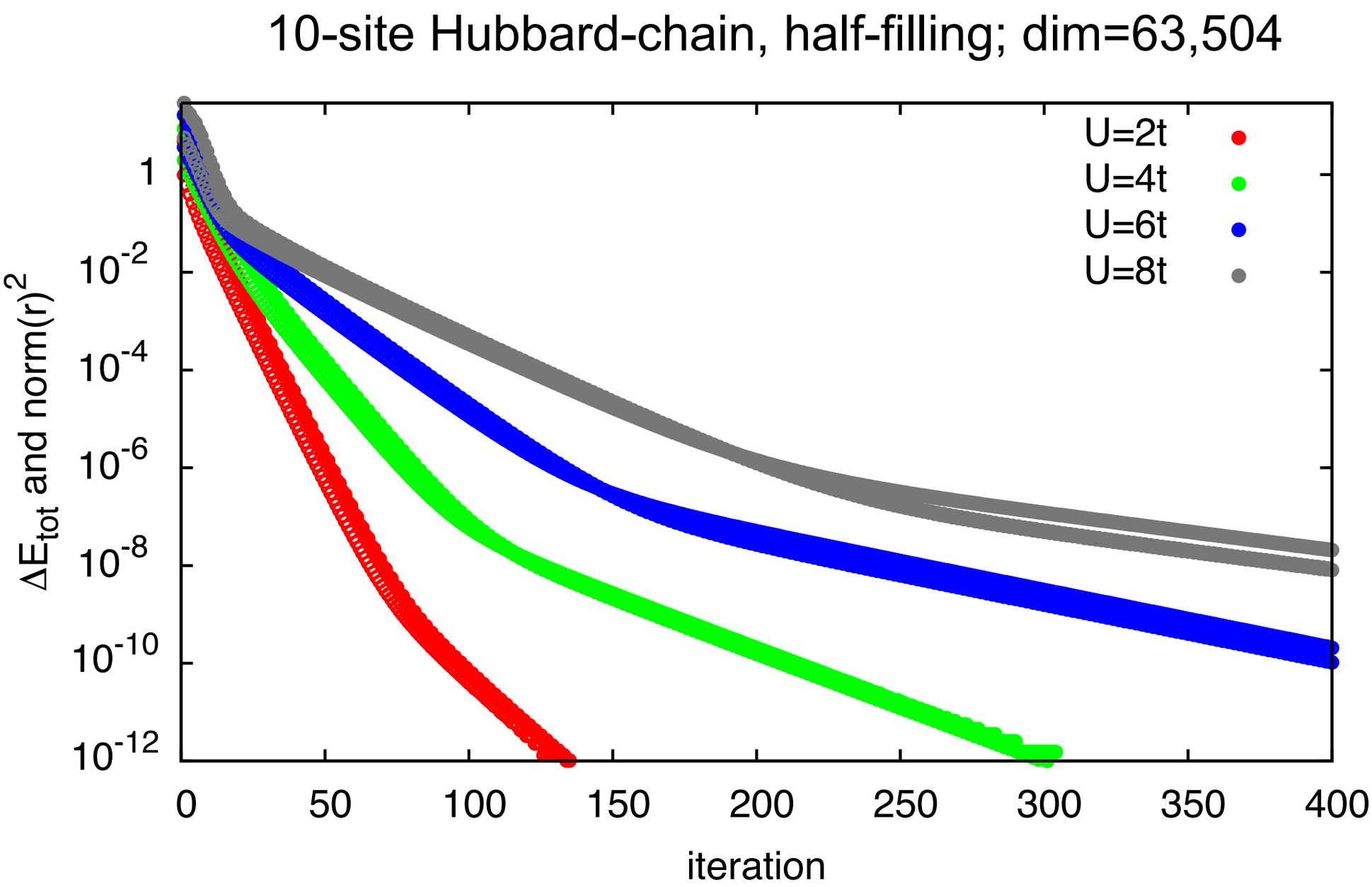
$$H|v_0\rangle = b_1 |v_1\rangle + a_0 |v_0\rangle$$

$$H_{\mathrm{span}(|\psi\rangle, H|\psi\rangle)} = \begin{pmatrix} a_0 & b_1 \\ b_1 & a_1 \end{pmatrix}$$

diagonalize to find lowest eigenvector

iterate!

convergence



Lanczos idea

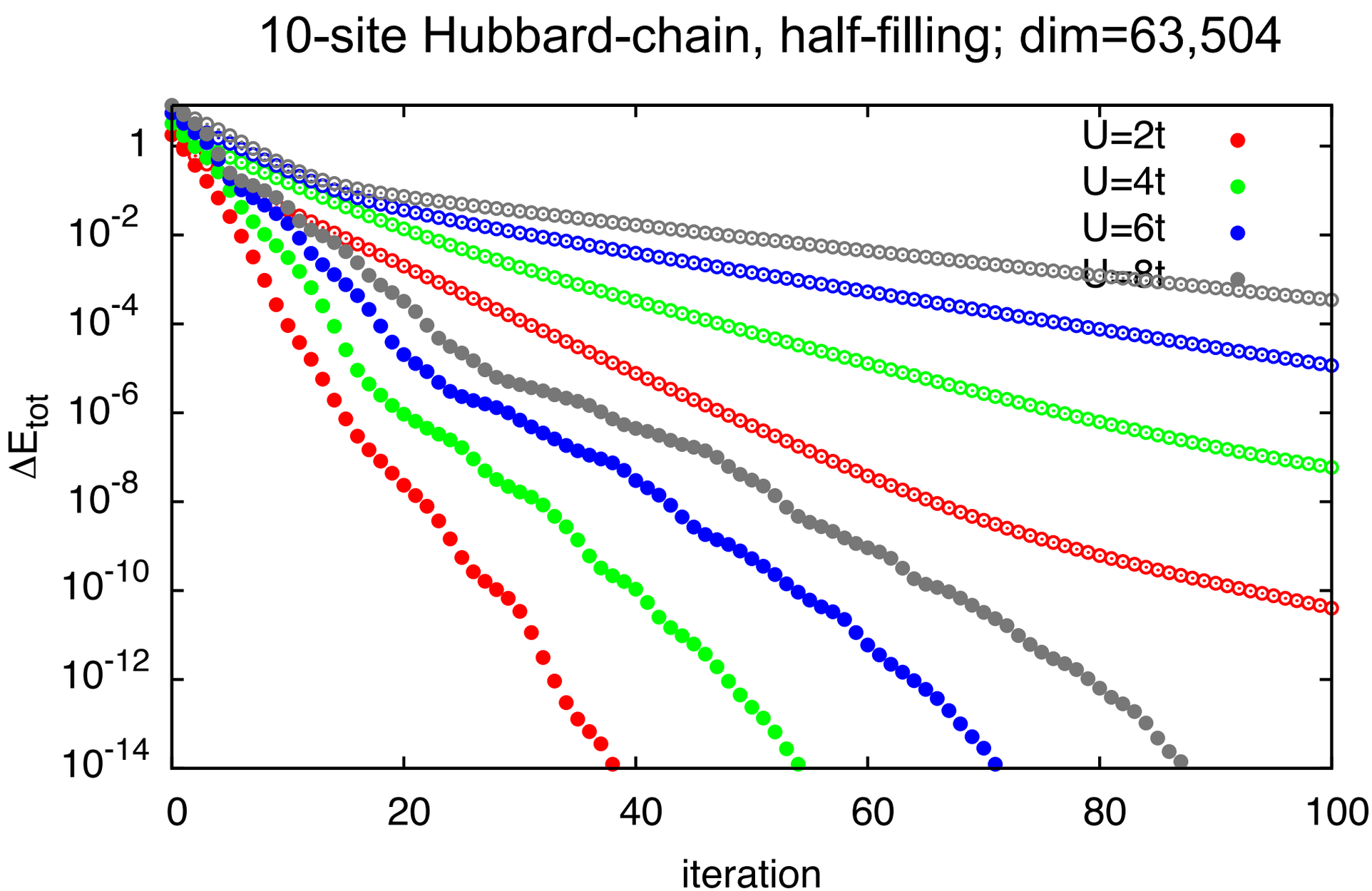
minimize on span $(|\psi_0\rangle, H|\psi_0\rangle)$ to obtain $|\psi_1\rangle$
minimize on span $(|\psi_1\rangle, H|\psi_1\rangle) \in$ span $\left(|\psi_0\rangle, H|\psi_0\rangle, H^2|\psi_0\rangle\right)$
minimize on span $(|\psi_2\rangle, H|\psi_2\rangle) \in$ span $\left(|\psi_0\rangle, H|\psi_0\rangle, H^2|\psi_0, H^3|\psi_0\rangle\right)$
etc.

instead of L-fold iterative minimization on two-dimensional subspaces
minimize energy on *L+1 dimensional* **Krylov space**

$$\mathcal{K}^L(\psi_0\rangle) = \text{span}\left(|\psi_0\rangle, H|\psi_0\rangle, H^2|\psi_0\rangle, \ldots, H^L|\psi_0\rangle\right)$$

more variational degrees of freedom $\Rightarrow$ even faster convergence

convergence to ground state



Lanczos iteration

construct orthonormal basis in Krylov space

$$b_{n+1}|v_{n+1}\rangle = |\tilde{v}_{n+1}\rangle = H|v_n\rangle - \sum_{i=0}^{n} |v_i\rangle\langle v_i|H|v_n\rangle$$

define: $\quad a_n := \langle v_n|H|v_n\rangle \qquad b_n := \sqrt{\langle \tilde{v}_n|\tilde{v}_n\rangle}$

$$\langle v_m| : \qquad b_{n+1}\,\delta_{m,n+1} = \langle v_m|H|v_n\rangle - \sum_{i=0}^{n}\langle v_m|H|v_n\rangle\,\delta_{m,i}$$

$$\langle v_m|H|v_n\langle = \begin{cases} \langle v_m|H|v_n\rangle & \text{for } m < n \\ a_n & \text{for } m = n \\ b_{n+1} & \text{for } m = n+1 \\ 0 & \text{for } m > n+1 \end{cases} \qquad H = \begin{pmatrix} a_0 & ? & ? & \cdots & ? \\ b_1 & a_1 & ? & & ? \\ 0 & b_2 & a_2 & & ? \\ & & & & \\ 0 & 0 & 0 & & a_L \end{pmatrix}$$

H has upper Hessenberg form
symmetric/hermitian ⇒ tridiagonal

Lanczos iteration

orthonormal basis in Krylov space

$$
\begin{aligned}
& |v_0\rangle \\
b_1\,|v_1\rangle \quad &= \quad H|v_0\rangle - a_0|v_0\rangle \\
b_2\,|v_2\rangle \quad &= \quad H|v_1\rangle - a_1|v_1\rangle - b_1|v_0\rangle \\
b_3\,|v_3\rangle \quad &= \quad H|v_2\rangle - a_2|v_2\rangle - b_2|v_1\rangle \\
& \cdots
\end{aligned}
$$

$$
H|v_n\rangle = b_n|v_{n-1}\rangle + a_n|v_n\rangle + b_{n+1}|v_{n+1}\rangle
$$

$$
H_{\mathcal{K}^L(|v_0\rangle)} = \begin{pmatrix}
a_0 & b_1 & 0 & 0 & & 0 & 0 \\
b_1 & a_1 & b_2 & 0 & \cdots & 0 & 0 \\
0 & b_2 & a_2 & b_3 & & 0 & 0 \\
0 & 0 & b_3 & a_3 & & 0 & 0 \\
 & \vdots & & & \ddots & \vdots & \\
0 & 0 & 0 & 0 & & a_{L-1} & b_L \\
0 & 0 & 0 & 0 & \cdots & b_L & a_L
\end{pmatrix}
$$

Lanczos algorithm

```
v=init
b0=norm2(v)
scal(1/b0,v)
w=0
w=w+H*v
a[0]=dot(v,w)
axpy(-a[0],v,w)
b[1]=norm2(w)
for n=1,2,...
  if abs(b[n])<eps then exit
  scal(1/b[n],w)
  scal( -b[n],v)
  swap(v,w)
  w=w+H*v
  a[n]=dot(v,w)
  axpy(-a[n],v,w)
  b[n+1]=norm2(w)
  diag(a[0]..a[n], b[1]..b[n])
  if converged then exit
end
```

not part of tridiagonal matrix

$\mathtt{v}= |v_0\rangle$

$\mathtt{w}= H|v_0\rangle$

$\mathtt{w}= |\tilde{v}_1\rangle = H|v_0\rangle - a_0|v_0\rangle$

invariant subspace

$\mathtt{w}= |v_n\rangle$

$\mathtt{v}= -b_n|v_{n-1}\rangle$

$\mathtt{w}= H|v_n\rangle - b_n|v_{n-1}\rangle$

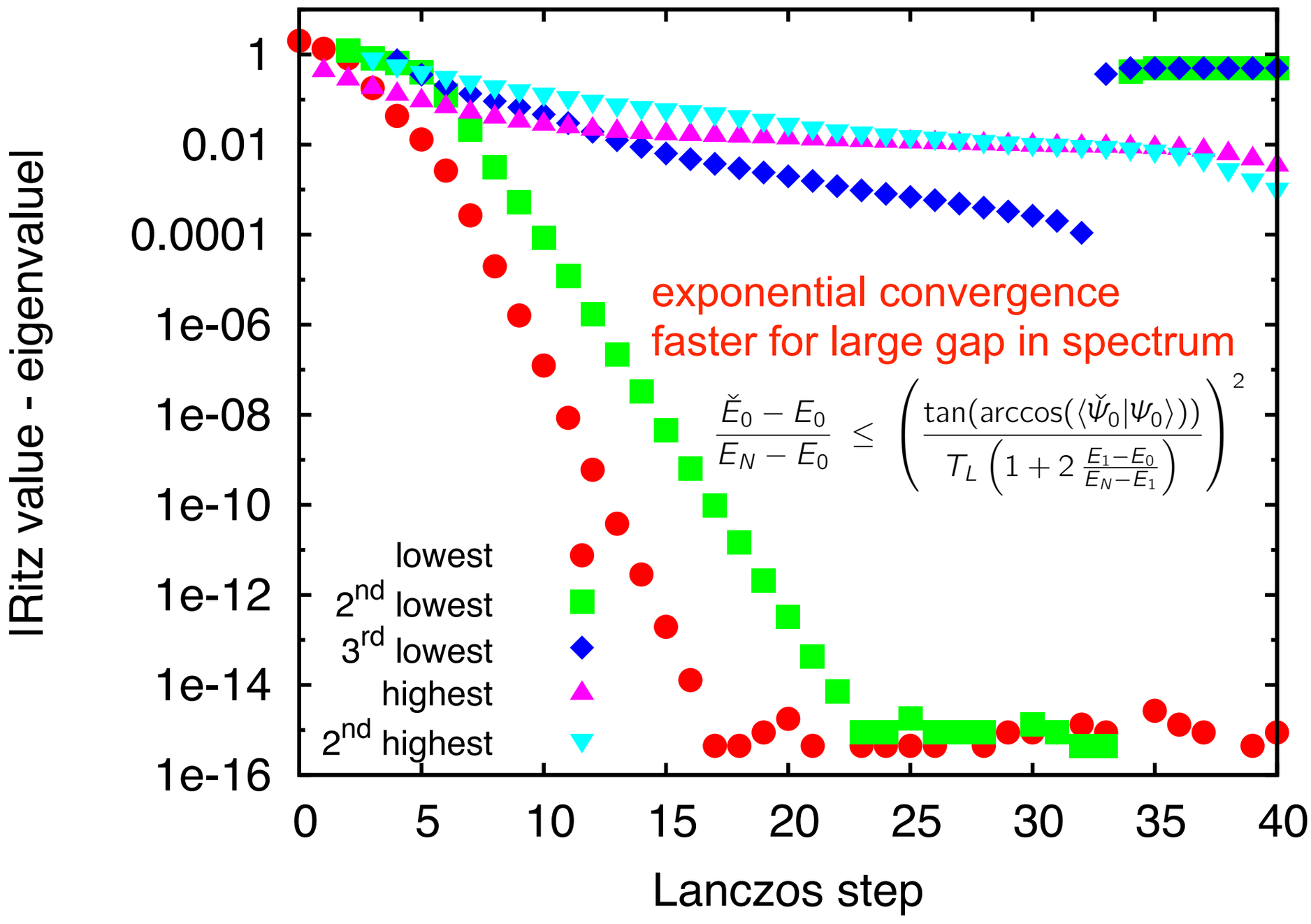
$\mathtt{a[n]}= \langle v_n|H|v_n\rangle - b_n\langle v_n|v_{n-1}\rangle$

$\mathtt{w}= |\tilde{v}_{n+1}\rangle$

getting a_{n+1} needs another $H|v\rangle$

convergence to extremal eigenvalues

toy problem: matrix with eigenvalues -3, -3, -2.5, -2,-1.99, -1.98, ... -0.01, 0



convergence of Ritz values

E_n: eigenvalues of H in ascending order, n=0,...

$E^{(L)}_n$: eigenvalues of Lanczos matrix $H^{(L)}$ (Ritz values)

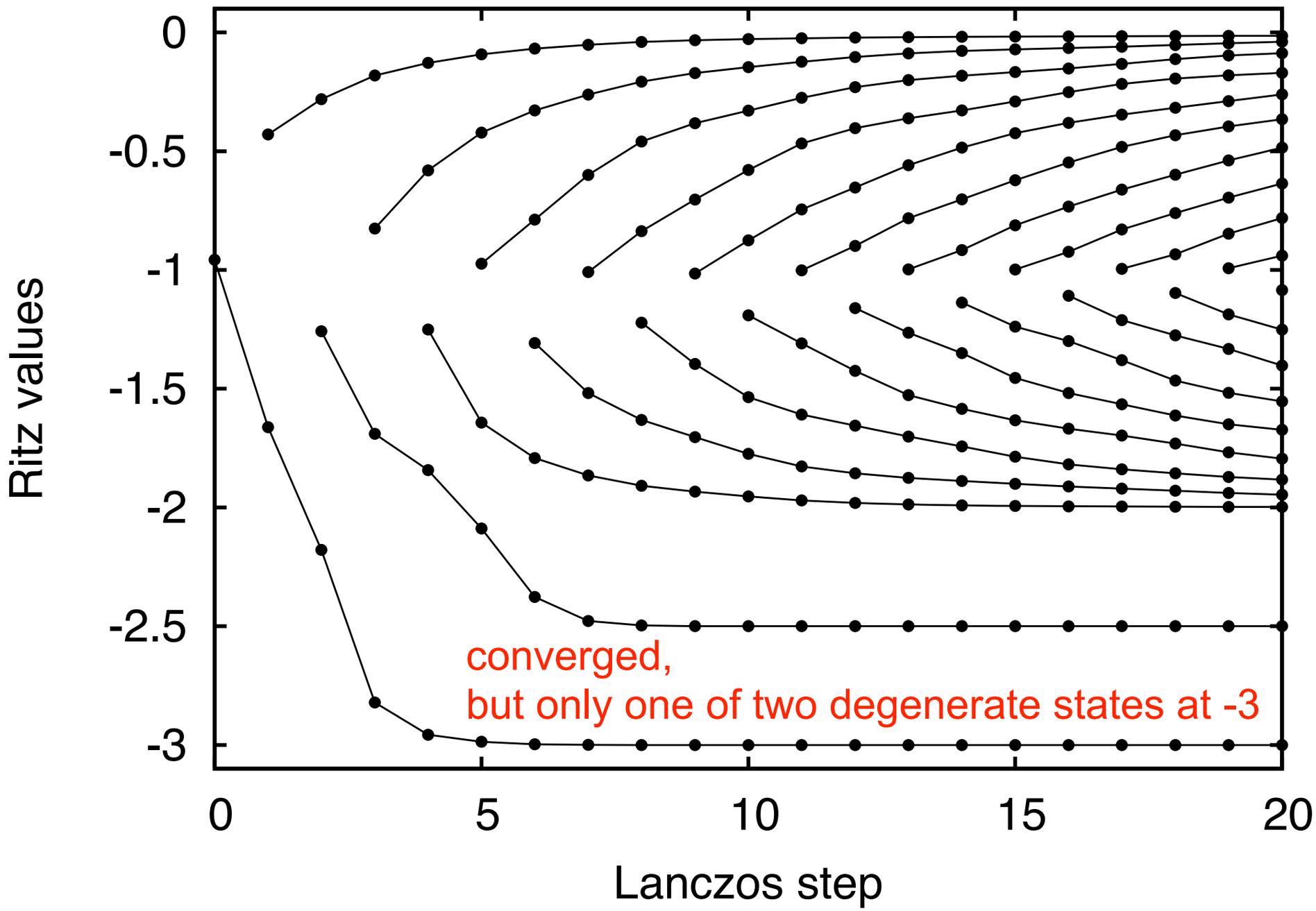
Ritz value n approaches eigenvalue n with increasing L from above:

$$E_n \leq E_n^{(L+1)} \leq E_n^{(L)}$$

general basis-set methods: MacDonald's theorem
Phys. Rev. **43**, 830 (1933)

spectrum of tridiagonal matrix

toy problem: matrix with eigenvalues -3, -3, -2.5, -2,-1.99, -1.98, ... -0.01, 0



Krylov space cannot contain degenerate states

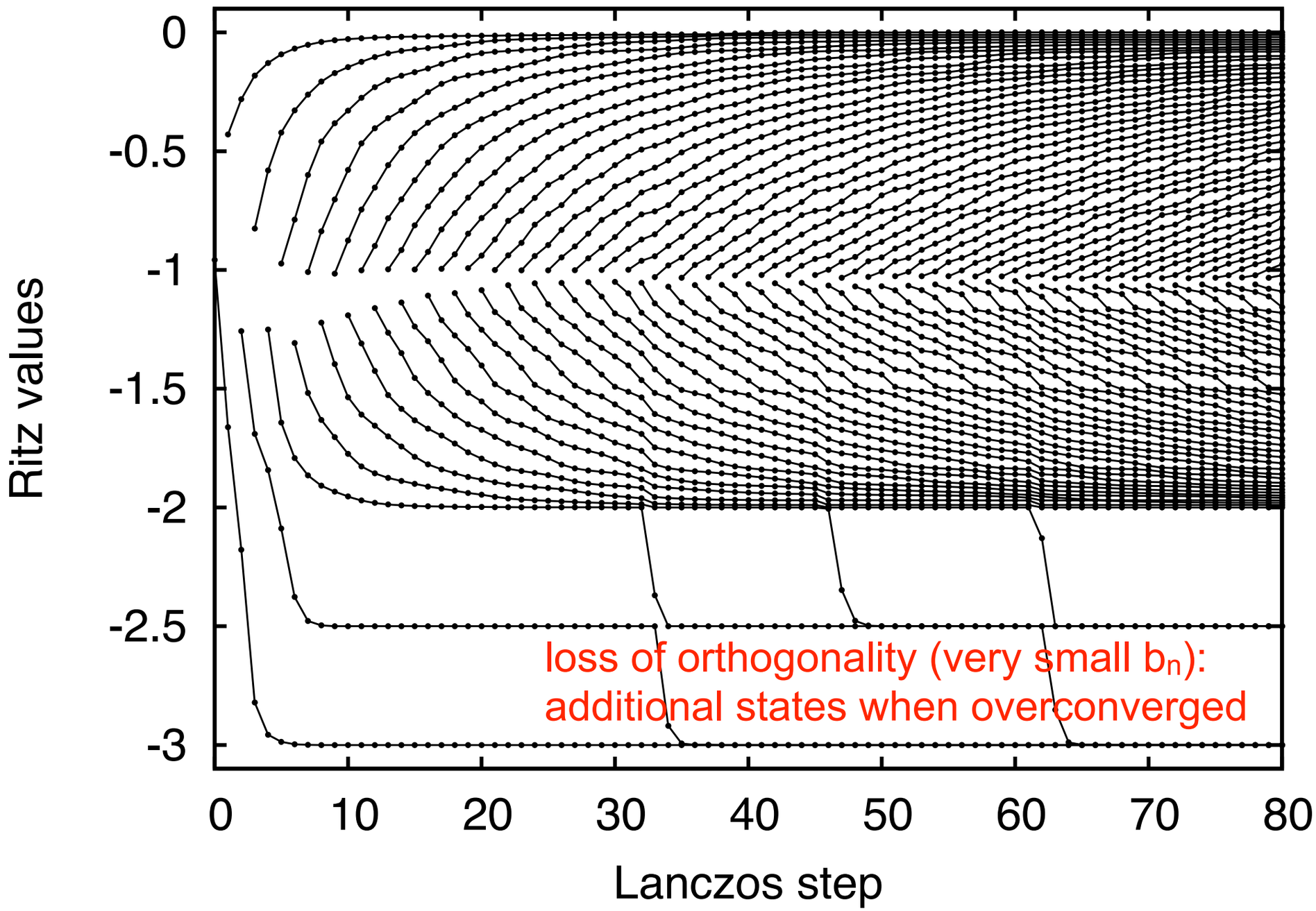
assume $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are degenerate eigenstates with eigenvalue ε,
then their expansion in the orthonormal basis of the Krylov space is

$$\langle v_0|H^n|\varphi_i\rangle = \varepsilon^n \langle v_0|\varphi_i\rangle$$

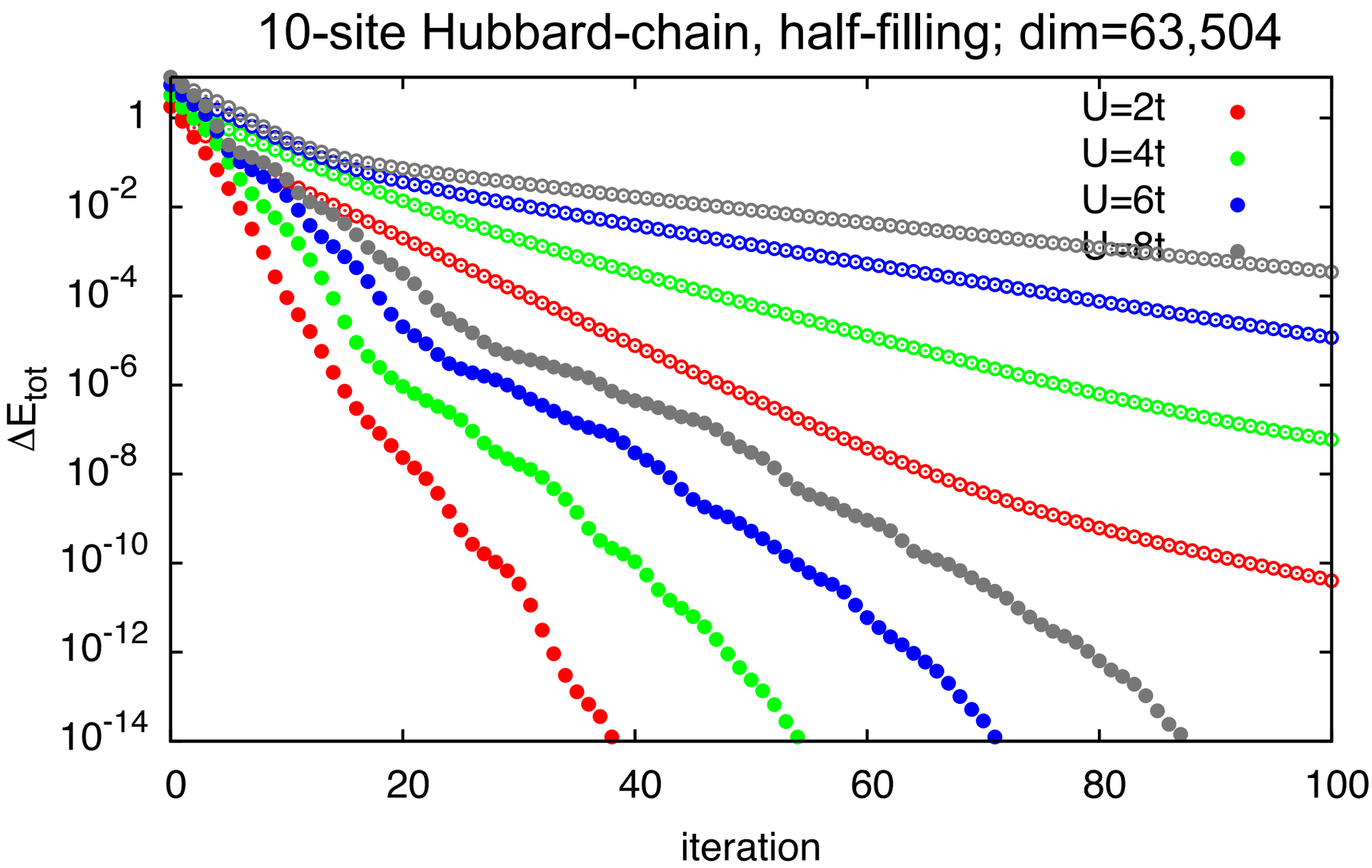
$\Rightarrow |\varphi_1\rangle$ and $|\varphi_2\rangle$ are identical up to normalization

loss of orthogonality

toy problem: matrix with eigenvalues -3, -3, -2.5, -2,-1.99, -1.98, ... -0.01, 0

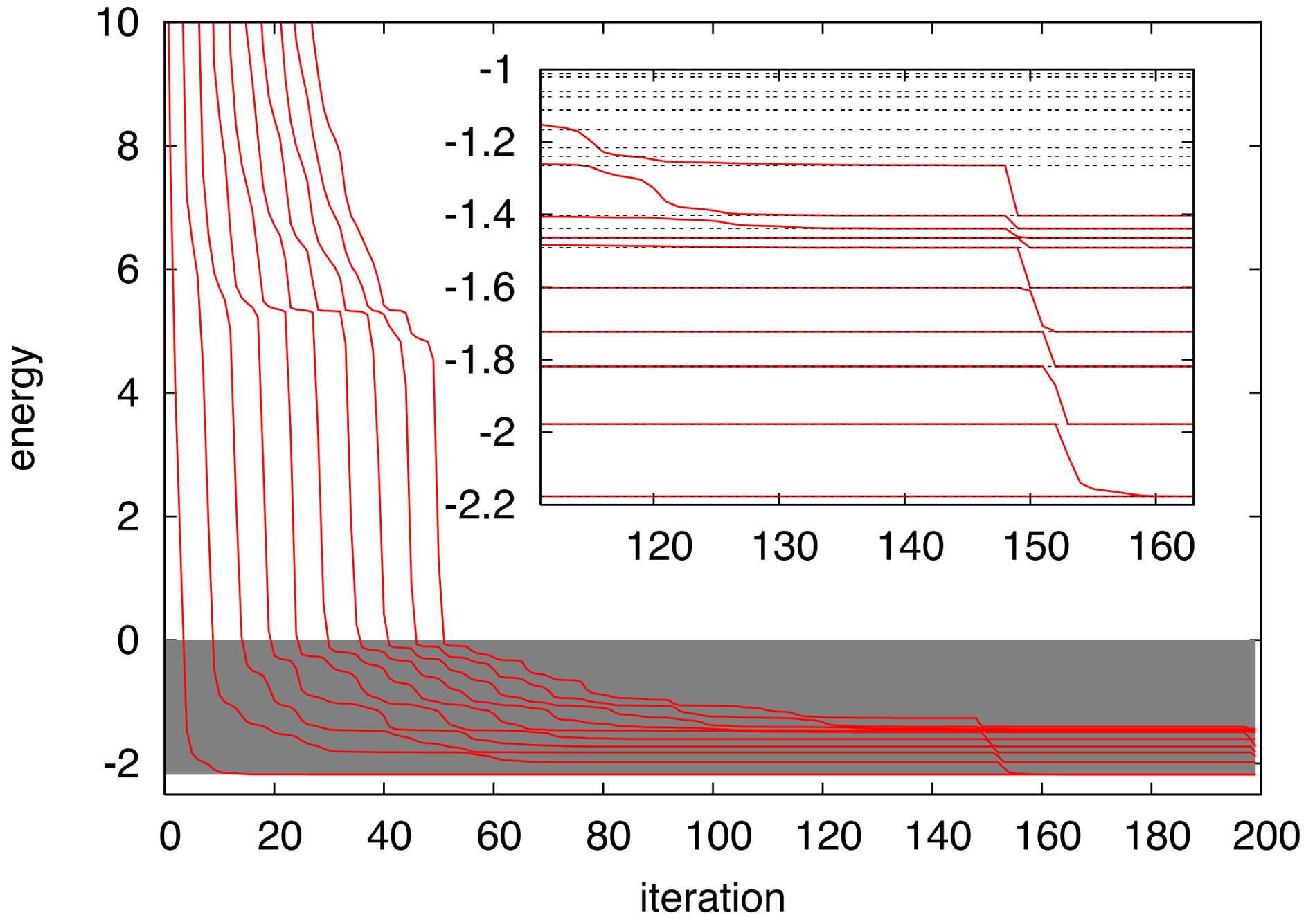


convergence to ground state



$$\frac{\check{E}_0 - E_0}{E_N - E_0} \leq \left(\frac{\tan(\arccos(\langle \check{\psi}_0 | \psi_0 \rangle))}{T_L\left(1 + 2\,\frac{E_1 - E_0}{E_N - E_1}\right)} \right)^2$$

over-convergence: ghost states



$$b_{n+1}|v_{n+1}\rangle = H|v_n\rangle - a_n|v_n\rangle - bn|v_{n-1}\rangle$$

construction of eigenvectors

let $\check{\psi}_n = (\check{\psi}_{n,i})$ be the n^{th} eigenstate of the tridiagonal Lanczos matrix

$$H_{\mathcal{K}^L(|v_0\rangle)} = \begin{pmatrix} a_0 & b_1 & 0 & 0 & & 0 & 0 \\ b_1 & a_1 & b_2 & 0 & \cdots & 0 & 0 \\ 0 & b_2 & a_2 & b_3 & & 0 & 0 \\ 0 & 0 & b_3 & a_3 & & 0 & 0 \\ & \vdots & & & \ddots & \vdots & \\ 0 & 0 & 0 & 0 & & a_{L-1} & b_L \\ 0 & 0 & 0 & 0 & \cdots & b_L & a_L \end{pmatrix}$$

the approximate eigenvector is then given in the Lanczos basis

$$|\check{\psi}_n\rangle = \sum_{i=0}^{L} \check{\psi}_{n,i} |v_i\rangle$$

need all Lanczos basis vectors ⇒ need very large memory

instead: rerun Lanczos iteration from same $|v_0\rangle$

and accumulate eigenvector on the fly

spectral function

$$G_c(z) = \left\langle \psi_c \left| \frac{1}{z - H} \right| \psi_c \right\rangle = \sum_{n=0}^{N} \frac{\langle \psi_c | \psi_n \rangle \langle \psi_n | \psi_c \rangle}{z - E_n}$$

need to calculate entire spectrum?

resolvent / spectral function

$$G_c(z) = \left\langle \psi_c \left| \frac{1}{z - H} \right| \psi_c \right\rangle = \sum_{n=0}^{N} \frac{\langle \psi_c | \psi_n \rangle \langle \psi_n | \psi_c \rangle}{z - E_n}$$

$$\check{G}_c(z) = \left\langle \psi_c \left| \frac{1}{z - \check{H}_c} \right| \psi_c \right\rangle = \sum_{n=0}^{L} \frac{\langle \psi_c | \check{\psi}_n \rangle \langle \check{\psi}_n | \psi_c \rangle}{z - \check{E}_n}$$

$$z - \check{H}_c = \left(\begin{array}{c|cccccc} z - a_0 & -b_1 & 0 & 0 & \cdots & 0 & 0 \\ \hline -b_1 & z - a_1 & -b_2 & 0 & \cdots & 0 & 0 \\ 0 & -b_2 & z - a_2 & -b_3 & \cdots & 0 & 0 \\ 0 & 0 & -b_3 & z - a_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & z - a_{L-1} & -b_L \\ 0 & 0 & 0 & 0 & \cdots & -b_L & z - a_L \end{array} \right)$$

resolvent / spectral function

$$z - \check{H}_c = \begin{pmatrix} z - a_0 & B^{(1)\,T} \\ B^{(1)} & z - \check{H}_c^{(1)} \end{pmatrix}$$

inversion by partitioning

$$\begin{aligned} \left[(z - \check{H}_c)^{-1}\right]_{00} &= \left(z - a_0 - B^{(1)\,T}(z - \check{H}_c^{(1)})^{-1} B^{(1)}\right)^{-1} \\ &= \left(z - a_0 - b_1^2 \left[(z - \check{H}_c^{(1)})^{-1}\right]_{00}\right)^{-1} \end{aligned}$$

recursively

$$\check{G}_c(z) = \left[(z - \check{H}_c)^{-1}\right]_{00} = \cfrac{1}{z - a_0 - \cfrac{b_1^2}{z - a_1 - \cfrac{b_2^2}{z - a_2 - \cdots}}}$$

downfolding

partition Hilbert space

$$H = \begin{pmatrix} H_{00} & T_{01} \\ T_{10} & H_{11} \end{pmatrix}$$

resolvent

$$G(\varepsilon) = (\varepsilon - H)^{-1} = \begin{pmatrix} \varepsilon - H_{00} & -T_{01} \\ -T_{10} & \varepsilon - H_{11} \end{pmatrix}^{-1}$$

inverse of 2×2 block-matrix

$$G_{00}(\varepsilon) = \left(\varepsilon - \left[H_{00} + T_{01}(\varepsilon - H_{11})^{-1} T_{10}\right]\right)^{-1}$$

downfolded Hamiltonian

$$H_{\text{eff}} \approx H_{00} + T_{01}(\varepsilon_0 - H_{11})^{-1} T_{10}$$

good approximation: narrow energy range and/or small coupling

inversion by partitioning

2×2 matrix

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \qquad M^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

invert block-2×2 matrix

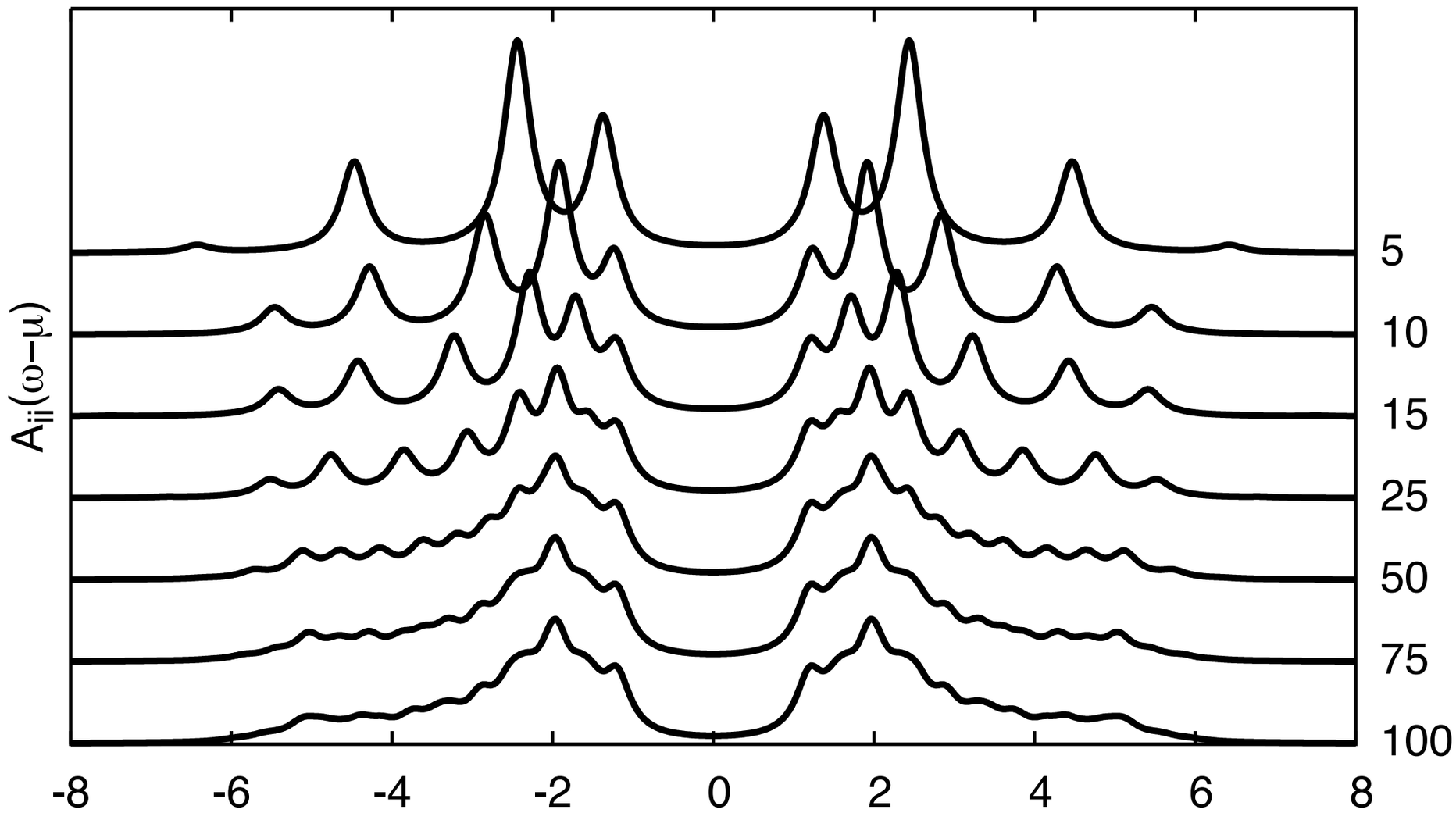
$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \quad M^{-1} = \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{pmatrix}$$

solve

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\begin{aligned} A\tilde{A} + B\tilde{C} &= 1 && = (A - BD^{-1}C)\tilde{A} \\ C\tilde{A} + D\tilde{C} &= 0 \quad \rightsquigarrow \quad \tilde{C} = -D^{-1}C\tilde{A} \end{aligned}$$

convergence: moments



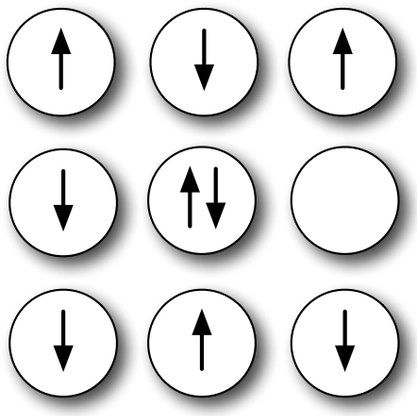
$$\int_{-\infty}^{\infty} d\omega\, \omega^m \check{A}(\omega) = \sum_{n=0}^{L} |\check{\psi}_{n,0}|^2 \check{E}_n^m = \sum_{n=0}^{L} \langle \Psi_c | \check{\psi}_n \rangle \langle \check{\psi}_n | \Psi_c \rangle \check{E}_n^m = \langle \Psi_c | \check{H}^m | \Psi_c \rangle$$

application to Hubbard model and shared-memory parallelization

dimension of many-body Hilbert space

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

solve finite clusters



$$\dim(H) = \begin{pmatrix} M \\ N_{\uparrow} \end{pmatrix} \times \begin{pmatrix} M \\ N_{\downarrow} \end{pmatrix}$$

M	$N_{\uparrow}$	$N_{\downarrow}$	dimension of Hilbert space	memory
2	1	1	4	
4	2	2	36	
6	3	3	400	
8	4	4	4 900	
10	5	5	63 504	
12	6	6	853 776	6 MB
14	7	7	11 778 624	89 MB
16	8	8	165 636 900	1 263 MB
18	9	9	2 363 904 400	18 GB
20	10	10	34 134 779 536	254 GB
22	11	11	497 634 306 624	3708 GB
24	12	12	7 312 459 672 336	53 TB

choice of basis

real space: sparse Hamiltonian

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

hopping only connects states of same spin
interaction diagonal (even for long-range interaction!)

k-space

$$H = \sum_{k\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + \frac{U}{M} \sum_{k,k',q} c^{\dagger}_{k\uparrow} c_{k-q,\uparrow} c^{\dagger}_{k'\downarrow} c_{k'+q,\downarrow}$$

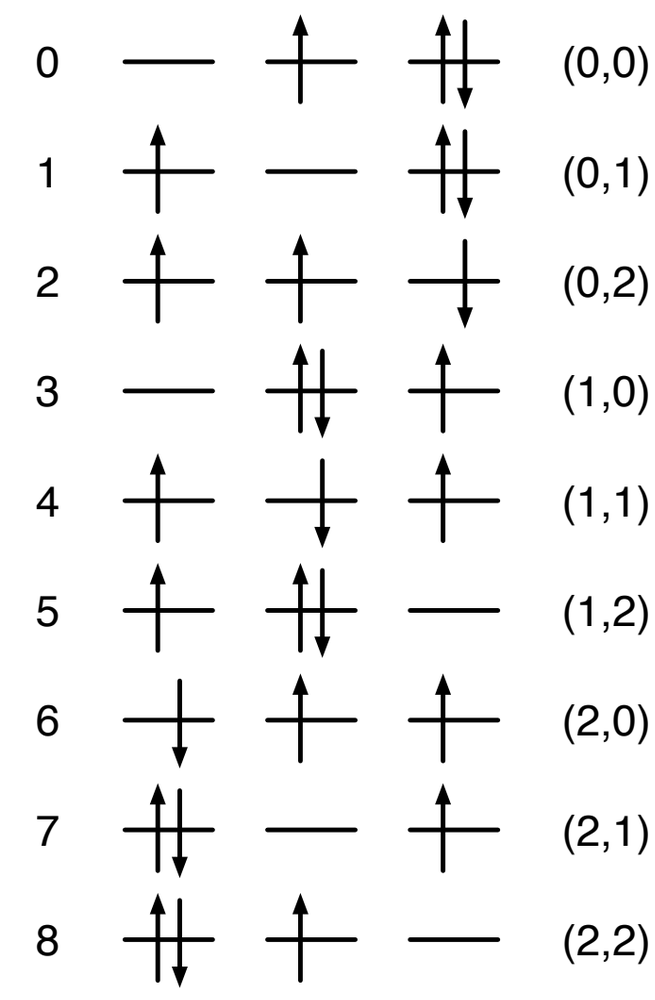
choice of basis

work with operators that create electrons in Wannier orbitals

$$|\{n_{i\sigma}\}\rangle = \prod_{i=0}^{L-1} \left(c_{i\downarrow}^{\dagger}\right)^{n_{i\downarrow}} \left(c_{i\uparrow}^{\dagger}\right)^{n_{i\uparrow}} |0\rangle$$

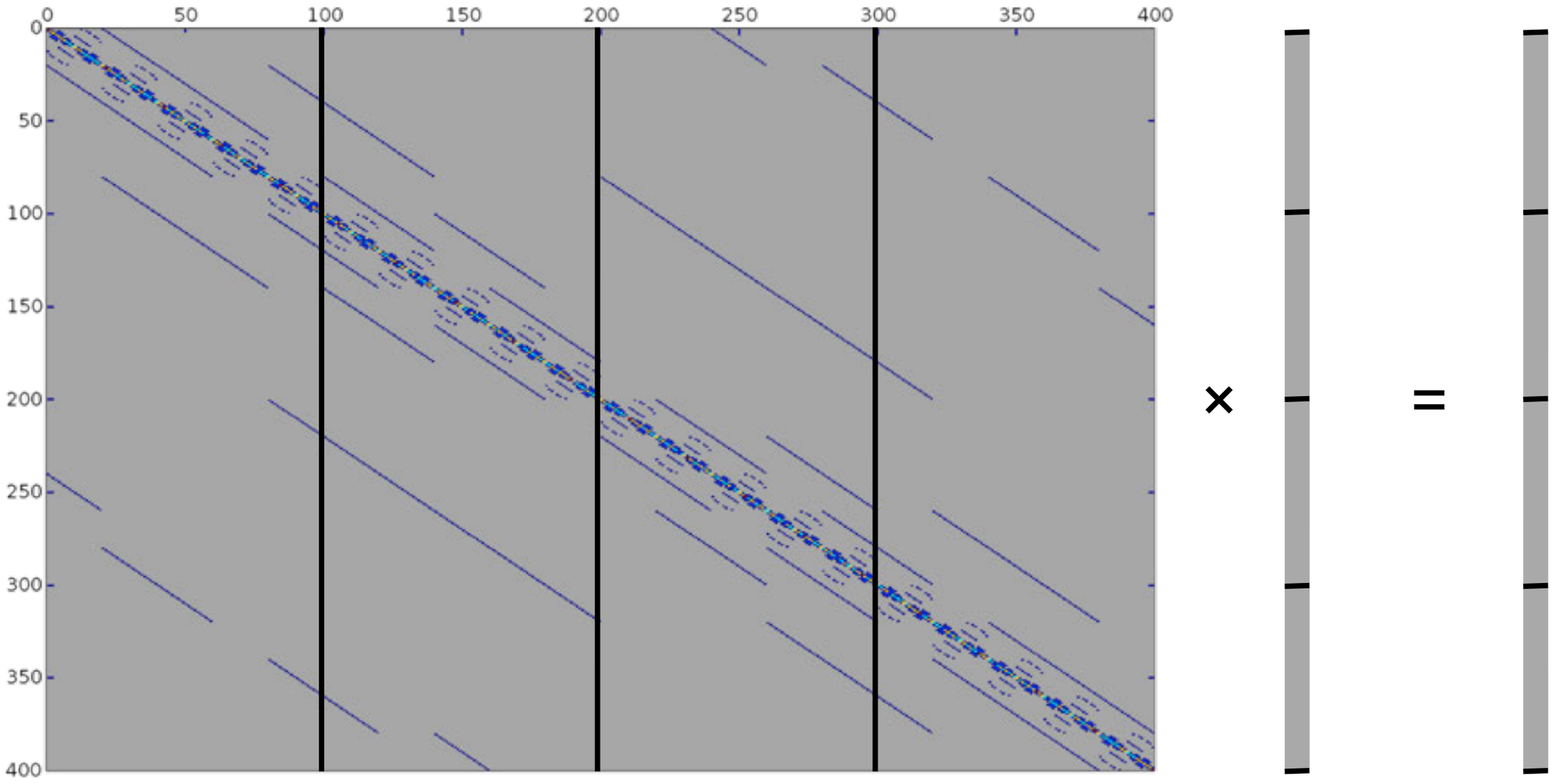
$\mathtt{m}_\uparrow$	bits	state	$\mathtt{i}_\uparrow$
0	000		
1	001		
2	010		
3	011	$c_{0\uparrow}^{\dagger} c_{1\uparrow}^{\dagger} \|0\rangle$	0
4	100		
5	101	$c_{0\uparrow}^{\dagger} c_{2\uparrow}^{\dagger} \|0\rangle$	1
6	110	$c_{1\uparrow}^{\dagger} c_{2\uparrow}^{\dagger} \|0\rangle$	2
7	111		

$\mathtt{m}_\downarrow$	bits	state	$\mathtt{i}_\downarrow$
0	000		
1	001	$c_{0\downarrow}^{\dagger} \|0\rangle$	0
2	010	$c_{1\downarrow}^{\dagger} \|0\rangle$	1
3	011		
4	100	$c_{2\downarrow}^{\dagger} \|0\rangle$	2
5	101		
6	110		
7	111		



sparse matrix-vector product

$$H \quad |\Psi_i\rangle \quad = \quad |\Psi_{i+1}\rangle$$



sparse matrix-vector product: OpenMP

$$w = w + H\,v \qquad H = \sum_{\langle ij\rangle,\sigma} t_{i,j}\, c^{\dagger}_{j,\sigma} c_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

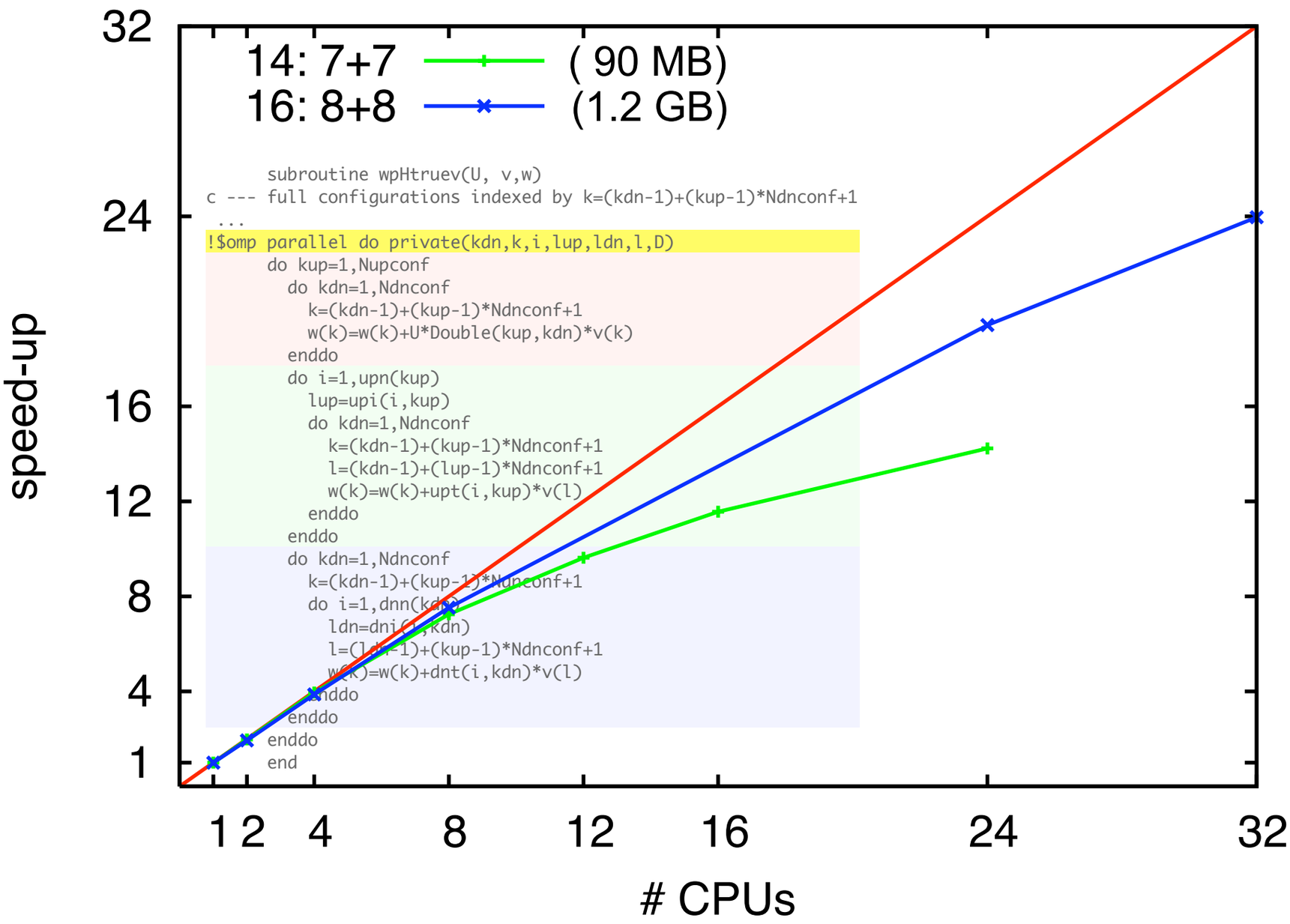
```
      subroutine wpHtruev(U, v,w)
c --- full configurations indexed by k=(kdn-1)+(kup-1)*Ndnconf+1
 ...
!$omp parallel do private(kdn,k,i,lup,ldn,l,D)
      do kup=1,Nupconf
        do kdn=1,Ndnconf
          k=(kdn-1)+(kup-1)*Ndnconf+1
          w(k)=w(k)+U*Double(kup,kdn)*v(k)
        enddo
        do i=1,upn(kup)
          lup=upi(i,kup)
          do kdn=1,Ndnconf
            k=(kdn-1)+(kup-1)*Ndnconf+1
            l=(kdn-1)+(lup-1)*Ndnconf+1
            w(k)=w(k)+upt(i,kup)*v(l)
          enddo
        enddo
        do kdn=1,Ndnconf
          k=(kdn-1)+(kup-1)*Ndnconf+1
          do i=1,dnn(kdn)
            ldn=dni(i,kdn)
            l=(ldn-1)+(kup-1)*Ndnconf+1
            w(k)=w(k)+dnt(i,kdn)*v(l)
          enddo
        enddo
      enddo
      end
```

$$U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

$$\sum_{\langle ij\rangle,\sigma=\uparrow} t_{i,j}\, c^{\dagger}_{j,\sigma} c_{i,\sigma}$$

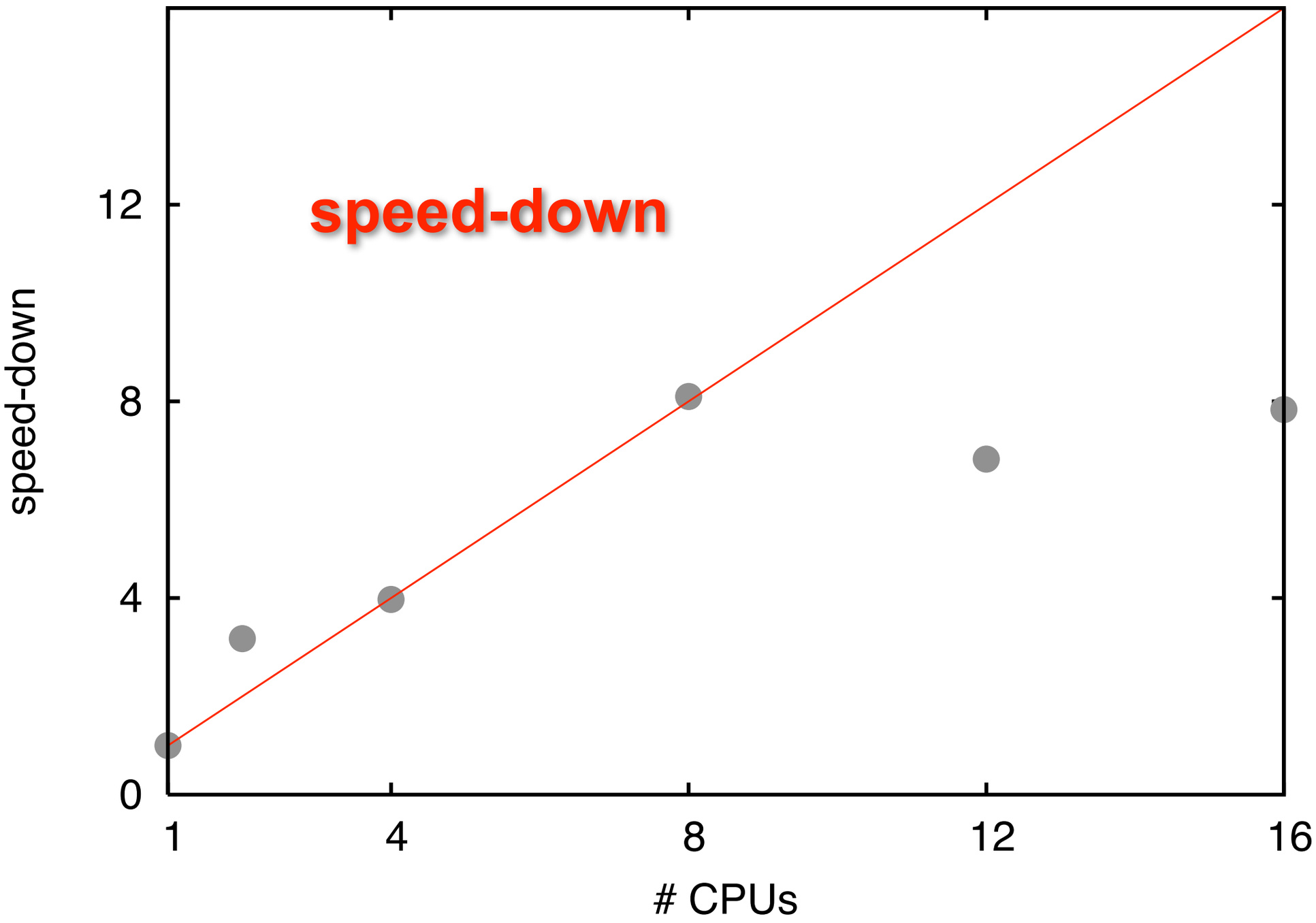
$$\sum_{\langle ij\rangle,\sigma=\downarrow} t_{i,j}\, c^{\dagger}_{j,\sigma} c_{i,\sigma}$$

OpenMP on Jump



distributed memory

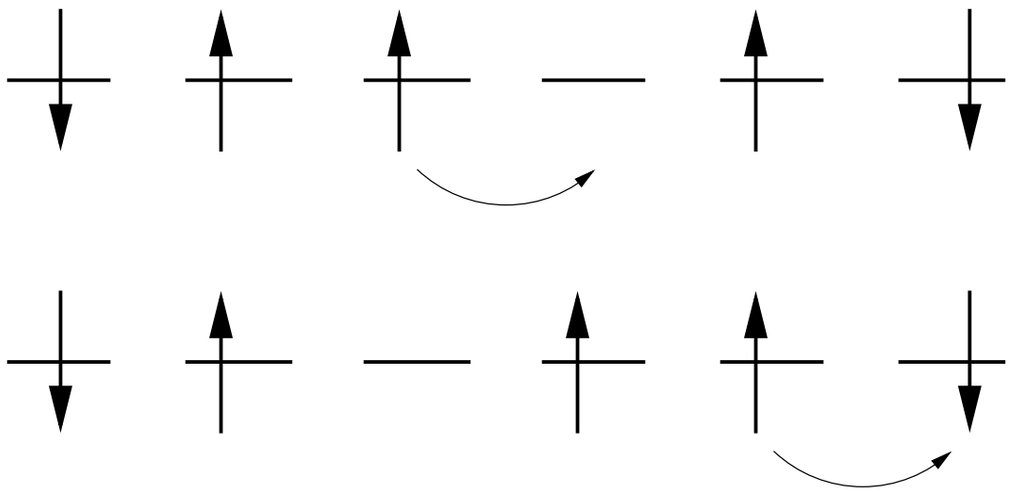
MPI-2: one-sided communication



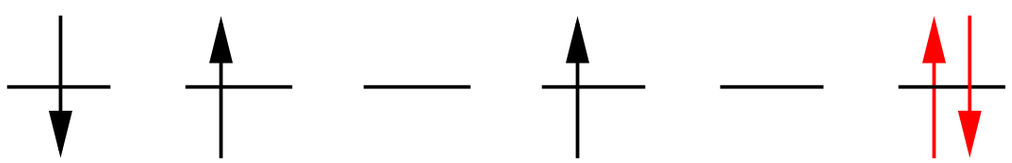
Hubbard model

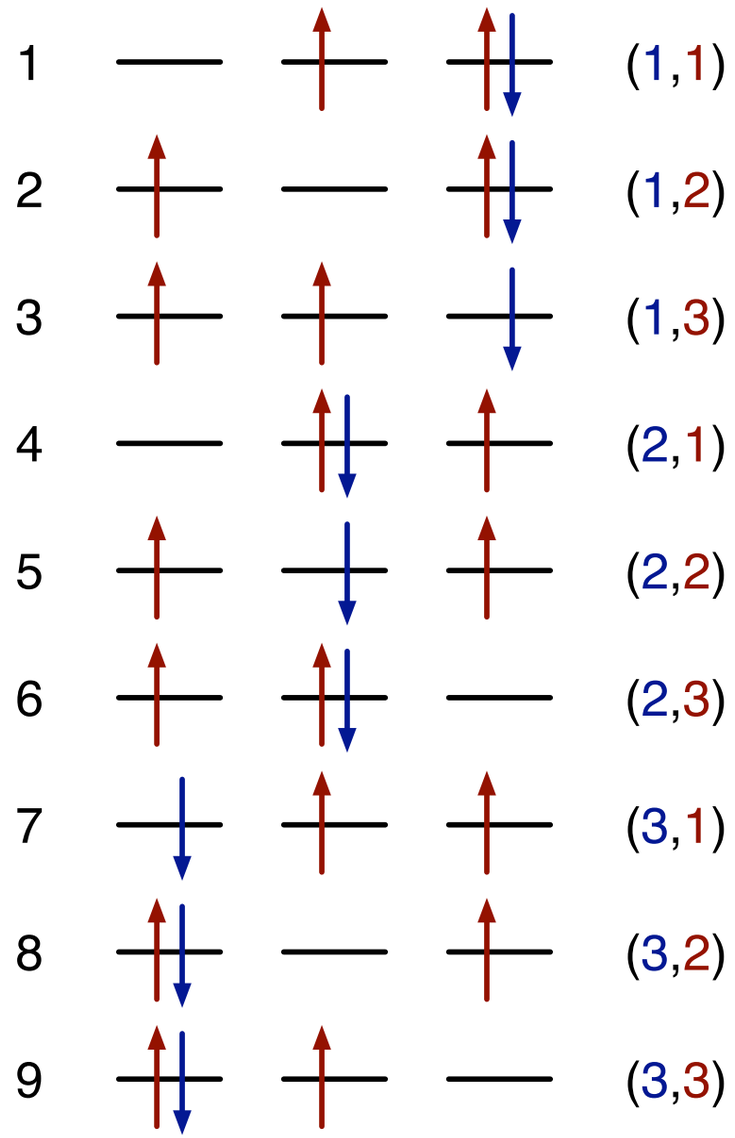
$$H = \sum_{\langle ij \rangle, \sigma} \; t_{i,j} \, c^{\dagger}_{j,\sigma} c_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

hopping: spin unchanged

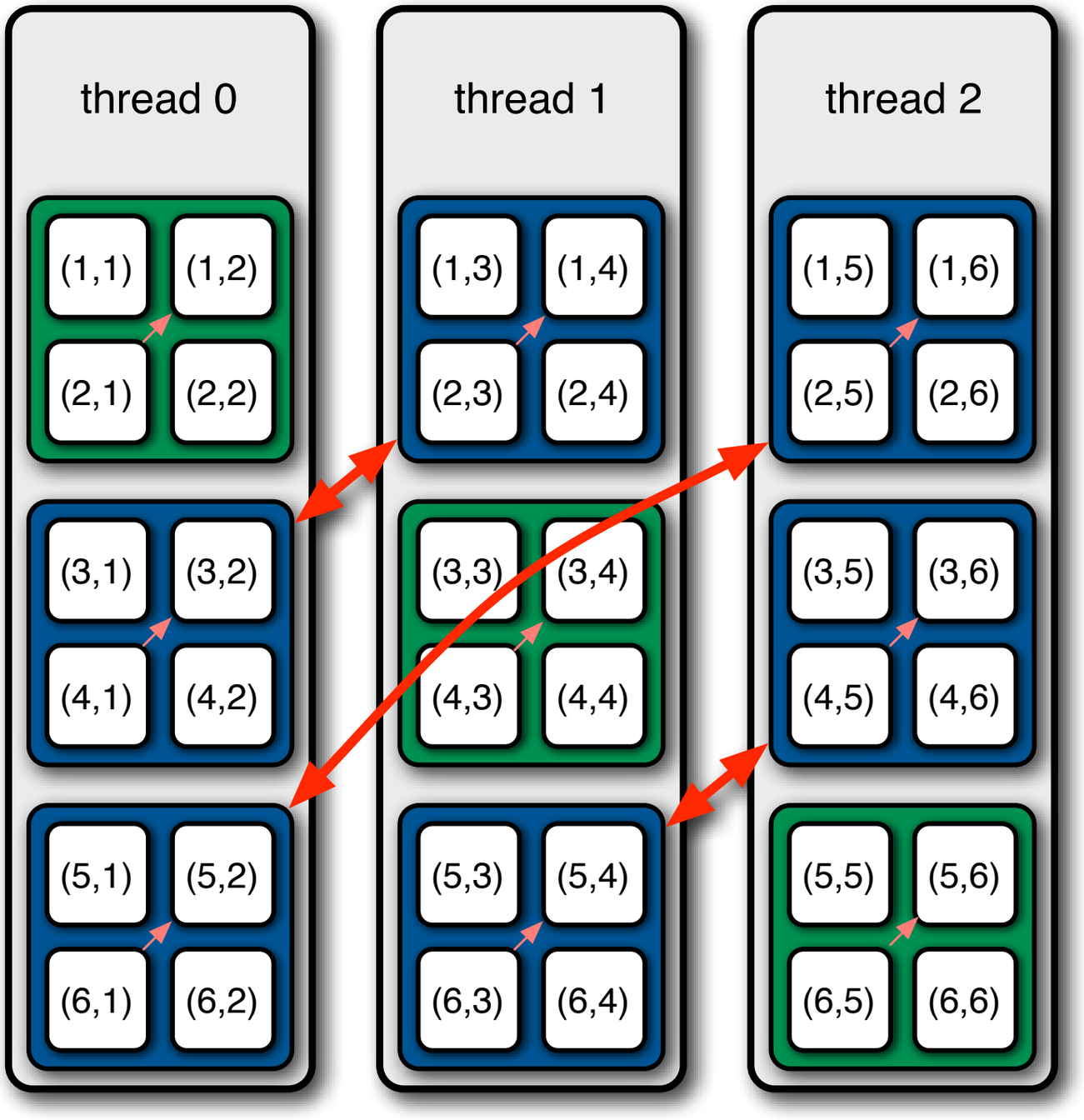


interaction diagonal





Idea: matrix transpose of $v(i_{\downarrow},i_{\uparrow})$



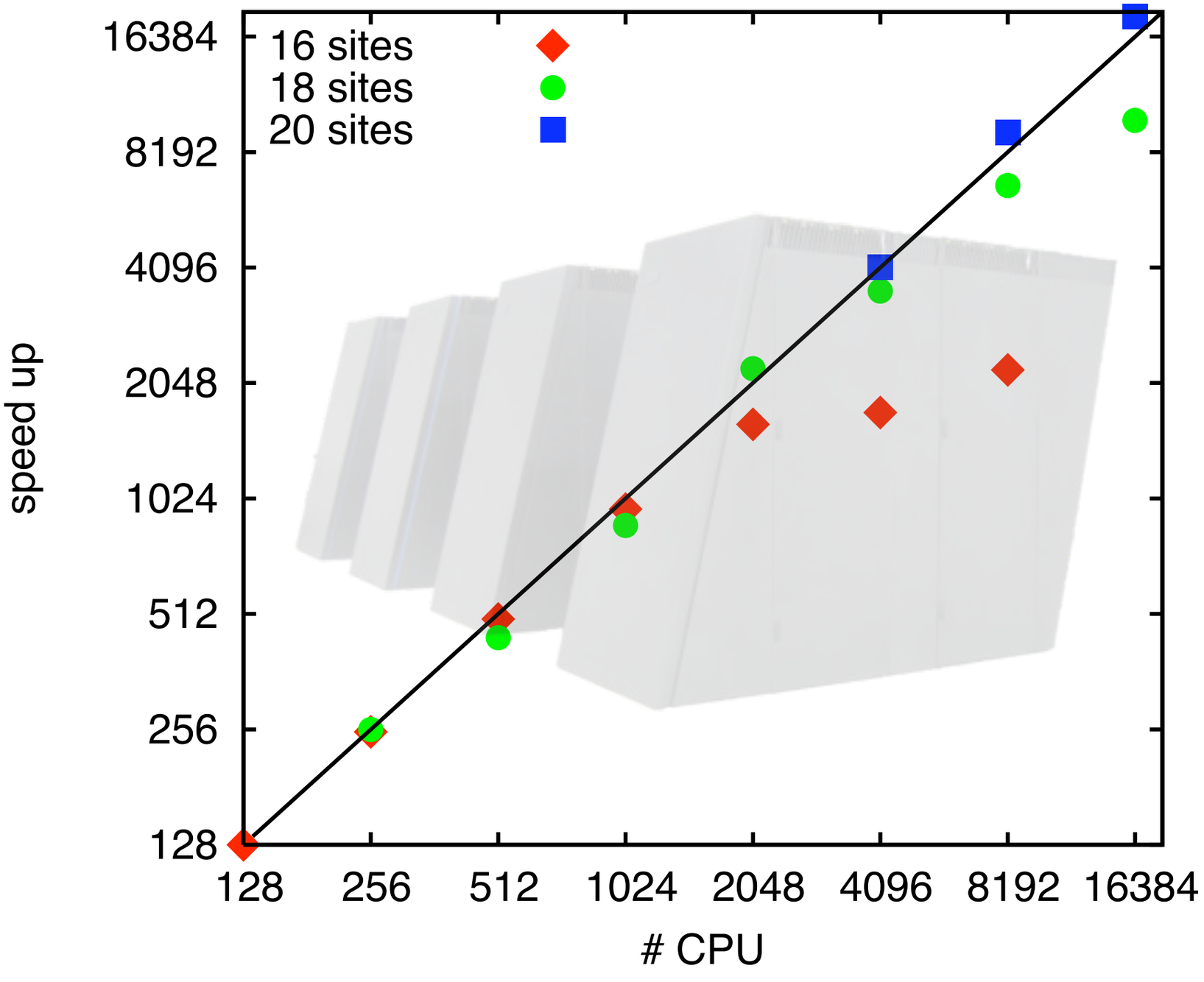
Lanczos-vector as matrix:
$v(i_{\downarrow},i_{\uparrow})$

before transpose: ↓-hops local
after transpose: ↑-hops local

implementation:

`MPI_alltoall` $(N_{\downarrow} = N_{\uparrow})$
`MPI_alltoallv` $(N_{\downarrow} \neq N_{\uparrow})$

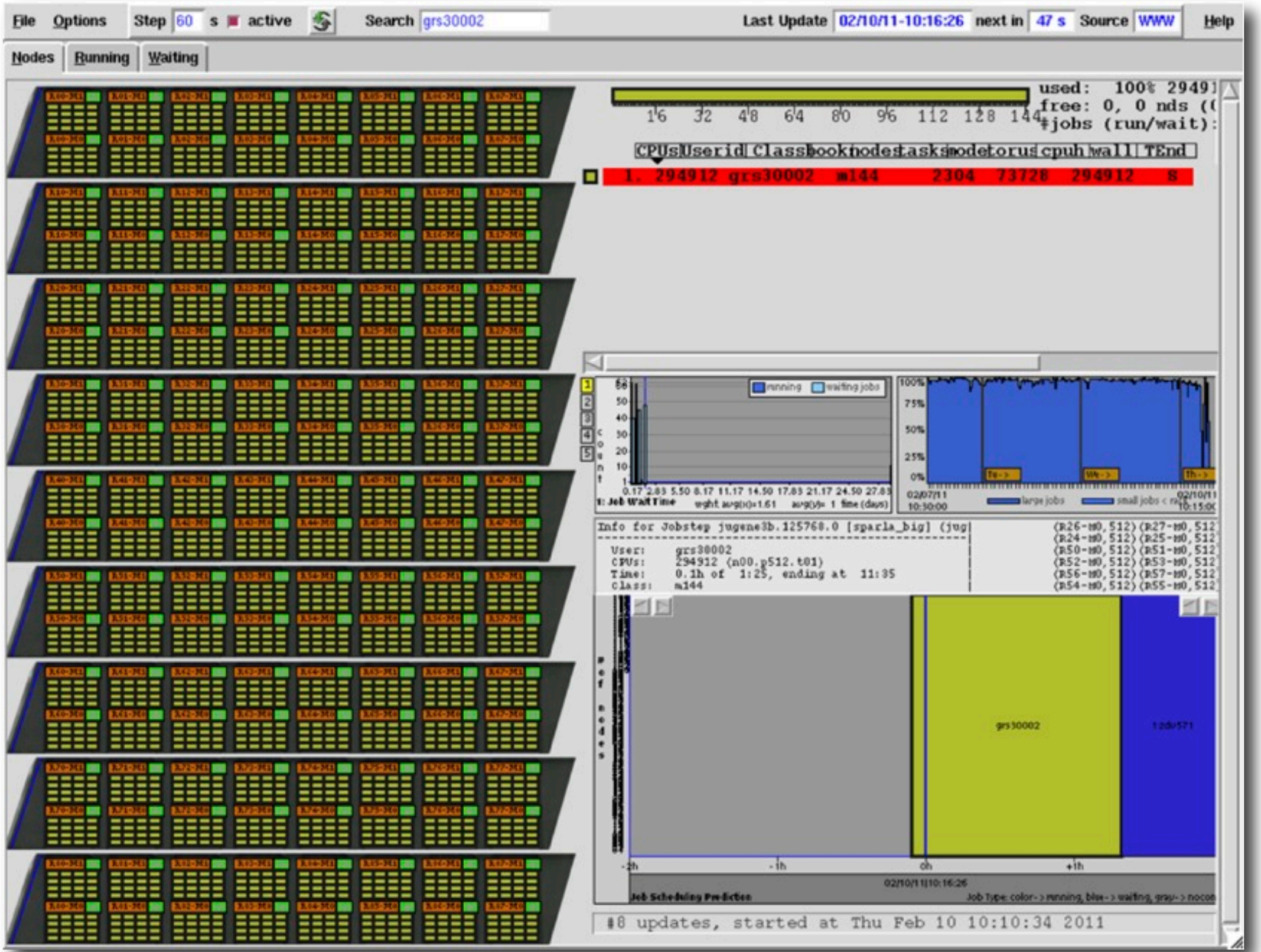
Implementation on IBM BlueGene/P



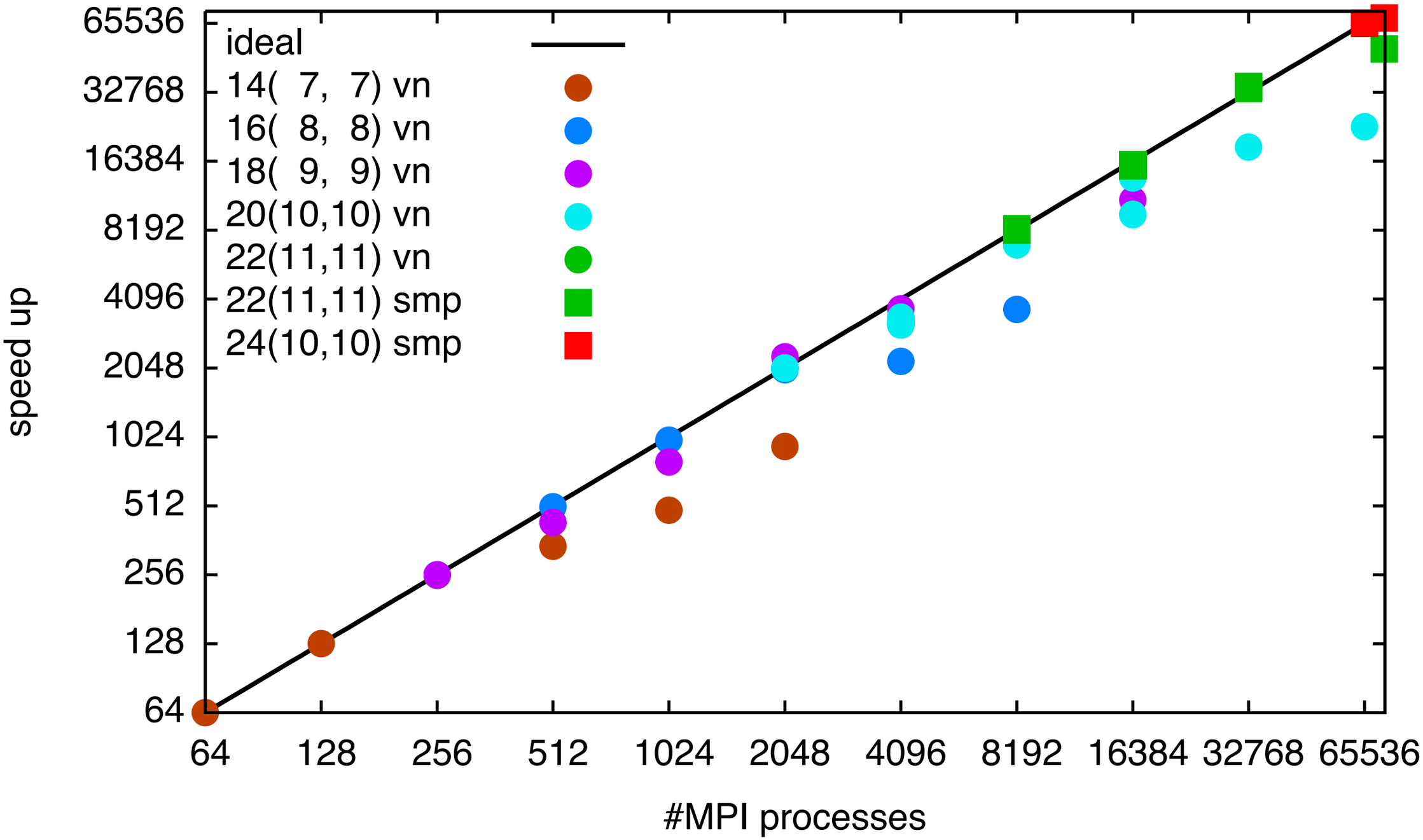
sites	memory
16	1 GB
18	18 GB
20	254 GB

Adv. Parallel Computing **15**, 601 (2008)

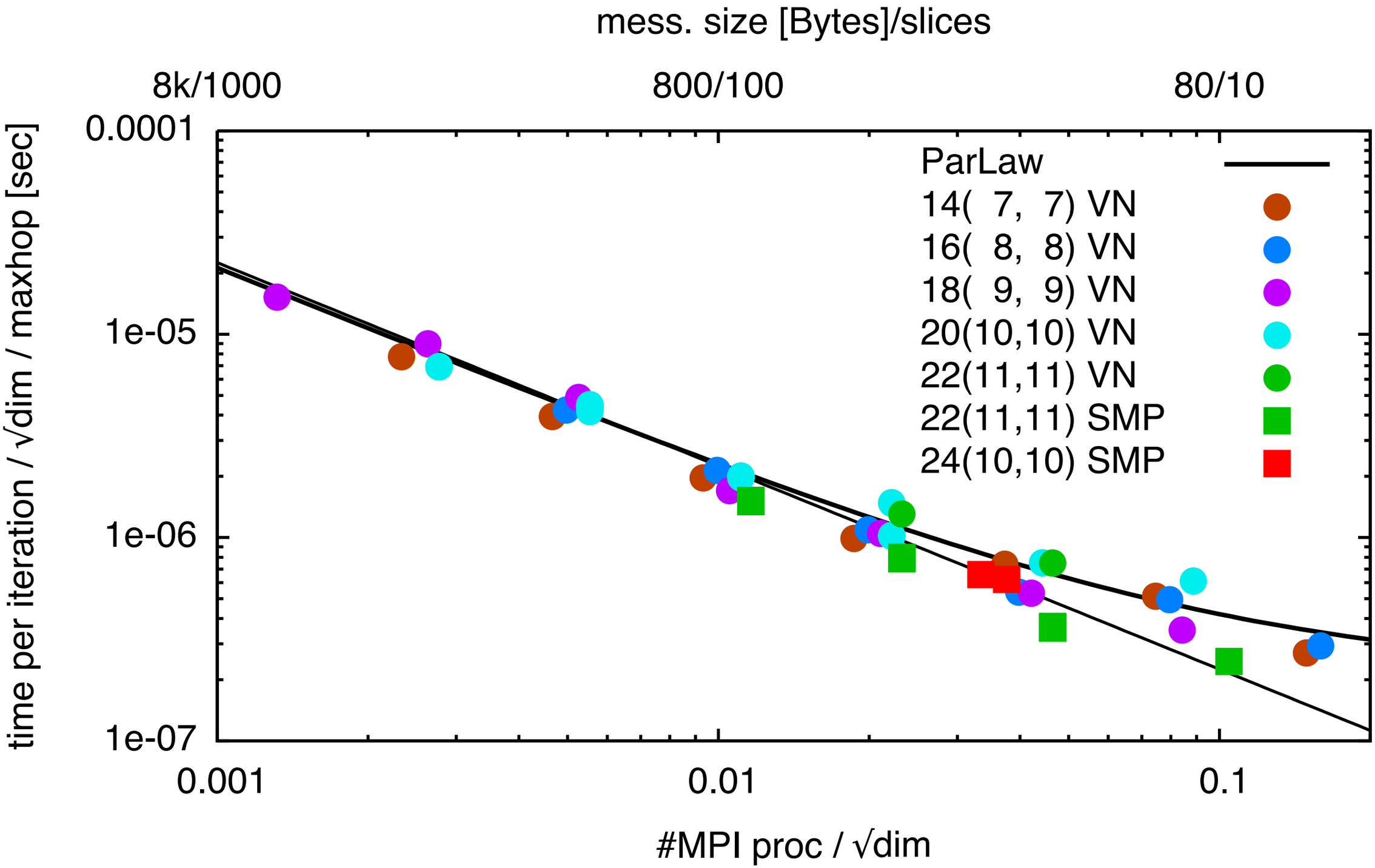
performance on full Jugene?



performance on full Jugene!



performance on full Jugene!



Spin-Systems

pairwise interaction

$$\sum_{\langle j,k \rangle} J_{jk}\, \mathbf{S}_j \mathbf{S}_k$$

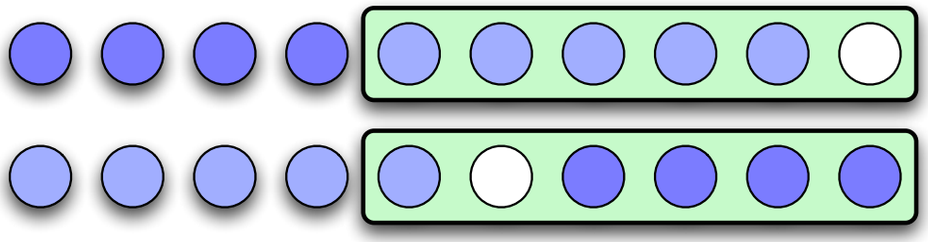
spin configurations

$$\underbrace{100100}_{i_>}\ \underbrace{1100111}_{i_<}$$

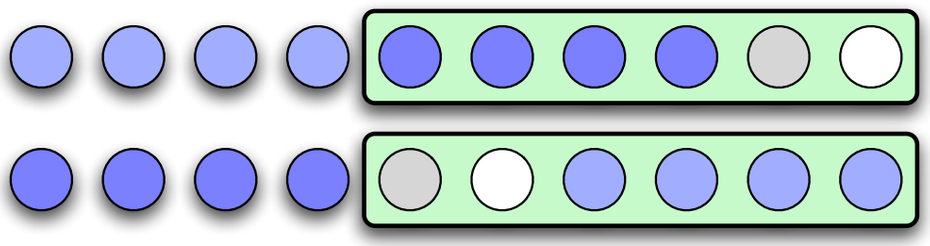
matrix transpose via `MPI_alltoallv` or systolic algorithm

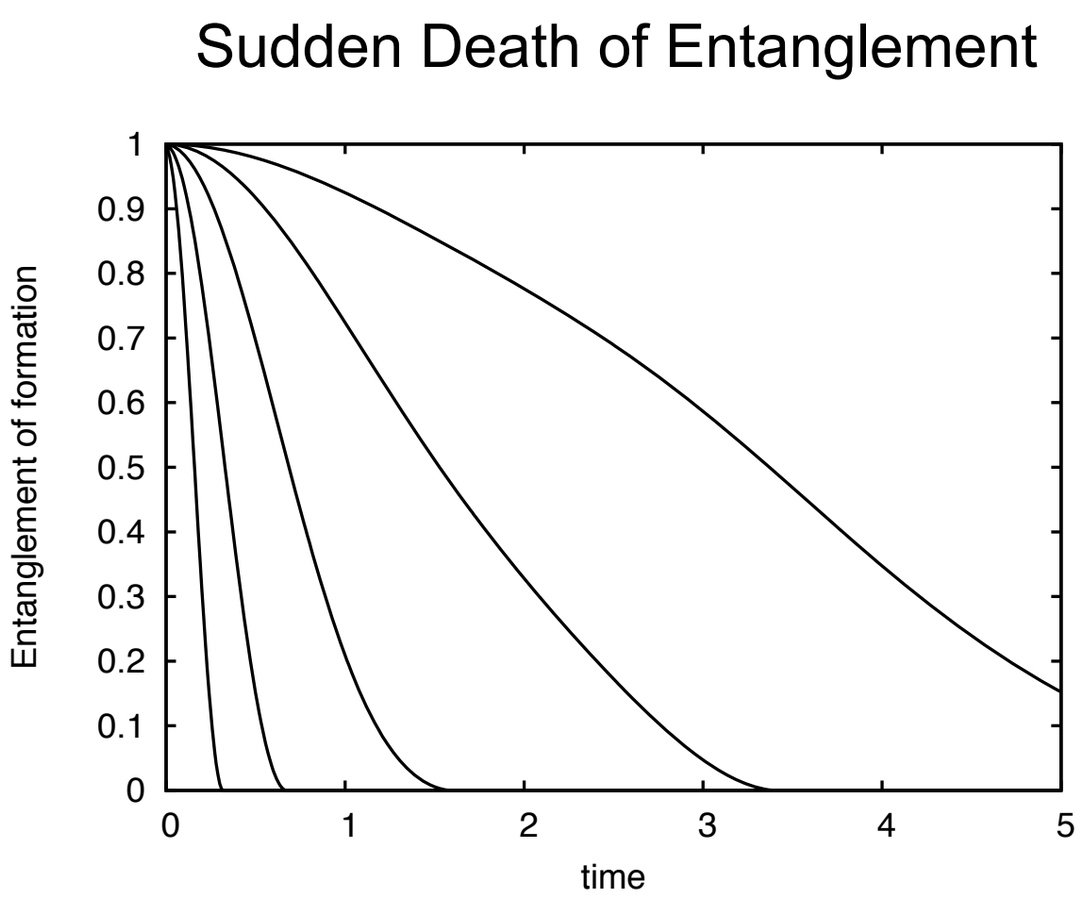
decoherence: single spin

$$H = \mu_B B_0 S_0^z + \sum_k A_k\, \mathbf{S}_k \mathbf{S}_0$$



decoherence: entanglement fidelity of 2-qubit gates





transpose for spins

43 210	43 210	43 210	43 210
00 000	01 000	10 000	11 000
00 001	01 001	10 001	11 001
00 010	01 010	10 010	11 010
00 011	01 011	10 011	11 011
00 100	01 100	10 100	11 100
00 101	01 101	10 101	11 101
00 110	01 110	10 110	11 110
00 111	01 111	10 111	11 111

0	8	16	24
1	9	17	25
2	10	18	26
3	11	19	27
4	12	20	28
5	13	21	29
6	14	22	30
7	15	23	31

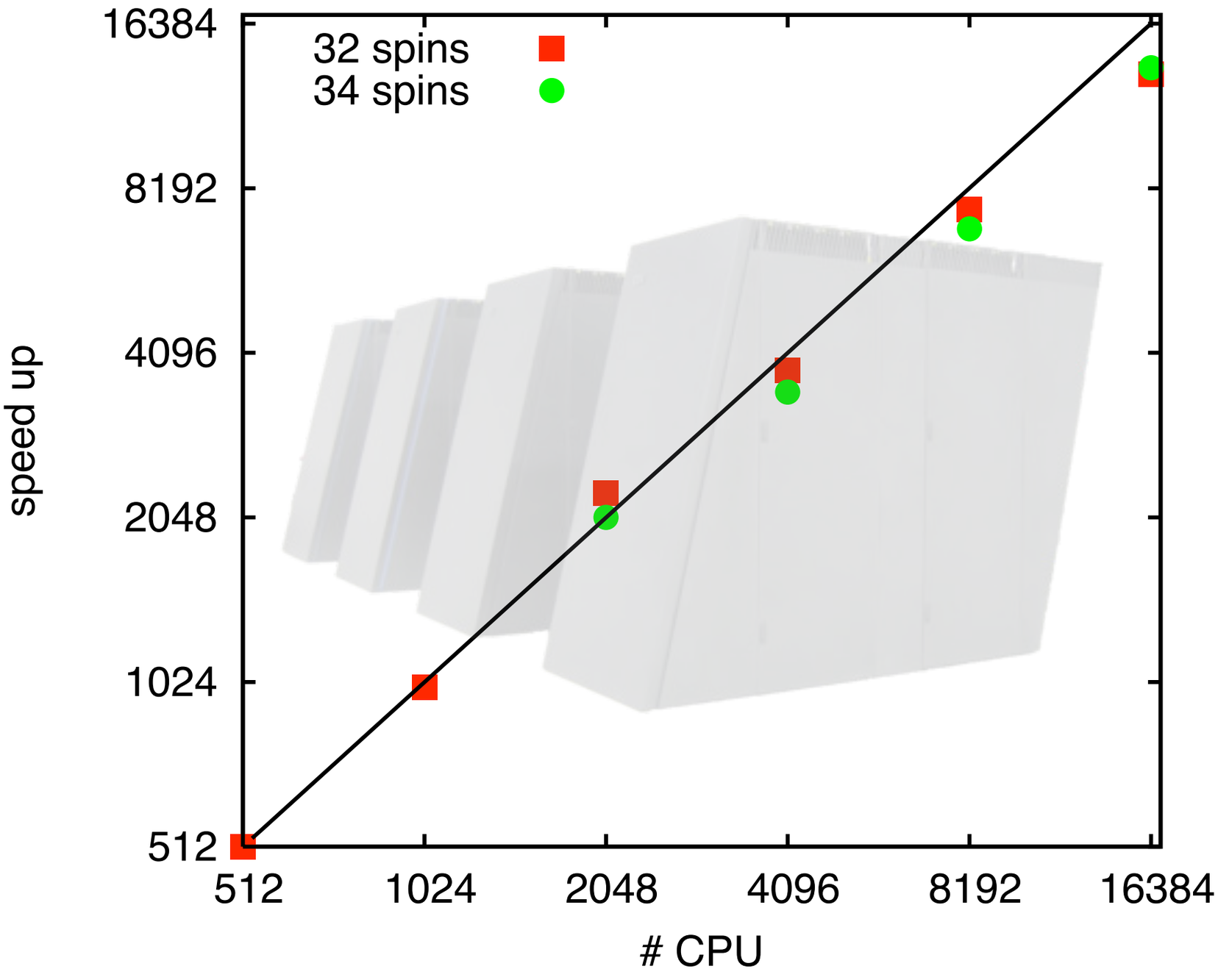
MPI_alltoall

21 043	21 043	21 043	21 043
00 000	01 000	10 000	11 000
00 100	01 100	10 100	11 100
00 001	01 001	10 001	11 001
00 101	01 101	10 101	11 101
00 010	01 010	10 010	11 010
00 110	01 110	10 110	11 110
00 011	01 011	10 011	11 011
00 111	01 111	10 111	11 111

0	2	4	6
1	3	5	7
8	10	12	14
9	11	13	15
16	18	20	22
17	19	21	23
24	26	28	30
25	27	29	31

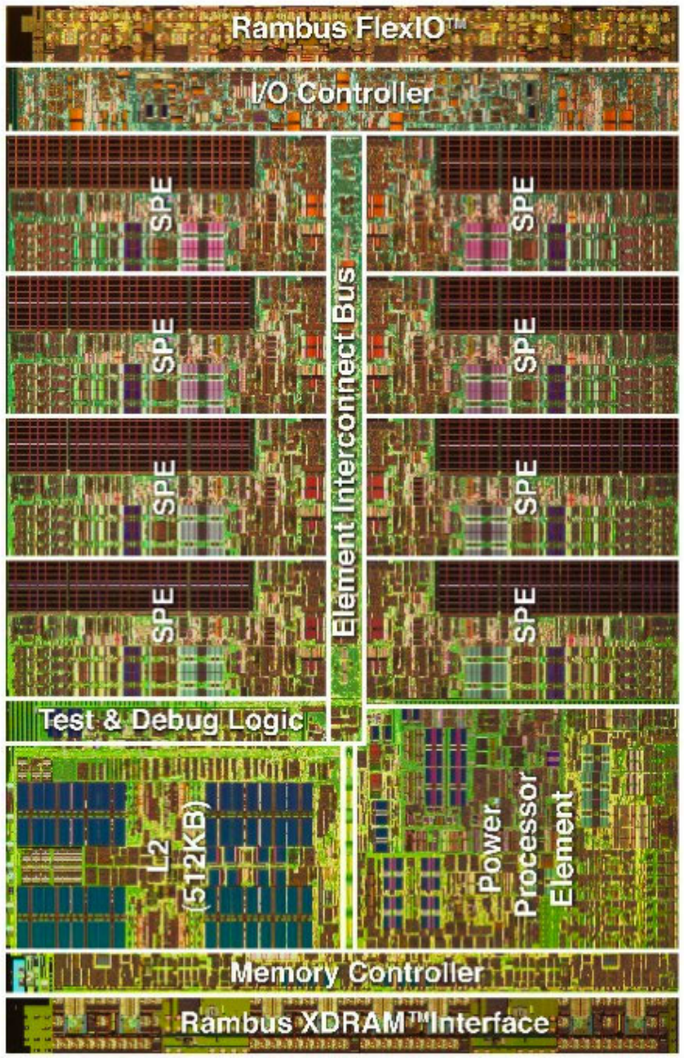
bit reordering: 43 210 ---> 21 034 -> 21 430 (mirror $i_<$)

Heisenberg model on IBM BlueGene/P



spins	memory
32	32 GB
34	256 GB

Cell Broadband Engine



1 Power Processor
8 SPE with 256 kB
fast local store each

spin models

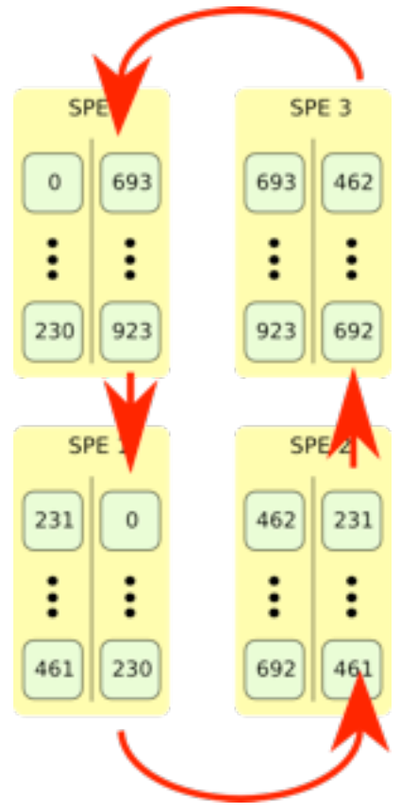
additional partitioning
of local memory

spin configurations

$$\underbrace{100100}_{i_{\text{distr}}}\ \underbrace{1100111}_{i_{\text{cell}}}\ \underbrace{101001}_{i_{\text{SPE}}}$$

Lanczos on Cell

rotate spin-slice
through local store



JUICE report; FZJ-ZAM-IB-13
PARA 2008, Trondheim

DMFT and optimal bath-parametrization

reminder: single-site DMFT

Hubbard model

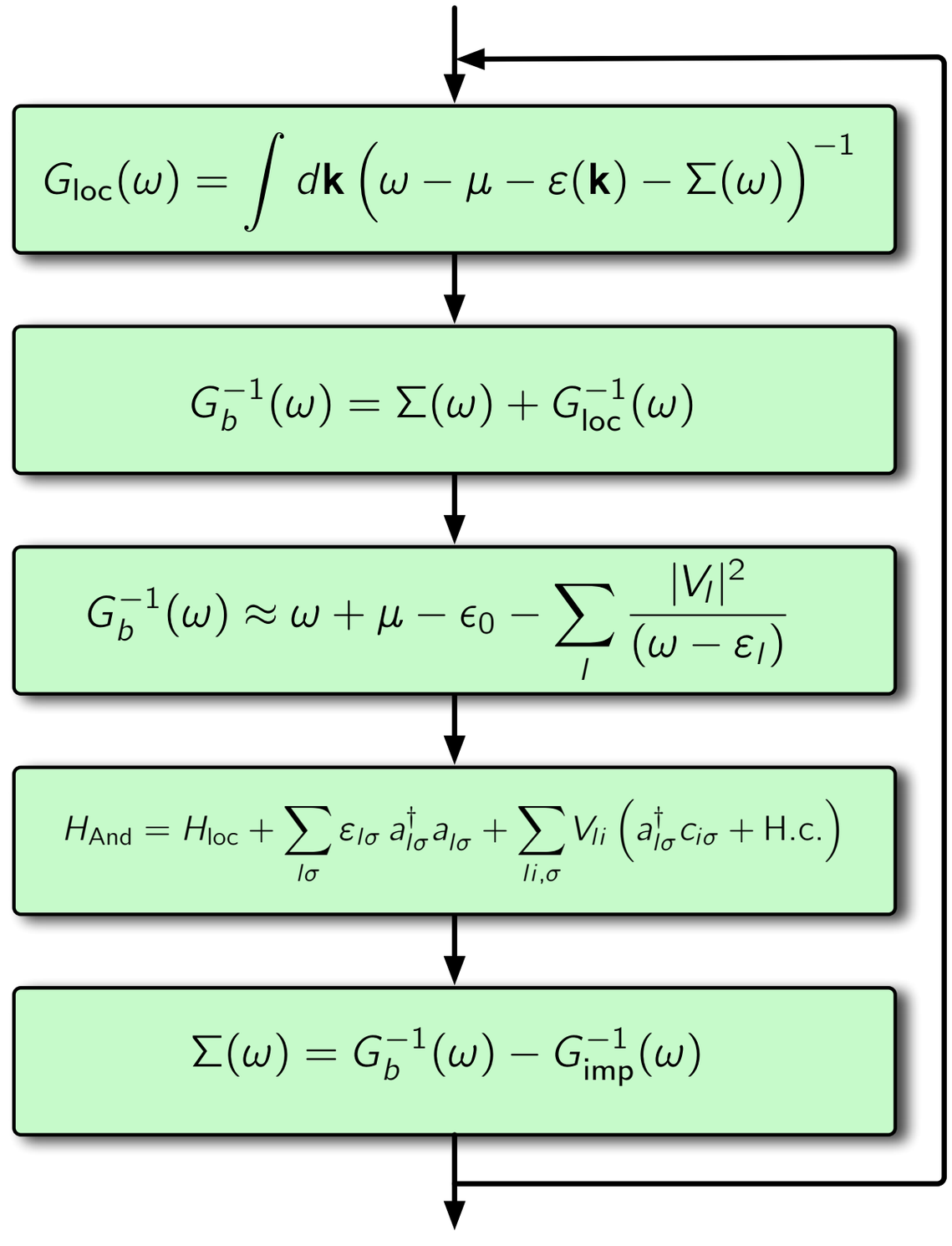
$$H = -\sum_{ij\sigma} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Bloch: $e^{-ik}\ 1\ e^{ik}\ e^{2ik}\ e^{3ik}\ e^{4ik}$

$$c^{\dagger}_{k\sigma} = \sum e^{ikr_i} c^{\dagger}_{i\sigma} \Rightarrow H(\mathbf{k}) = \epsilon(\mathbf{k})$$

project to single site: $\int d\mathbf{k}\, H(\mathbf{k}) = \epsilon_0$

$$H_{\text{loc}} = \epsilon_0 + U\, n_{\uparrow} n_{\downarrow}$$



bath parametrization

$$G_b^{-1}(\omega) = G_{\text{loc}}^{-1}(\omega) + \Sigma(\omega) = \omega + \mu - \int_{-\infty}^{\infty} d\omega' \, \frac{\Delta(\omega')}{\omega - \omega'}$$

$$G_{\text{And}}^{-1}(\omega) = \omega + \mu - \sum_{l=1}^{N_b} \frac{V_l^2}{\omega - \varepsilon_l}$$

how to determine bath parameters ε_l and V_l?

$$H_{\text{And}}^0 = \begin{pmatrix} 0 & V_1 & V_2 & V_3 & \cdots \\ V_1 & \varepsilon_1 & 0 & 0 & \\ V_2 & 0 & \varepsilon_2 & 0 & \\ V_3 & 0 & 0 & \varepsilon_3 & \\ \vdots & & & & \ddots \end{pmatrix}$$

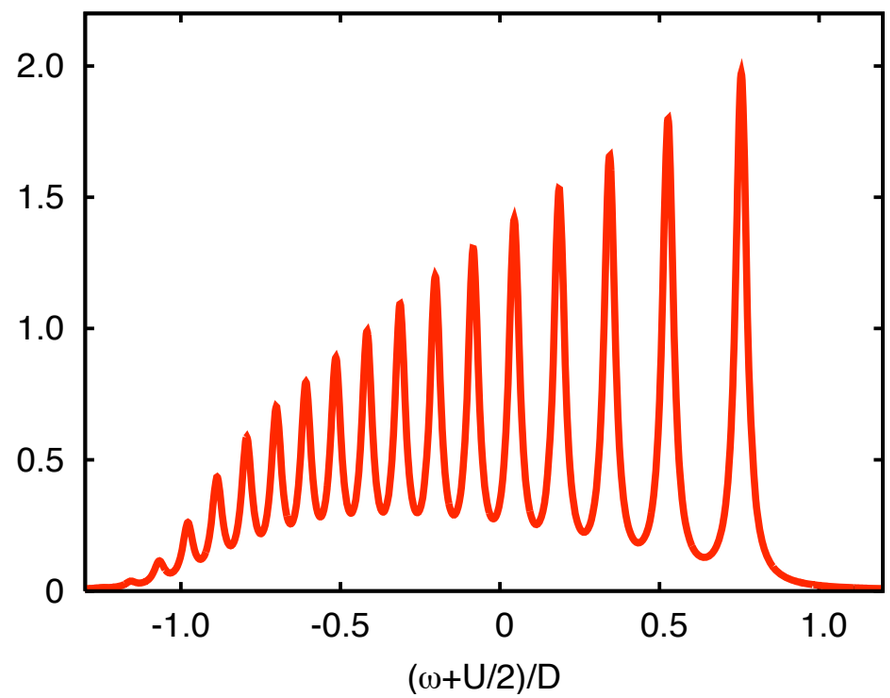
$$H_{\text{And}} = \varepsilon_0 \sum_\sigma n_\sigma + U n_\uparrow n_\downarrow + \sum_\sigma \sum_{l=1}^{N_b} \left(\varepsilon_l n_{l\sigma} + V_l \left(a_{l\sigma}^\dagger c_\sigma + c_\sigma^\dagger a_{l\sigma} \right) \right)$$

use Lanczos parameters

Bethe lattice: $$\int d\omega' \frac{\Delta(\omega')}{\omega - \omega'} = t^2 G_{\mathrm{imp}}(\omega)$$

$$t^2 G^{<}(\omega) + t^2 G^{>}(\omega) = \frac{t^2 {b_0^{<}}^2}{\omega + a_0^{<} - \frac{{b_1^{<}}^2}{\omega + a_1^{<} - \cdots}} + \frac{t^2 {b_0^{>}}^2}{\omega - a_0^{>} - \frac{{b_1^{>}}^2}{\omega - a_1^{>} - \cdots}}$$

$$H^0_{\mathrm{And}} = \begin{pmatrix}
0 & t^2 b_0^{<} & & & \cdots & t^2 b_0^{>} & & \\
t^2 b_0^{<} & -a_0^{<} & b_1^{<} & & & & & \\
 & b_1^{<} & -a_1^{<} & b_2^{<} & & & & \\
 & & b_2^{<} & -a_2^{<} & \ddots & & & \\
\vdots & & & \ddots & \ddots & & & \\
t^2 b_0^{>} & & & & & a_0^{>} & b_1^{>} & \\
 & & & & & b_1^{>} & a_1^{>} & b_2^{>} \\
 & & & & & & b_2^{>} & a_2^{>} & \ddots \\
 & & & & & & & \ddots
\end{pmatrix}$$



fit on imaginary axis

fictitious temperature: Matsubara frequencies

$$\chi^2(\{V_l, \varepsilon_l\}) = \sum_{n=0}^{n_{\max}} w(i\omega_n) \left| \mathcal{G}^{-1}(i\omega_n) - \mathcal{G}^{-1}_{\mathrm{And}}(i\omega_n) \right|^2$$

weight function $w(i\omega_n)$:

- emphasize region close to real axis
- make sum converge for $n \to \infty$ (sum rule)

reminder: single-site DMFT

Hubbard model

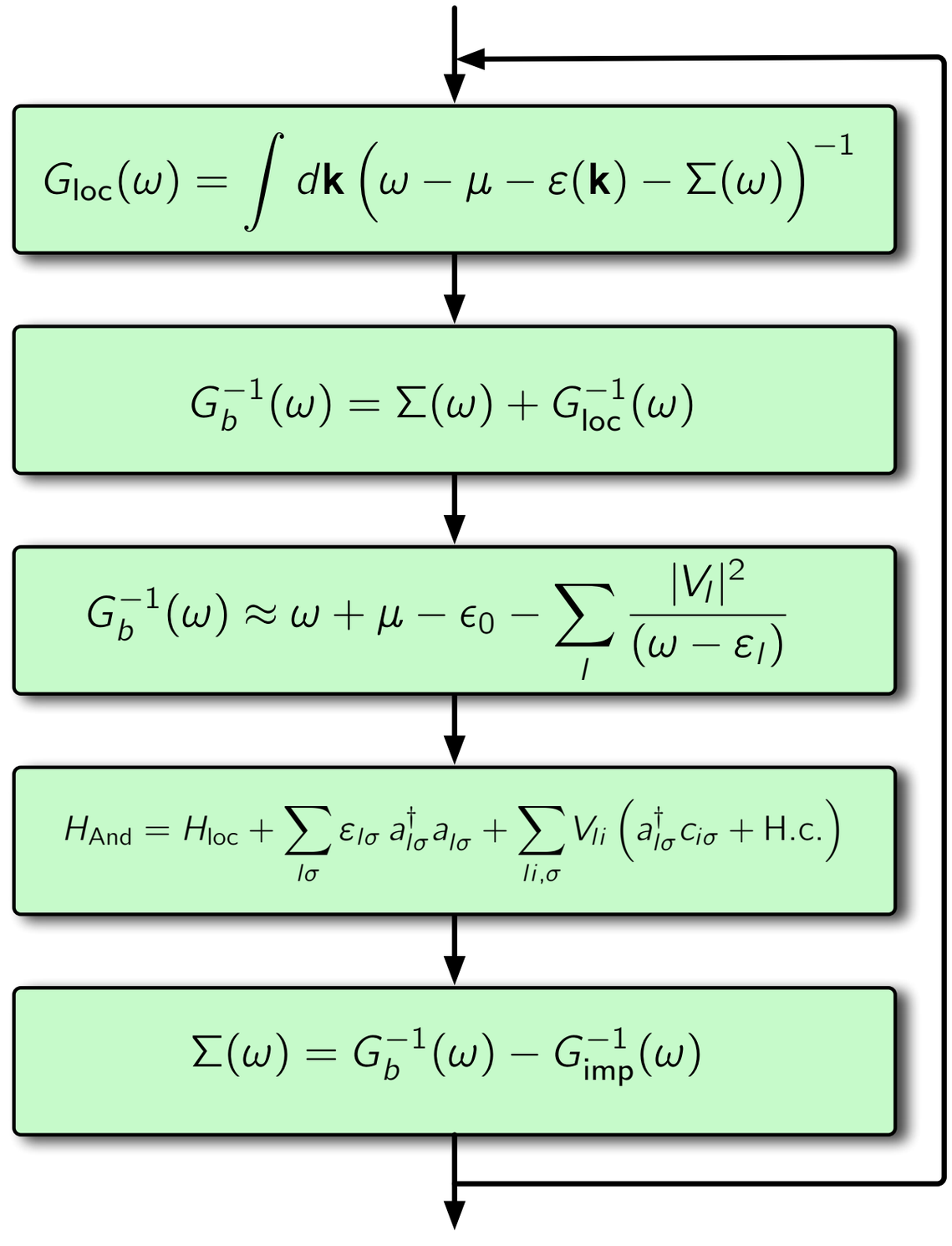
$$H = -\sum_{ij\sigma} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Bloch: $e^{-ik}\ 1\ e^{ik}\ e^{2ik}\ e^{3ik}\ e^{4ik}$

$$c^{\dagger}_{k\sigma} = \sum e^{ikr_i} c^{\dagger}_{i\sigma} \Rightarrow H(\mathbf{k}) = \epsilon(\mathbf{k})$$

project to single site: $\int d\mathbf{k}\, H(\mathbf{k}) = \epsilon_0$

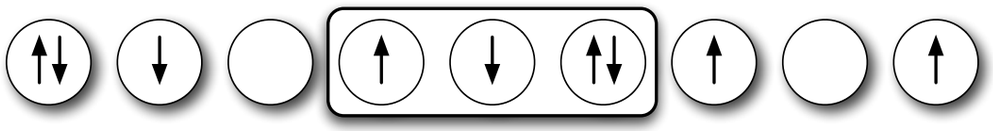
$$H_{\text{loc}} = \epsilon_0 + U\, n_{\uparrow} n_{\downarrow}$$



DMFT for clusters

Hubbard model

$$H = -\sum_{ij\sigma} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

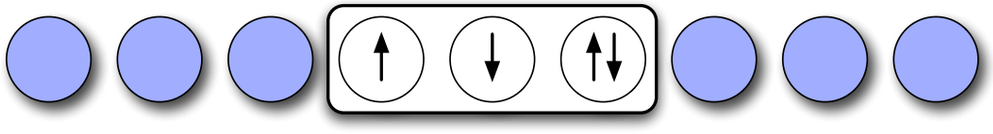


Bloch: $e^{-ik}\ 1\ e^{ik}\ e^{2ik}\ e^{3ik}\ e^{4ik}$

$$c^{\dagger}_{\tilde{k}\sigma} = \sum e^{i\tilde{k}r_i} c^{\dagger}_{i\sigma} \Rightarrow \mathbf{H}(\tilde{\mathbf{k}})$$

project to cluster: $\int d\tilde{\mathbf{k}}\, \mathbf{H}(\tilde{\mathbf{k}}) = \mathbf{H}_c$

$$H_{\mathrm{loc}} = \mathbf{H}_c + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



$$\boldsymbol{G}(\omega) = \int d\tilde{\mathbf{k}} \left(\omega + \mu - \mathbf{H}(\tilde{\mathbf{k}}) - \boldsymbol{\Sigma}_c(\omega)\right)^{-1}$$

$$\mathbf{G}_b^{-1}(\omega) = \boldsymbol{\Sigma}_c(\omega) + \mathbf{G}^{-1}(\omega)$$

$$\mathbf{G}_b^{-1}(\omega) \approx \omega + \mu - \mathbf{H}_c - \boldsymbol{\Gamma}\,[\omega - \mathbf{E}]^{-1}\boldsymbol{\Gamma}^{\dagger}$$

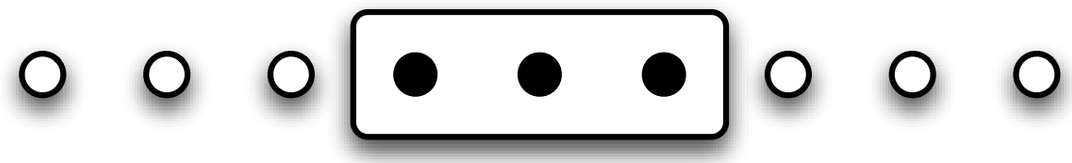
$$H_{\mathrm{And}} = H_{\mathrm{loc}} + \sum_{lm,\sigma} E_{lm,\sigma}\, a^{\dagger}_{l\sigma} a_{m\sigma} + \sum_{li,\sigma} \Gamma_{li} \left(a^{\dagger}_{l\sigma} c_{i\sigma} + \mathrm{H.c.}\right)$$

$$\boldsymbol{\Sigma}_c(\omega) = \mathbf{G}_b^{-1}(\omega) - \mathbf{G}_c^{-1}(\omega)$$

DCA

3-site cluster

$$\mathbf{H}(\tilde{k}) = -t \begin{pmatrix} 0 & e^{i\tilde{k}} & e^{-i\tilde{k}} \\ e^{-i\tilde{k}} & 0 & e^{i\tilde{k}} \\ e^{i\tilde{k}} & e^{-i\tilde{k}} & 0 \end{pmatrix}$$



$$\mathbf{H}_c = \frac{3}{2\pi} \int_{-\pi/3}^{\pi/3} d\tilde{k}\, \mathbf{H}(\tilde{k}) = -\frac{3\sqrt{3}}{2\pi}\, t \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

translation symmetry
coarse-grained Hamiltonian

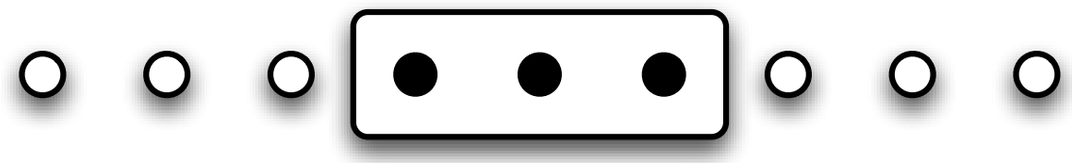
DCA

$$\mathbf{H}(\tilde{k}) = -t \begin{pmatrix} 0 & e^{i\tilde{k}} & e^{-i\tilde{k}} \\ e^{-i\tilde{k}} & 0 & e^{i\tilde{k}} \\ e^{i\tilde{k}} & e^{-i\tilde{k}} & 0 \end{pmatrix}$$

$$\mathbf{H}_c = \frac{3}{2\pi} \int_{-\pi/3}^{\pi/3} d\tilde{k}\, \mathbf{H}(\tilde{k}) = -\frac{3\sqrt{3}}{2\pi}\, t \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

translation symmetry
coarse-grained Hamiltonian

CDMFT

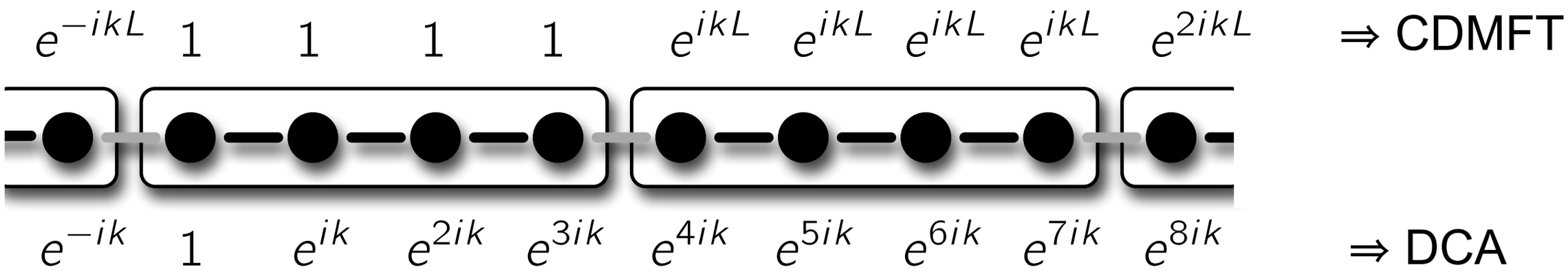


no translation symmetry
original Hamiltonian on cluster

$$\mathbf{H}(\tilde{k}) = -t \begin{pmatrix} 0 & 1 & e^{-3i\tilde{k}} \\ 1 & 0 & 1 \\ e^{3i\tilde{k}} & 1 & 0 \end{pmatrix}$$

$$\mathbf{H}_c = \frac{3}{2\pi} \int_{-\pi/3}^{\pi/3} d\tilde{k}\, \mathbf{H}(\tilde{k}) = -t \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

DCA – CDMFT



$$\tilde{c}^{\mathrm{CDMFT}}_{\mathrm{R}_i\sigma}(\tilde{\mathbf{k}}) = \sum_{\tilde{\mathrm{r}}} e^{-i\tilde{\mathrm{k}}\tilde{\mathrm{r}}}\, c_{\tilde{\mathrm{r}}+\mathrm{R}_i,\sigma}$$

$$\tilde{c}^{\mathrm{DCA}}_{\mathrm{R}_i\sigma}(\tilde{\mathbf{k}}) = \sum_{\tilde{\mathrm{r}}} e^{-i\tilde{\mathrm{k}}(\tilde{\mathrm{r}}+\mathrm{R}_i)}\, c_{\tilde{\mathrm{r}}+\mathrm{R}_i,\sigma}$$

gauge determines cluster method:

$$\tilde{c}_{\mathrm{R}_i\sigma}(\tilde{\mathbf{k}}) = \sum_{\tilde{\mathrm{r}}} e^{-i(\tilde{\mathrm{k}}\tilde{\mathrm{r}}+\varphi(\tilde{\mathrm{k}};\mathrm{R}_i))}\, c_{\tilde{\mathrm{r}}+\mathrm{R}_i,\sigma}$$

bath for cluster

$$H_{\mathrm{And}} = H_{\mathrm{clu}} + \sum_{l\sigma} \varepsilon_{l\sigma}\, a^{\dagger}_{l\sigma} a_{l\sigma} + \sum_{li,\sigma} \left(V_{l,i}\, a^{\dagger}_{l\sigma} c_{i\sigma} + \mathrm{H.c.} \right)$$

$$\mathbf{G}_b^{-1}(\omega) \approx \omega + \mu - \mathbf{H}_c - \sum_l \frac{\mathbf{V}_l\, \mathbf{V}_l^{\dagger}}{\omega - \varepsilon_l}$$

$$\mathbf{G}_b^{-1}(\omega) = \mathbf{\Sigma}_c(\omega) + \left(\int d\tilde{\mathbf{k}} \left(\omega + \mu - \mathbf{H}(\tilde{\mathbf{k}}) - \mathbf{\Sigma}_c(\omega) \right)^{-1} \right)^{-1}$$

expand up to $1/\omega^2$: **sum-rule**

$$\sum_l \mathbf{V}_l\, \mathbf{V}_l^{\dagger} = \int d\tilde{\mathbf{k}}\, \mathbf{H}^2(\tilde{\mathbf{k}}) - \left(\int d\tilde{\mathbf{k}}\, \mathbf{H}(\tilde{\mathbf{k}}) \right)^2$$

hybridization sum-rules: single-site

H with hopping t_n to the z_n n^{th}-nearest neighbors

$$\sum_l V_l^2 = \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} d^d\mathbf{k}\, \varepsilon_{\mathrm{k}}^2 = \sum_n z_n\, t_n^2$$

special case: Bethe lattice of coordination *z* with hopping $t/\sqrt{z}$

$$\sum_l V_l^2 = t^2$$

hybridization sum-rules: DCA

hybridizations diagonal in the cluster-momenta **K**:

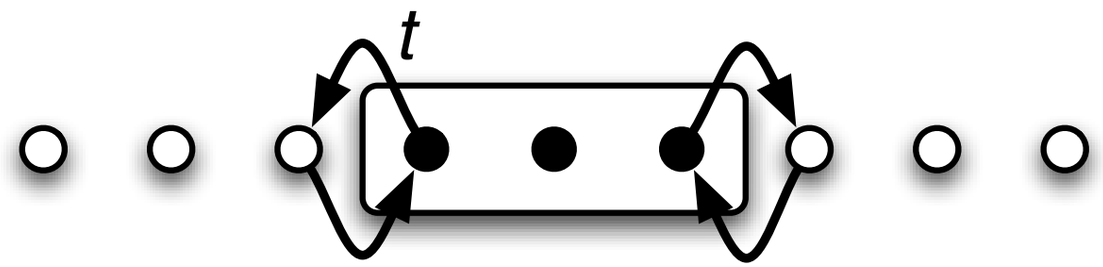
$$\sum_l |V_{l,\mathrm{K}}|^2 = \int d\tilde{\mathbf{k}}\, \varepsilon^2_{\mathrm{K}+\tilde{\mathrm{k}}} - \left(\int d\tilde{\mathbf{k}}\, \varepsilon_{\mathrm{K}+\tilde{\mathrm{k}}} \right)^2$$

all terms $V_{l,K}\, V_{l,K'}$ mixing different cluster momenta vanish

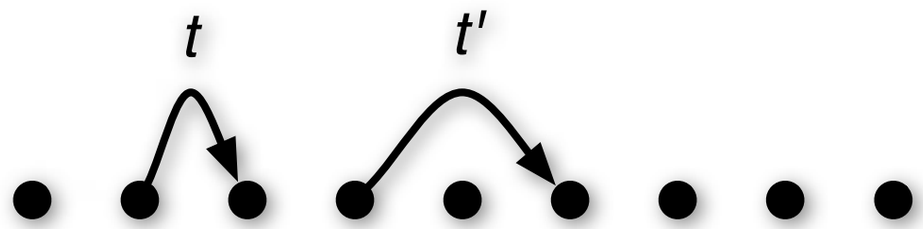
hybridization sum-rules: CDMFT

$$\mathbf{H}(\tilde{k}) = -t \begin{pmatrix} 0 & 1 & e^{-3i\tilde{k}} \\ 1 & 0 & 1 \\ e^{3i\tilde{k}} & 1 & 0 \end{pmatrix}$$

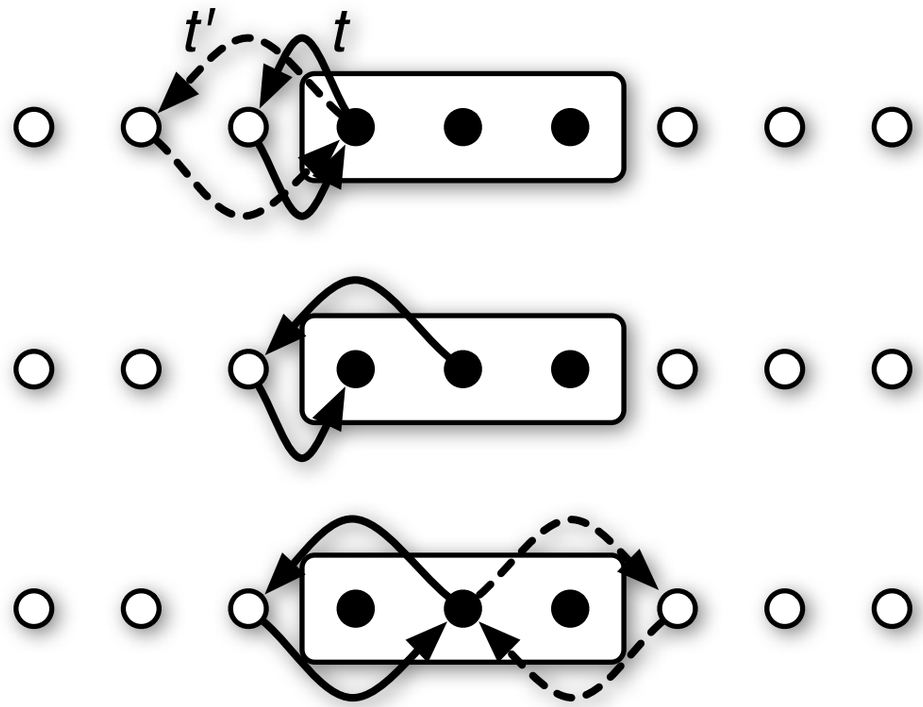
$$\sum_l \mathbf{V}_l \mathbf{V}_l^\dagger = \int d\tilde{\mathbf{k}}\, \mathbf{H}^2(\tilde{\mathbf{k}}) - \left(\int d\tilde{\mathbf{k}}\, \mathbf{H}(\tilde{\mathbf{k}}) \right)^2 = \begin{pmatrix} t^2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & t^2 \end{pmatrix}$$



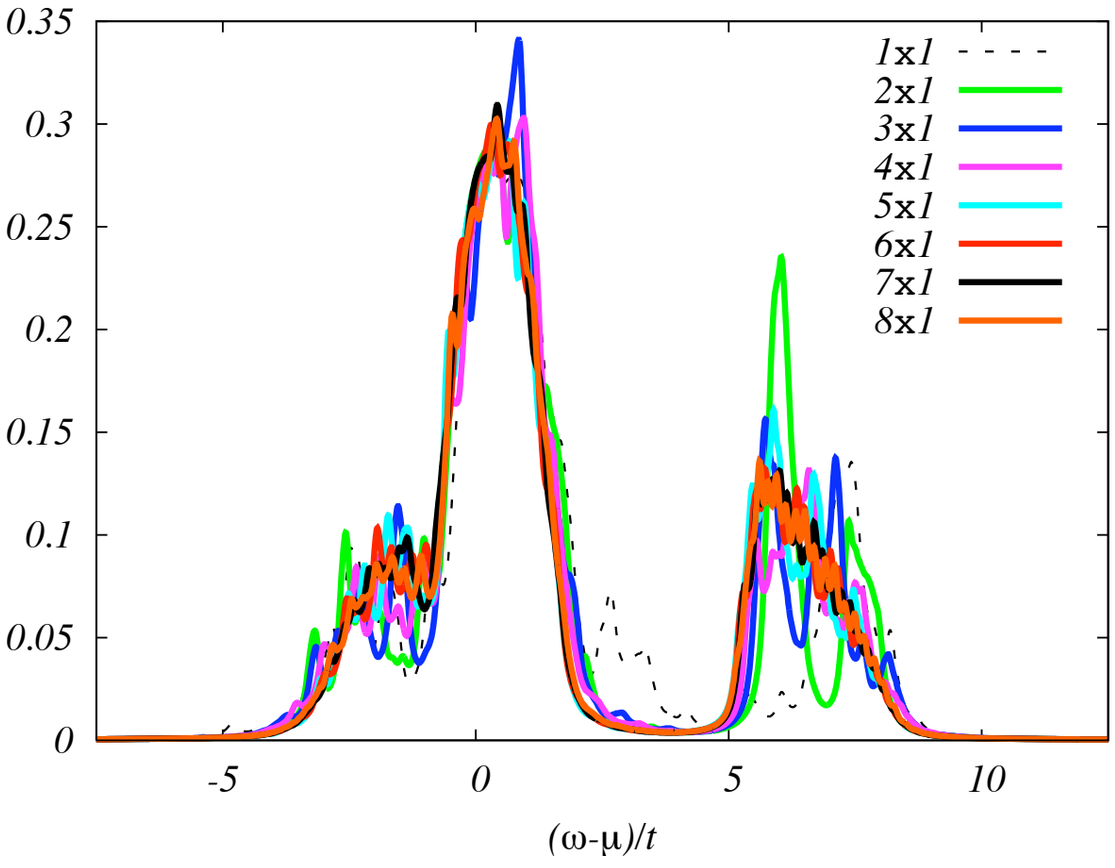
hybridization sum-rules: CDMFT



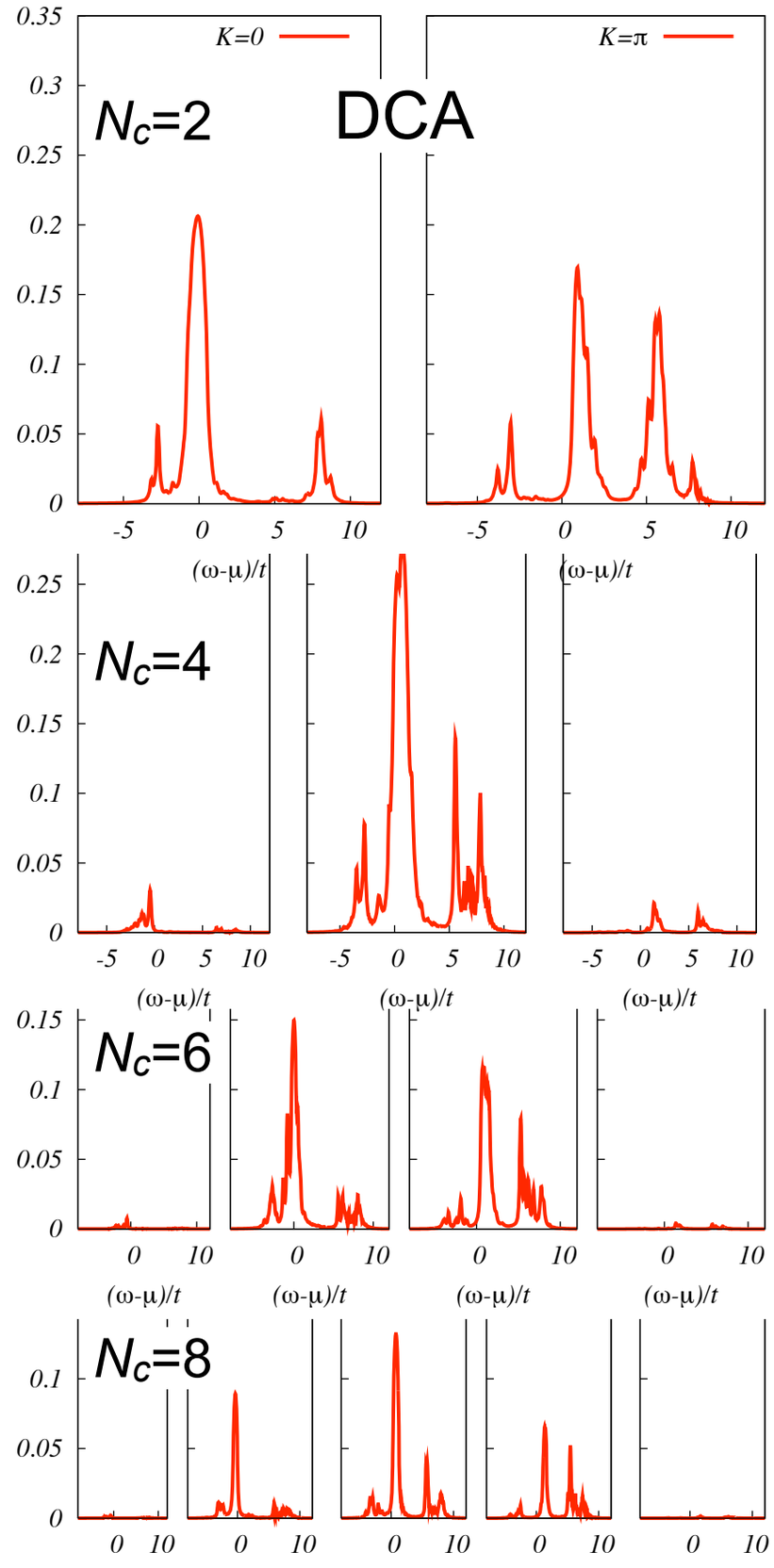
$$\left(\sum_l V_{l,i}\bar{V}_{l,j}\right) = \begin{pmatrix} t^2+t'^2 & t\,t' & 0 \\ t\,t' & 2t'^2 & t\,t' \\ 0 & t\,t' & t^2+t'^2 \end{pmatrix}$$



example: 1-d clusters



	CDMFT	DCA
hybridize	only surface	full cluster
strength	const.	$1/N_c^{2/d}$



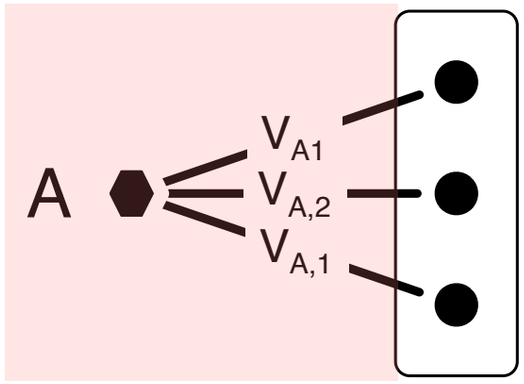
symmetry of bath

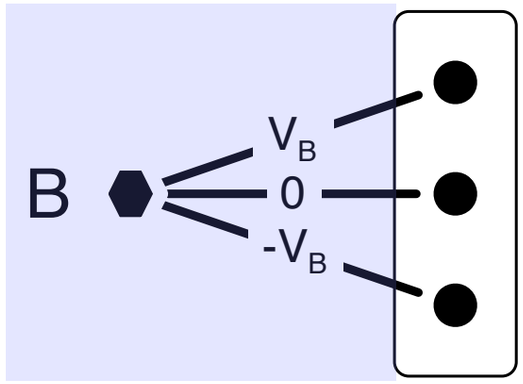
$$\mathbf{W} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{pmatrix}$$

irreducible representations: A (even), B (odd)

$$\mathbf{W}^\dagger \mathbf{G}_b^{-1} \mathbf{W} = \begin{pmatrix} G_{b,11}^{-1} + G_{b,13}^{-1} & \sqrt{2}\, G_{b,12}^{-1} & 0 \\ \sqrt{2}\, G_{b,21}^{-1} & G_{b,22}^{-1} & 0 \\ 0 & 0 & G_{b,11}^{-1} - G_{b,13}^{-1} \end{pmatrix}$$

block-diagonal





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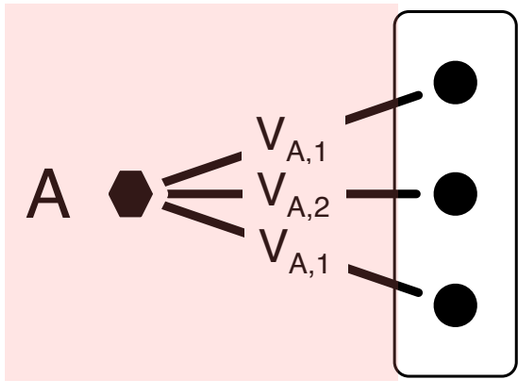
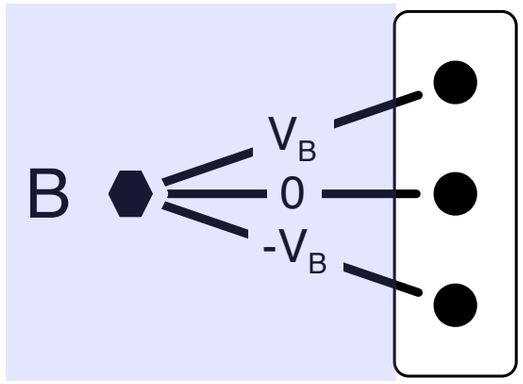
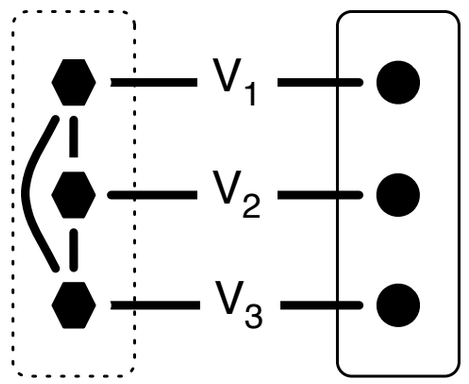
block-diagonal





cluster replica: 2A+B

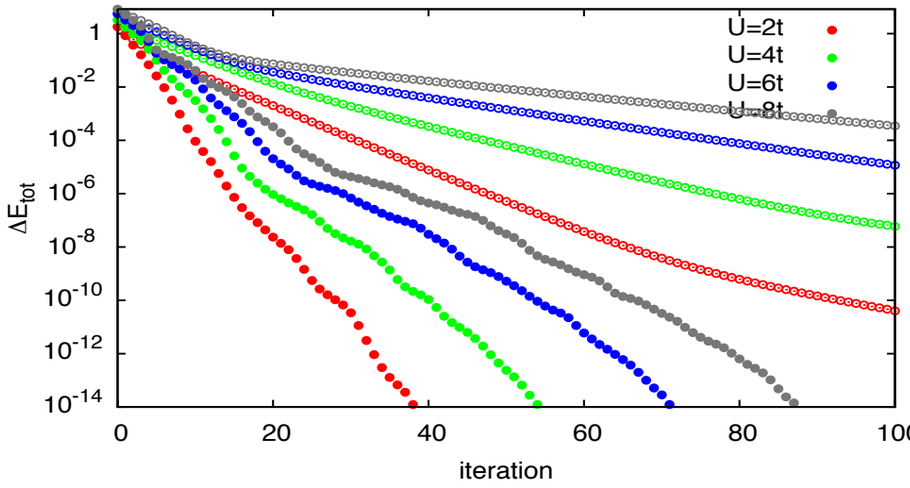


$$\begin{aligned} V_{A,1} &= (V_1 + V_3)/\sqrt{2} \\ V_{A,2} &= V_2 \\ V_B &= (V_1 - V_3)/\sqrt{2} \end{aligned}$$

summary

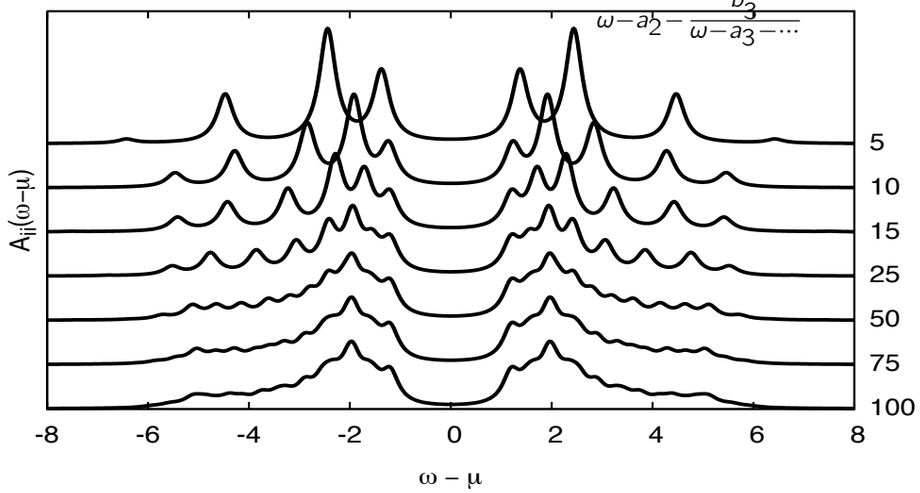
steepest descent ⇒ Krylov space

$$\frac{\delta E[\psi]}{\delta\langle\psi|} = \frac{H|\psi\rangle - E[\psi]|\psi\rangle}{\langle\psi|\psi\rangle} = |\psi_a\rangle \in \mathrm{span}\left(|\psi\rangle, H|\psi\rangle\right)$$

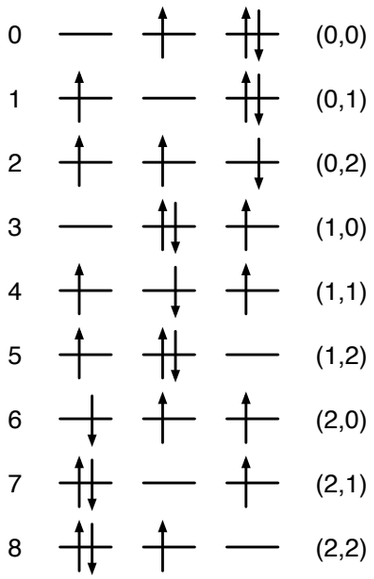


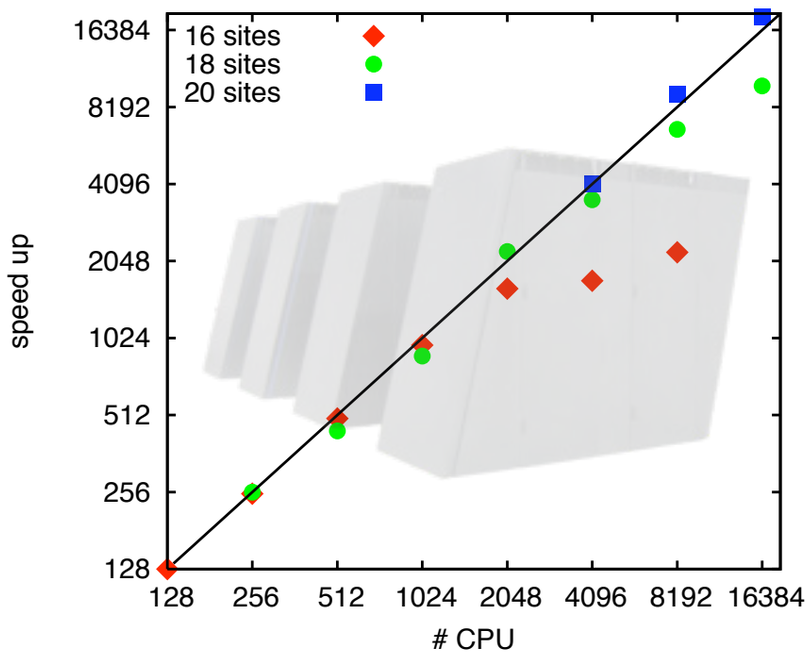
spectral function: moments

$$G_k(\omega) = \cfrac{b_0^2}{\omega - a_0 - \cfrac{b_1^2}{\omega - a_1 - \cfrac{b_2^2}{\omega - a_2 - \cfrac{b_3^2}{\omega - a_3 - \cdots}}}}$$

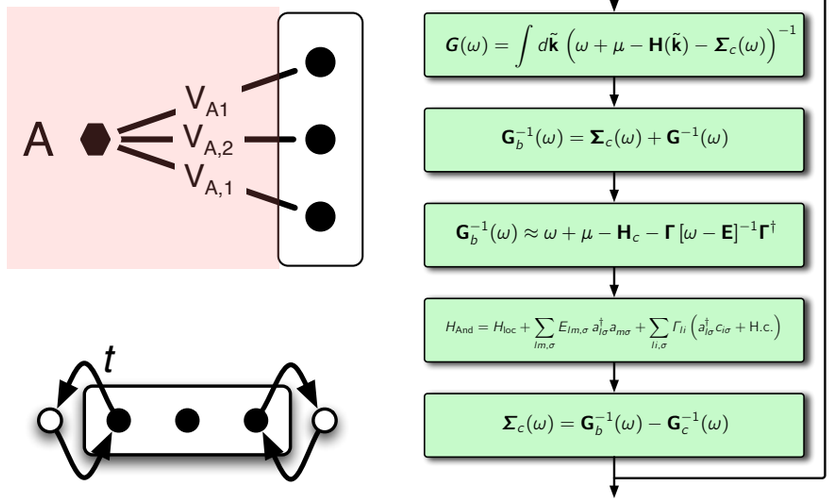


sparse Hamiltonian in Wannier representation



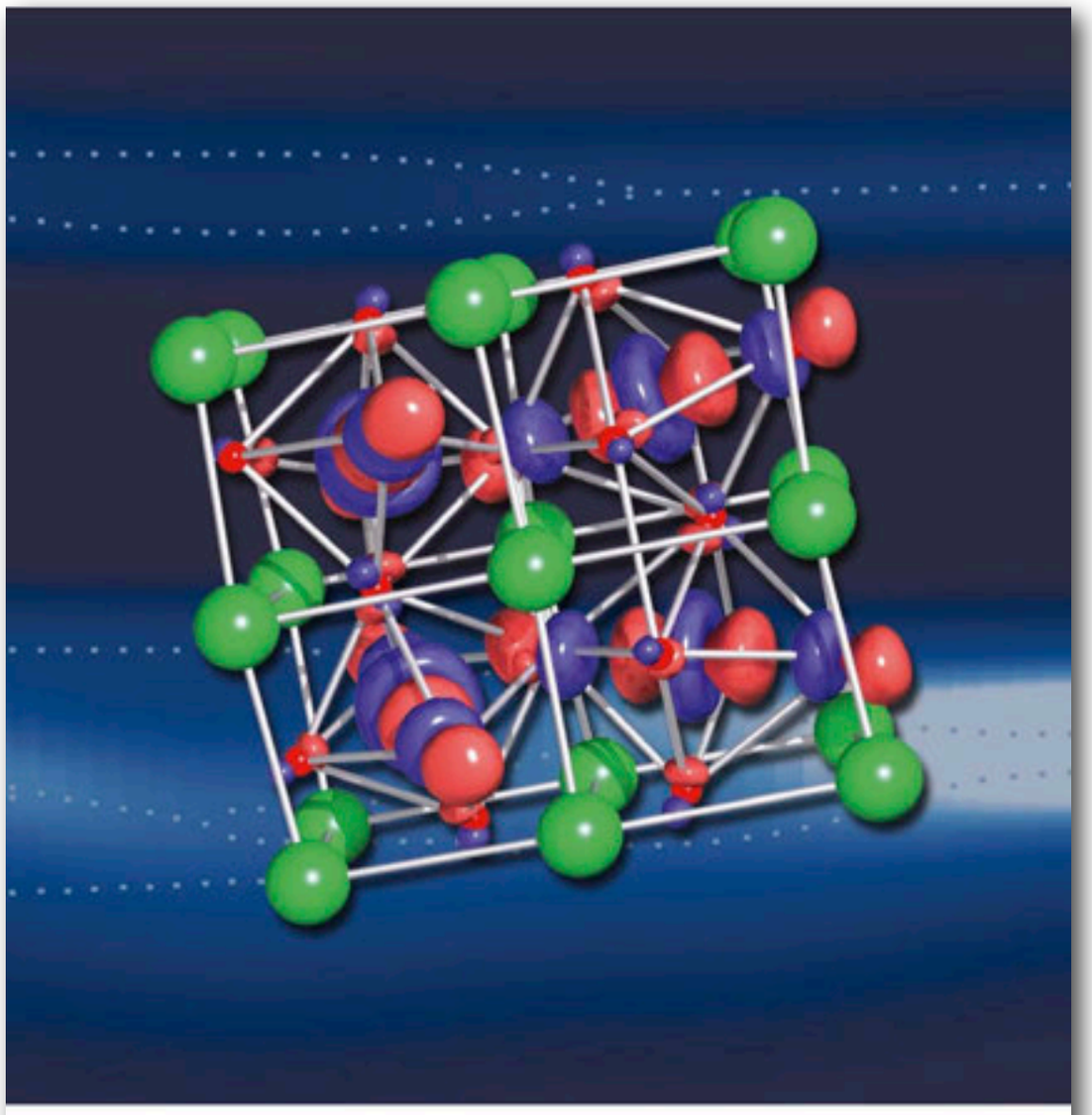


bath parametrization



$$\sum_l \mathbf{V}_l\,\mathbf{V}_l^\dagger = \int d\tilde{\mathbf{k}}\,\mathbf{H}^2(\tilde{\mathbf{k}}) - \left(\int d\tilde{\mathbf{k}}\,\mathbf{H}(\tilde{\mathbf{k}})\right)^2$$

reference



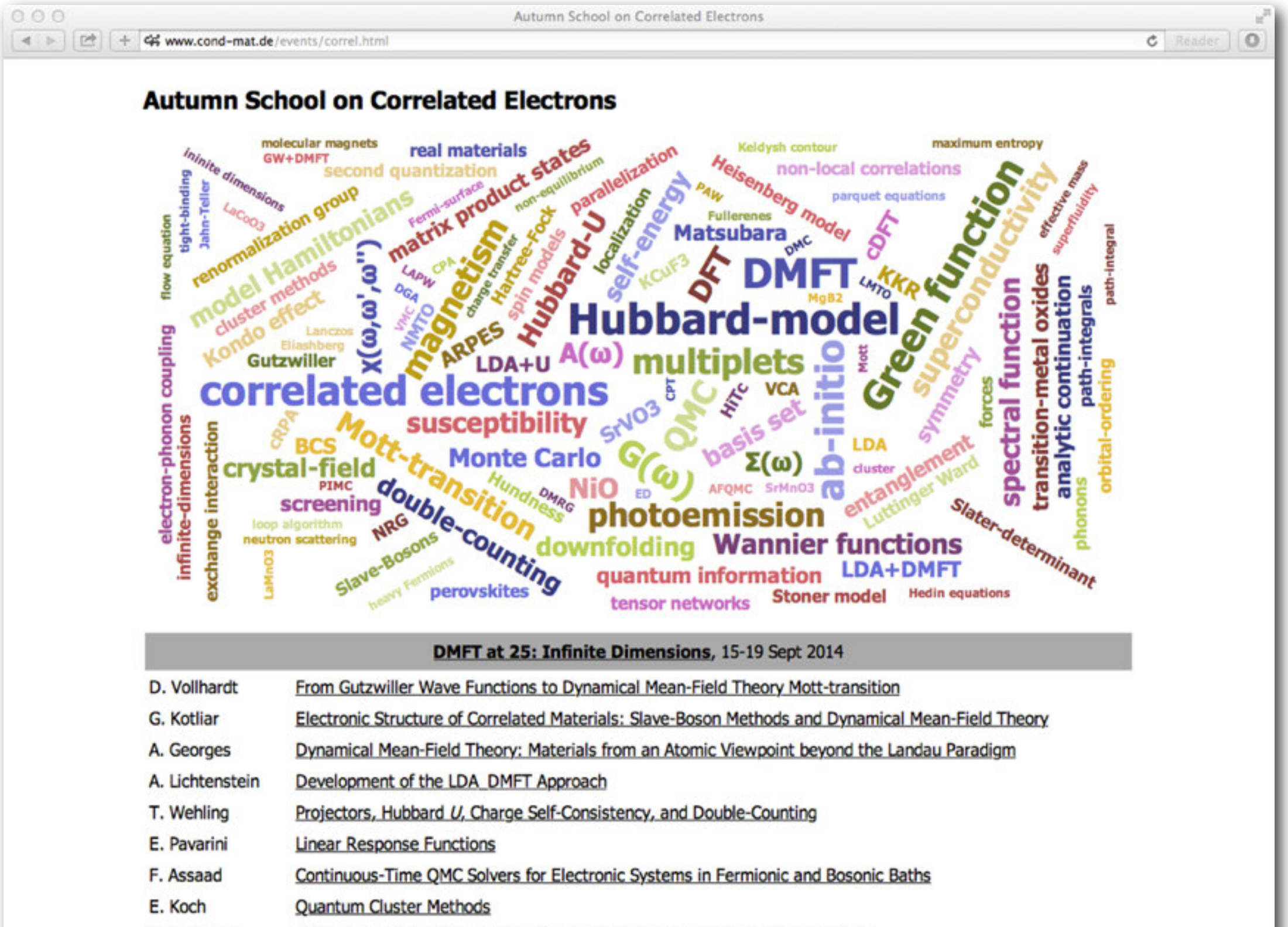
The LDA+DMFT approach to strongly correlated materials

Eva Pavarini, Erik Koch, Dieter Vollhardt, and Alexander Lichtenstein (Eds.)

German Research School for Simulation Sciences

JÜLICH FORSCHUNGSZENTRUM

www.cond-mat.de/events/correl.html



DMFT at 25: Infinite Dimensions, 15-19 Sept 2014	
D. Vollhardt	From Gutzwiller Wave Functions to Dynamical Mean-Field Theory Mott-transition
G. Kotliar	Electronic Structure of Correlated Materials: Slave-Boson Methods and Dynamical Mean-Field Theory
A. Georges	Dynamical Mean-Field Theory: Materials from an Atomic Viewpoint beyond the Landau Paradigm
A. Lichtenstein	Development of the LDA_DMFT Approach
T. Wehling	Projectors, Hubbard *U*, Charge Self-Consistency, and Double-Counting
E. Pavarini	Linear Response Functions
F. Assaad	Continuous-Time QMC Solvers for Electronic Systems in Fermionic and Bosonic Baths
E. Koch	Quantum Cluster Methods
M. Potthoff	Making Use of Self-Energy Functionals: The Variational Cluster Approximation