The Lanczos Method

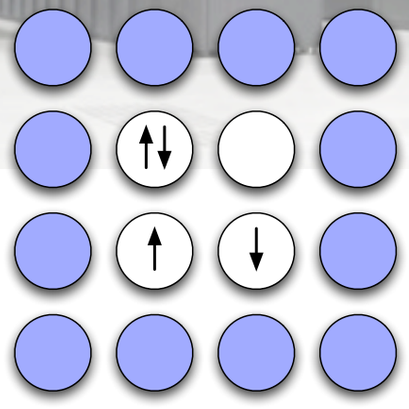
Erik Koch
Computational Materials Science
German Research School for Simulation Sciences, Jülich

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

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

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

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



German Research School
for Simulation Sciences

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

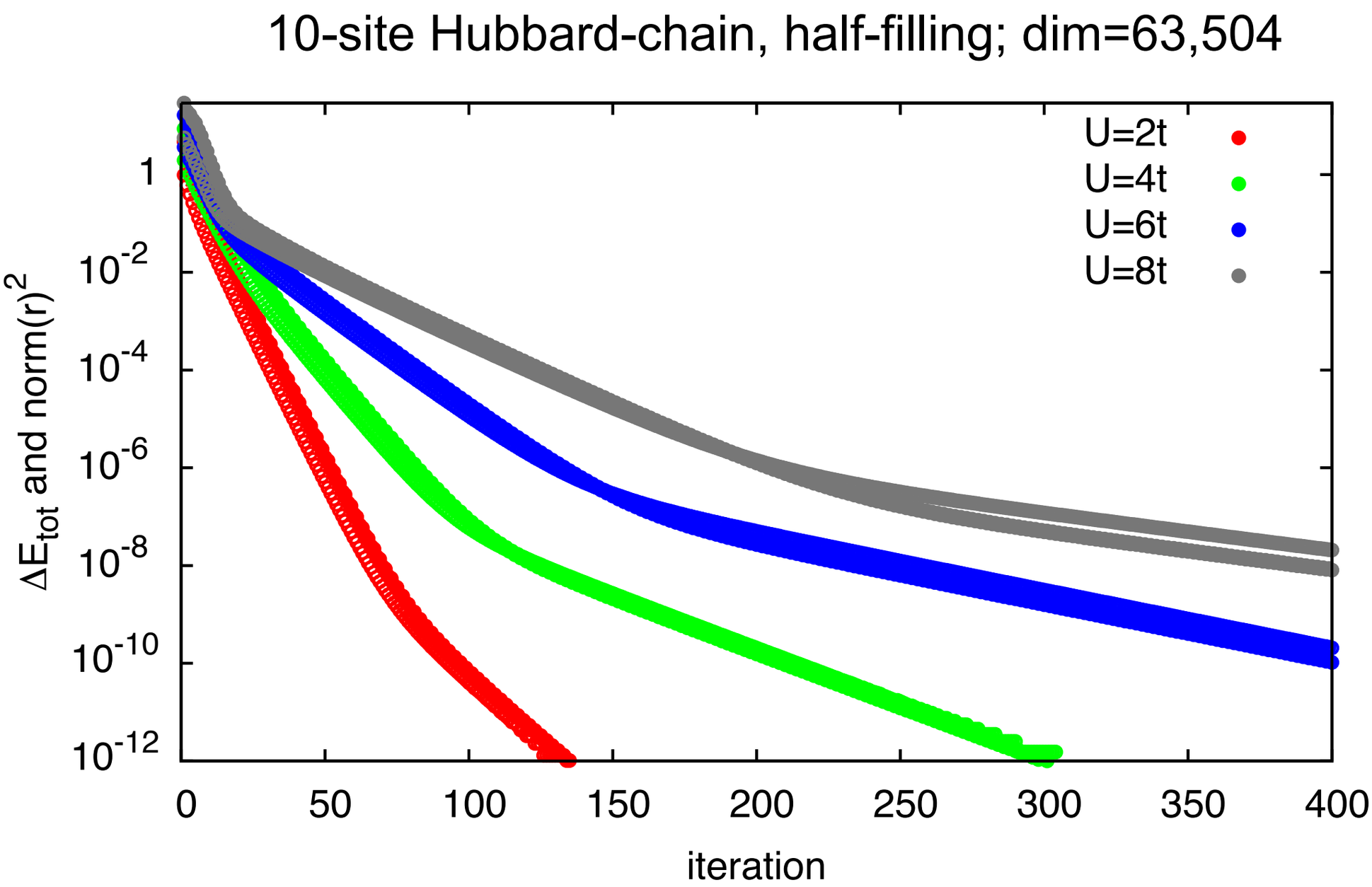
$$H|v_0\rangle = b_1 |v_1\rangle + a_0 |v_0\rangle$$

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

diagonalize to find lowest eigenvector

iterate!

convergence



Lanczos idea

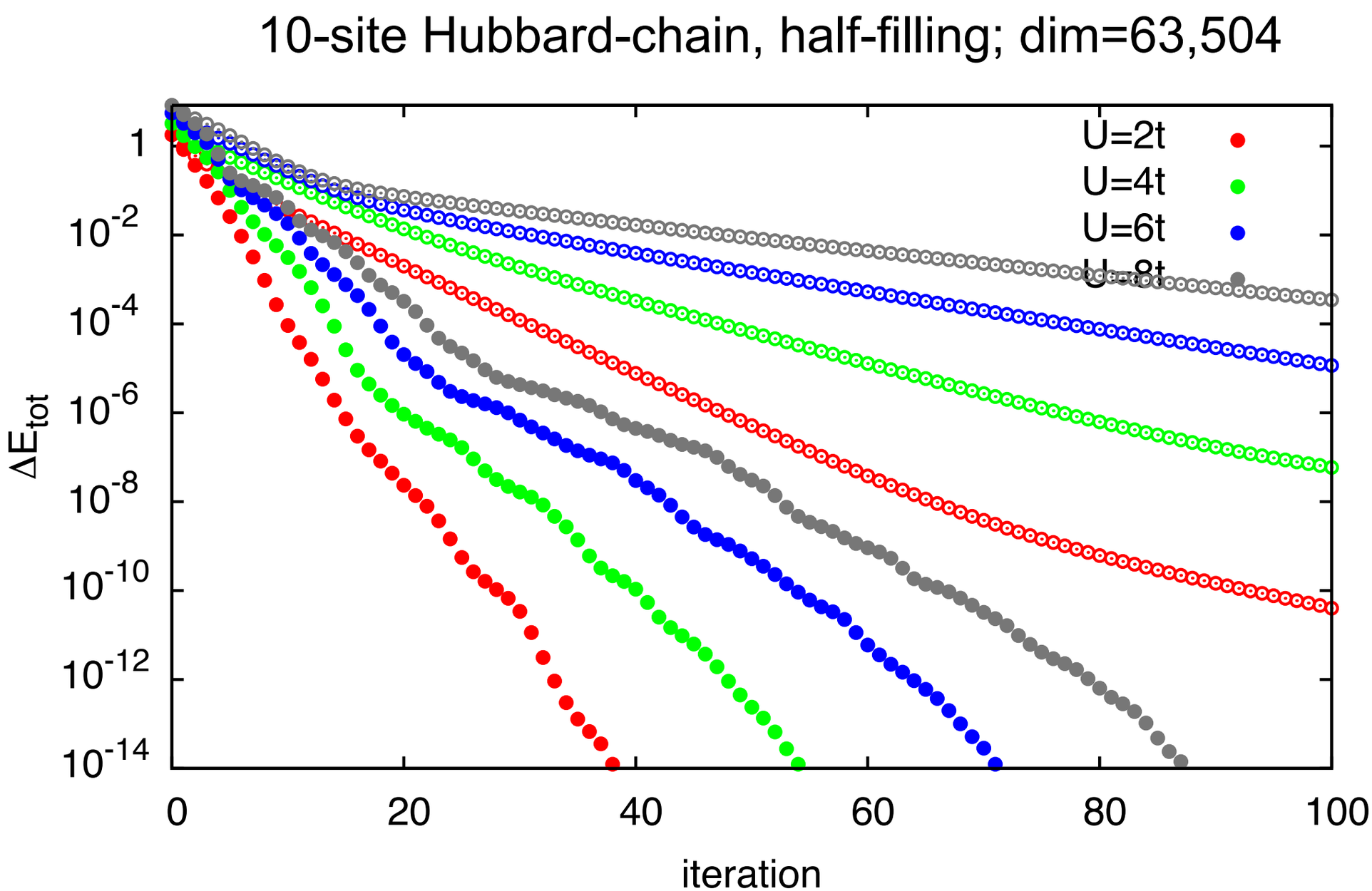
minimize on span $(|\psi_0\rangle, H|\psi_0\rangle)$ to obtain $|\psi_1\rangle$
minimize on span $(|\psi_1\rangle, H|\psi_1\rangle) \in$ span $\left(|\psi_0\rangle, H|\psi_0\rangle, H^2|\psi_0\rangle\right)$
minimize on span $(|\psi_2\rangle, H|\psi_2\rangle) \in$ span $\left(|\psi_0\rangle, H|\psi_0\rangle,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

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

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

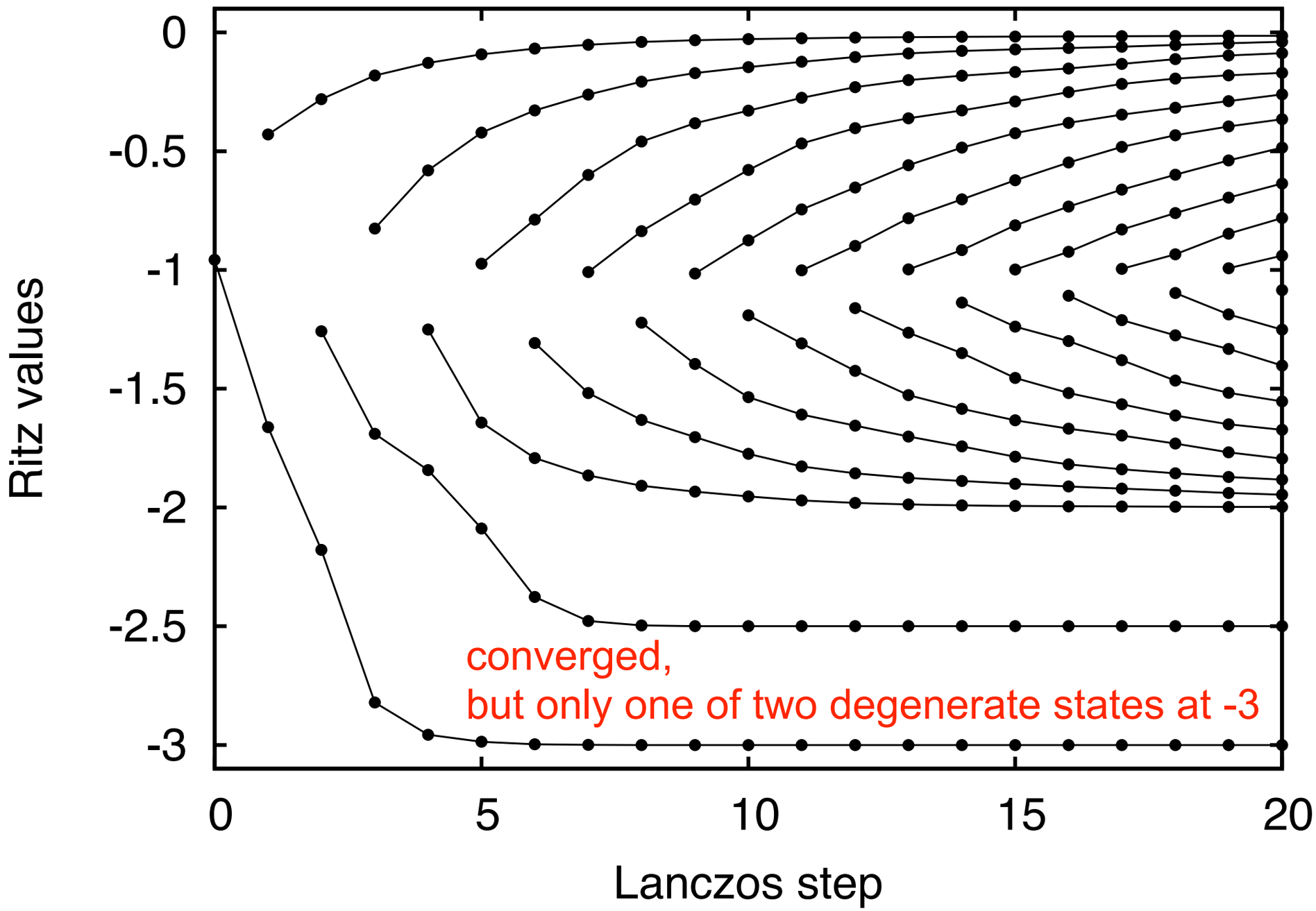
Ritz value n approaches eigenvalue n with increasing L from above:

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

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

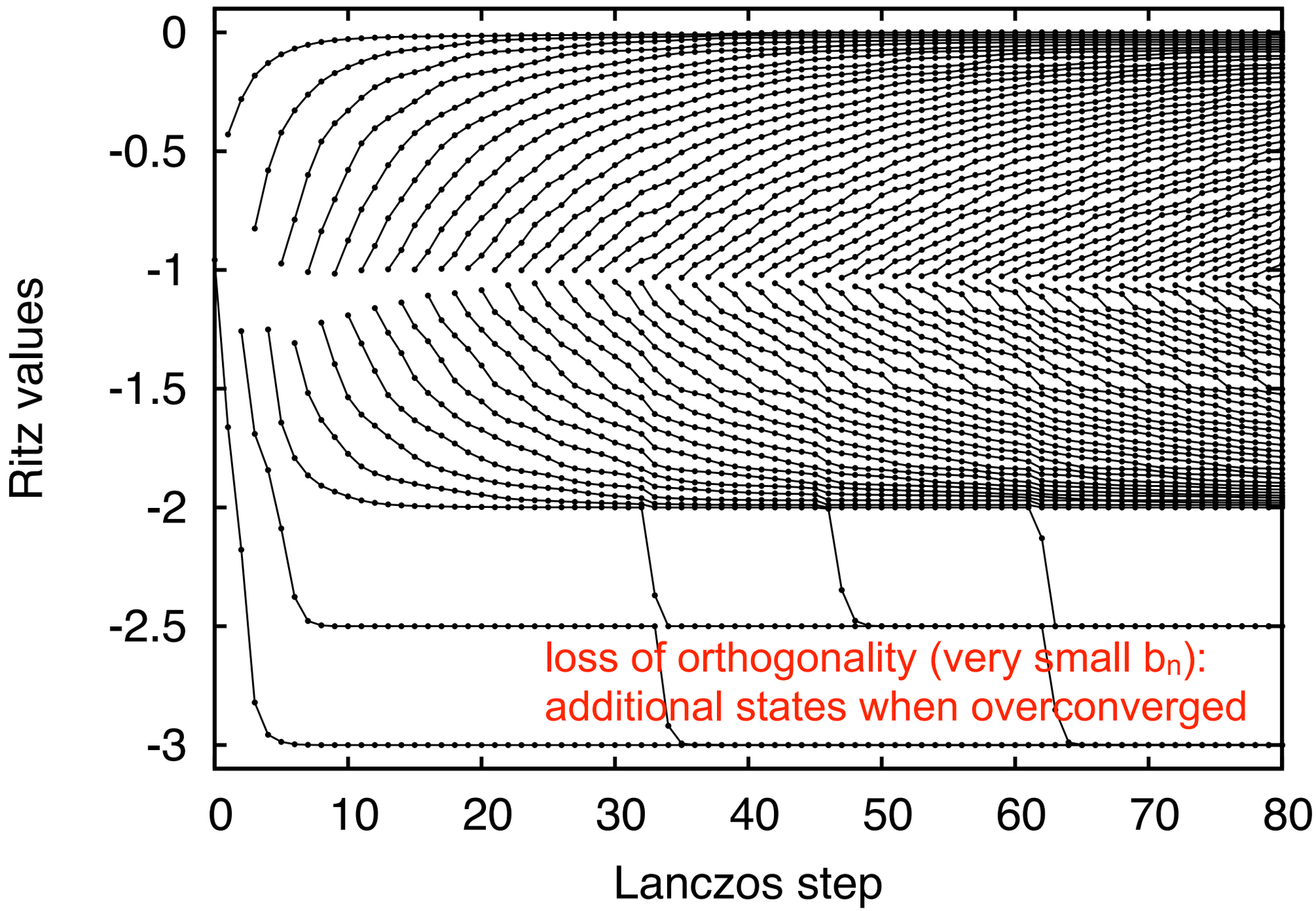
assume $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are degenerate eigenstates with eigenvalue ε, then their expansion in the orthonormal basis of the Krylov space is

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

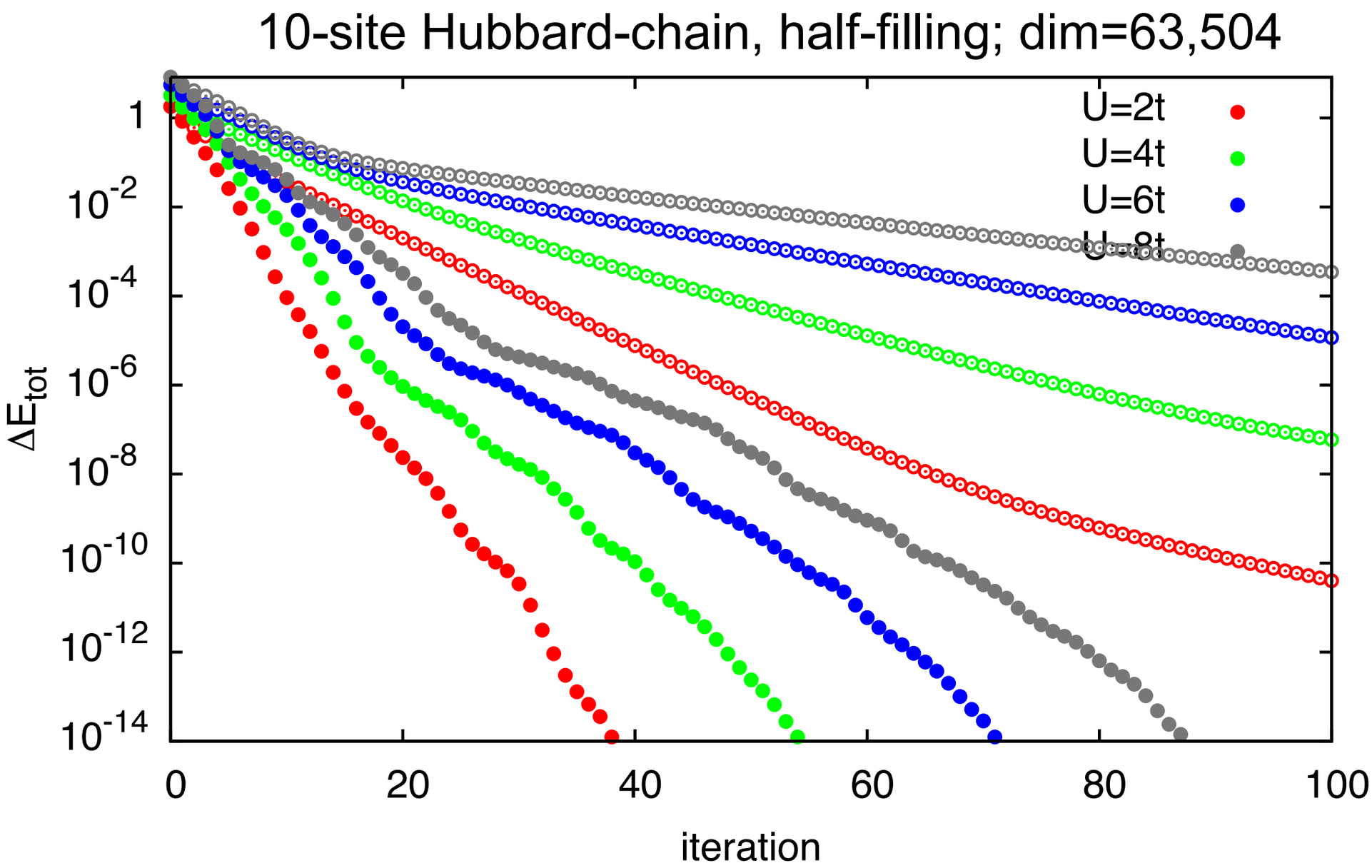
$\Rightarrow |\varphi_1\rangle$ and $|\varphi_2\rangle$ are identical up to normalization

loss of orthogonality

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



convergence to ground state



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

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

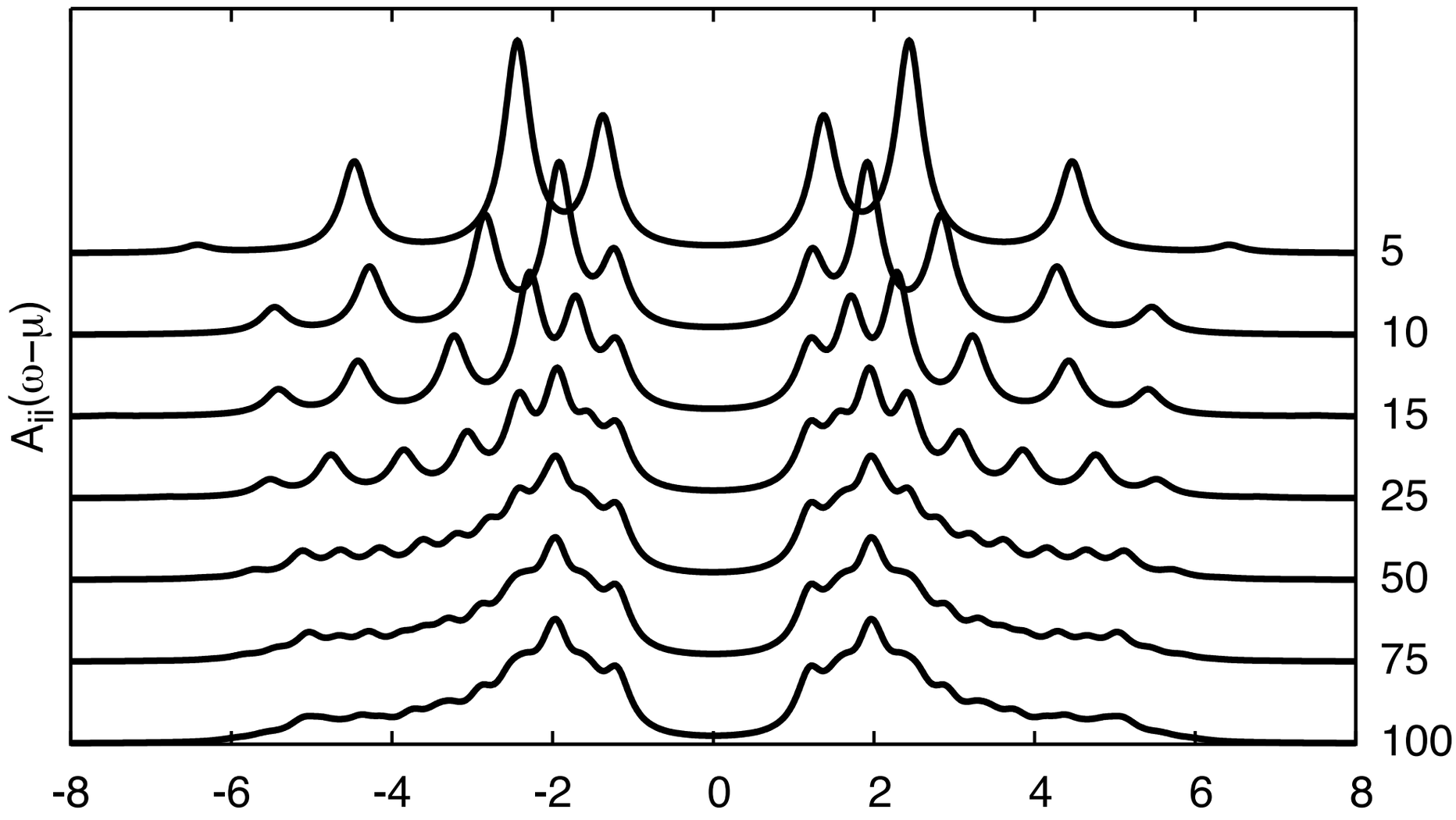
$$G_{00}(\varepsilon) = \left(\varepsilon - \left[H_{00} + T_{01}(\varepsilon - H_{11})^{-1} T_{10}\right]\right)^{-1}$$

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

convergence: moments



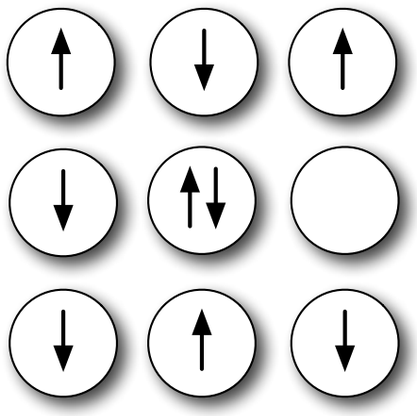
$$\int_{-\infty}^{\infty} d\omega\, \omega^m \check{A}(\omega) = \sum_{n=0}^{L} |\check{\psi}_{n,0}|^2 \check{E}_n^m = \sum_{n=0}^{L} \langle \Psi_c | \check{\psi}_n \rangle \langle \check{\psi}_n | \Psi_c \rangle \check{E}_n^m = \langle \Psi_c | \check{H}^m | \Psi_c \rangle$$

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

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

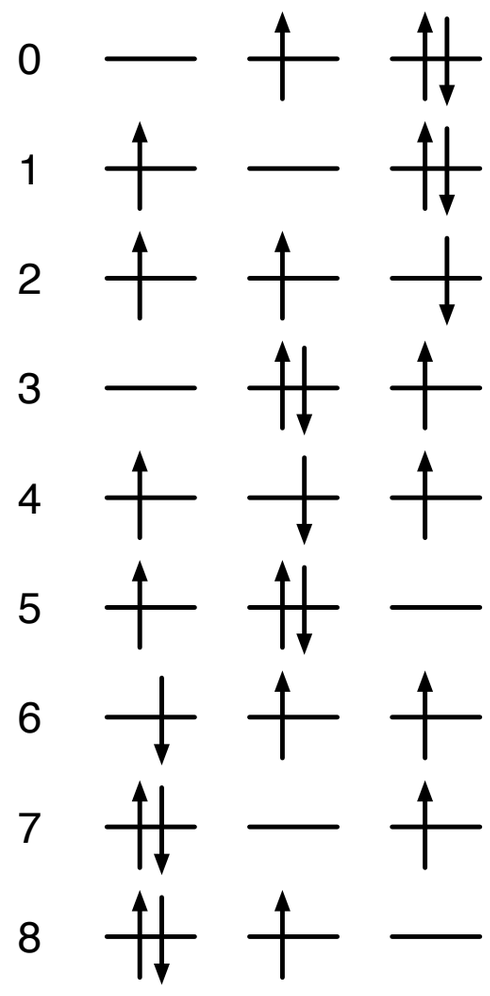
choice of basis

work with operators that create electrons in Wannier orbitals

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

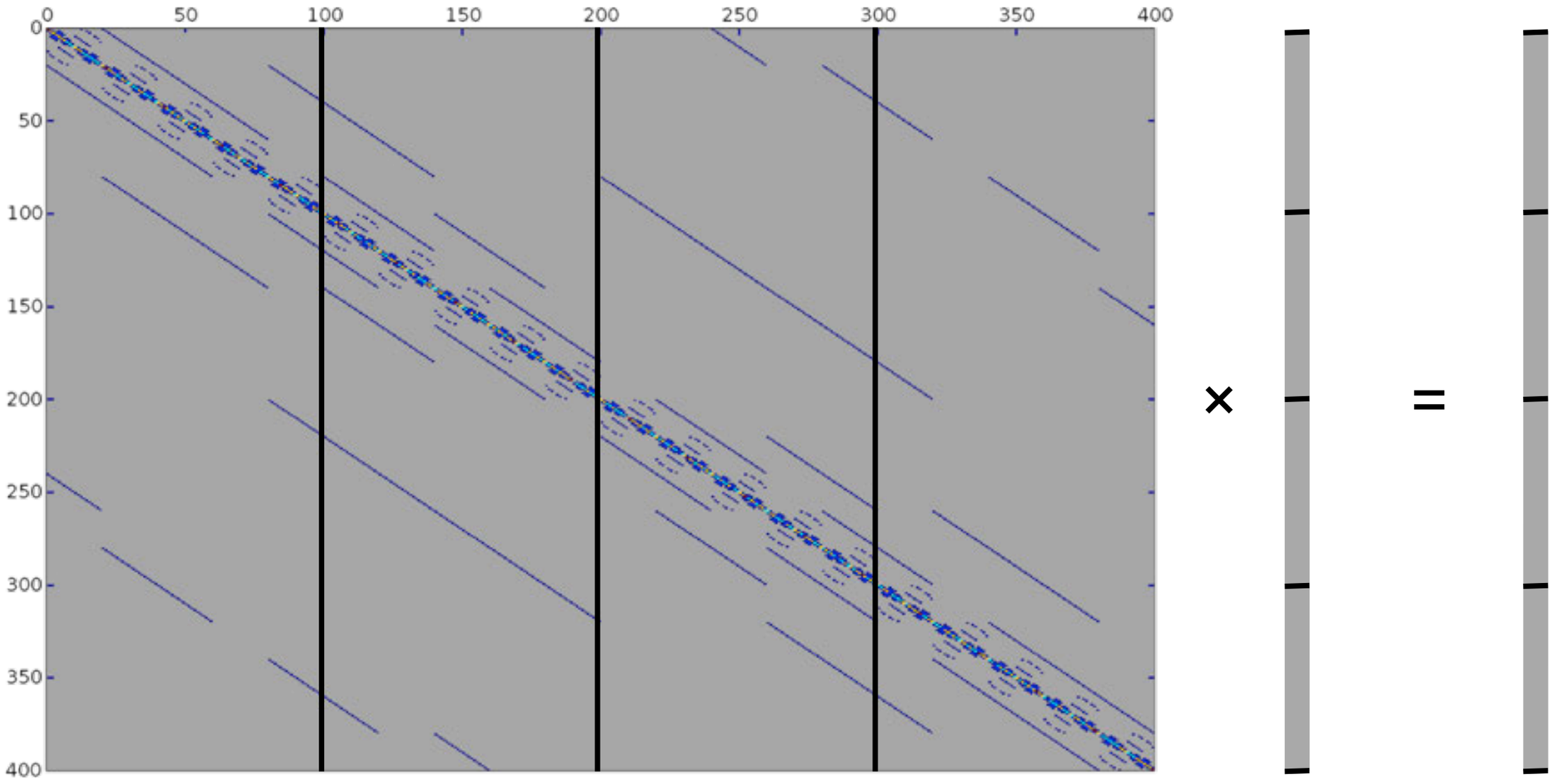
$\mathtt{m}_\uparrow$	bits	state	$\mathtt{i}_\uparrow$
0	000		
1	001		
2	010		
3	011	$c_{0\uparrow}^{\dagger} c_{1\uparrow}^{\dagger} \|0\rangle$	0
4	100		
5	101	$c_{0\uparrow}^{\dagger} c_{2\uparrow}^{\dagger} \|0\rangle$	1
6	110	$c_{1\uparrow}^{\dagger} c_{2\uparrow}^{\dagger} \|0\rangle$	2
7	111		

$\mathtt{m}_\downarrow$	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

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



sparse matrix-vector product: OpenMP

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

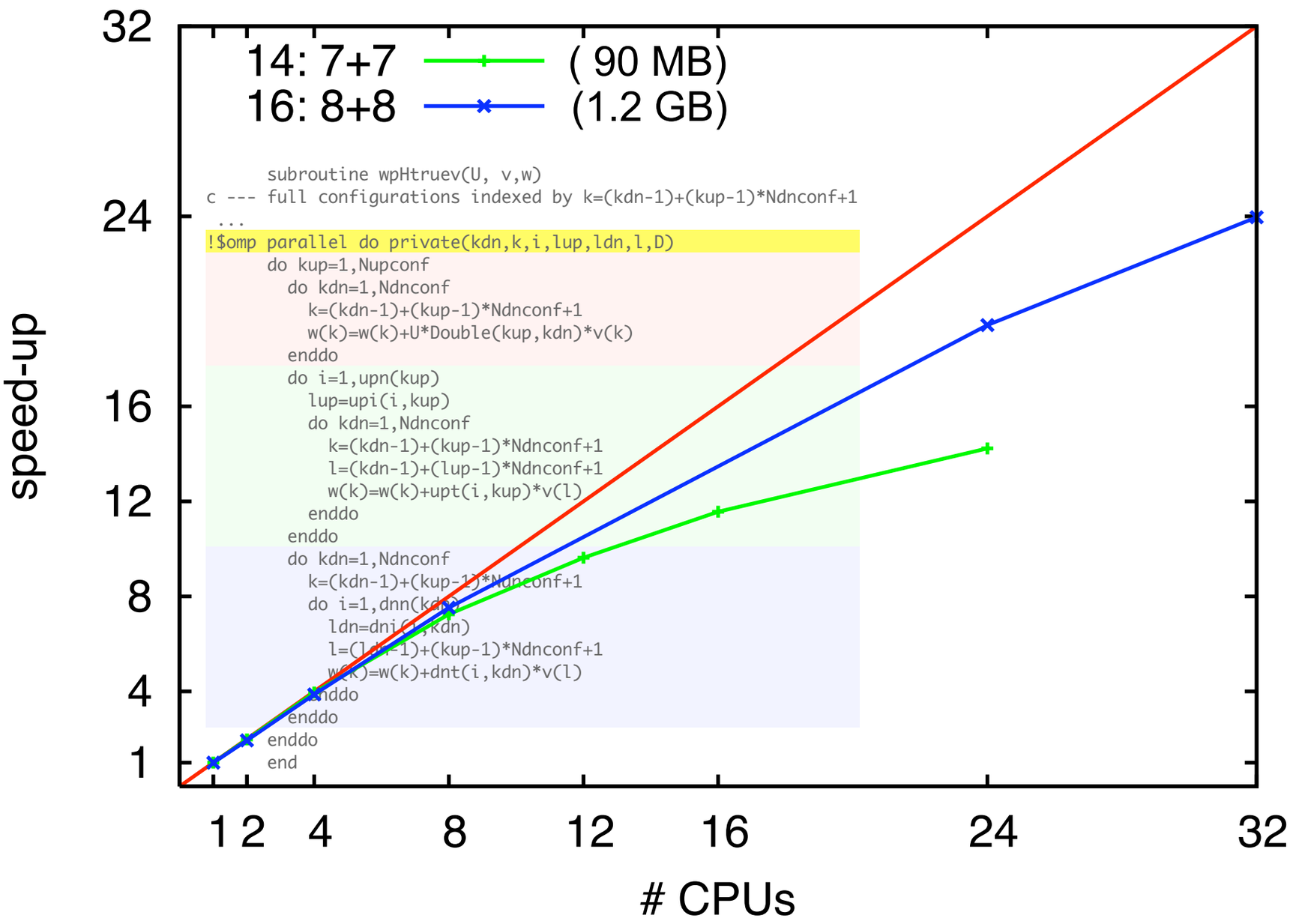
```
      subroutine wpHtruev(U, v,w)
c --- full configurations indexed by k=(kdn-1)+(kup-1)*Ndnconf+1
 ...
!$omp parallel do private(kdn,k,i,lup,ldn,l,D)
      do kup=1,Nupconf
        do kdn=1,Ndnconf
          k=(kdn-1)+(kup-1)*Ndnconf+1
          w(k)=w(k)+U*Double(kup,kdn)*v(k)
        enddo
  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

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

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

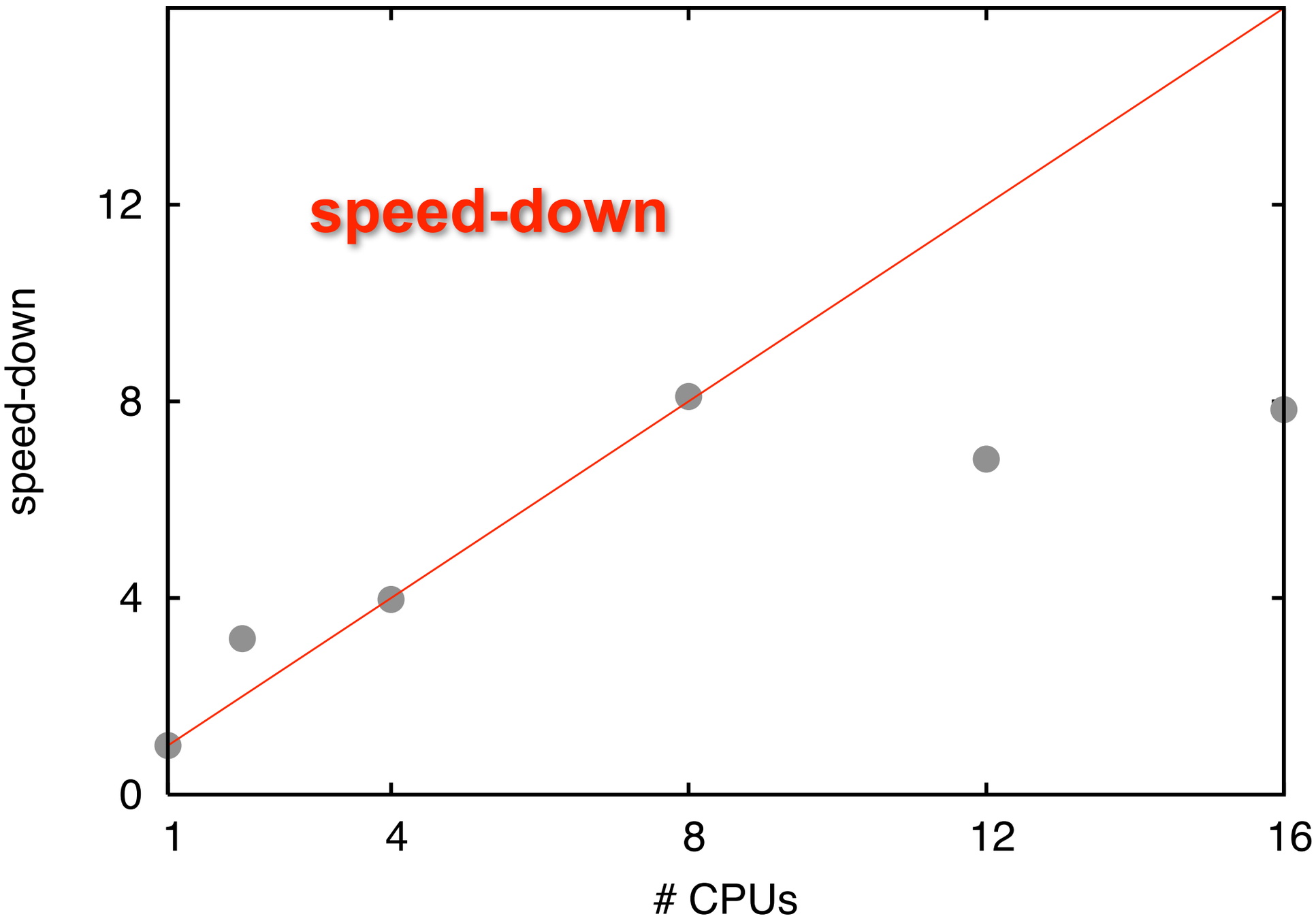
$$\sum_{\langle ij\rangle,\sigma=\downarrow} t_{i,j}\, c^{\dagger}_{j,\sigma} c_{i,\sigma}$$

OpenMP on Jump



distributed memory

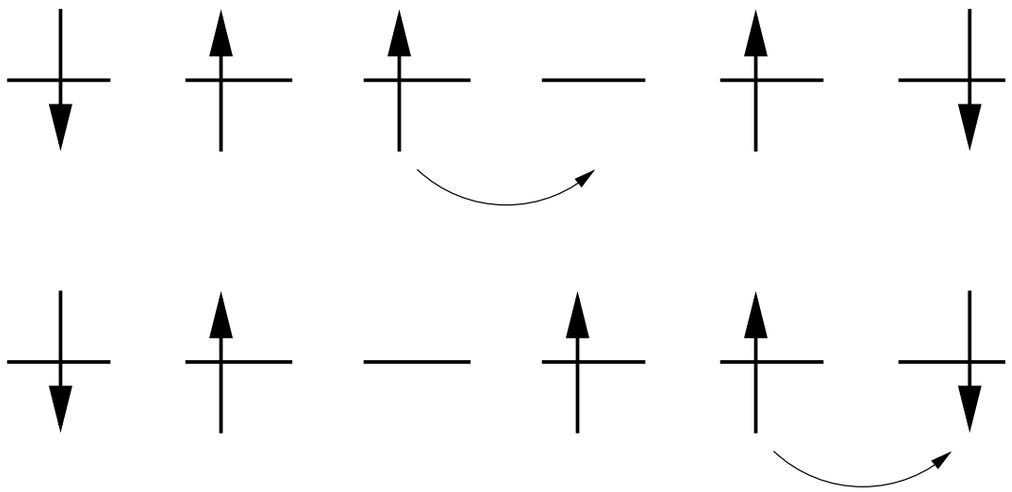
MPI-2: one-sided communication



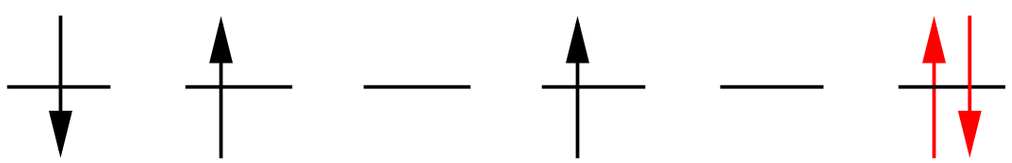
Hubbard model

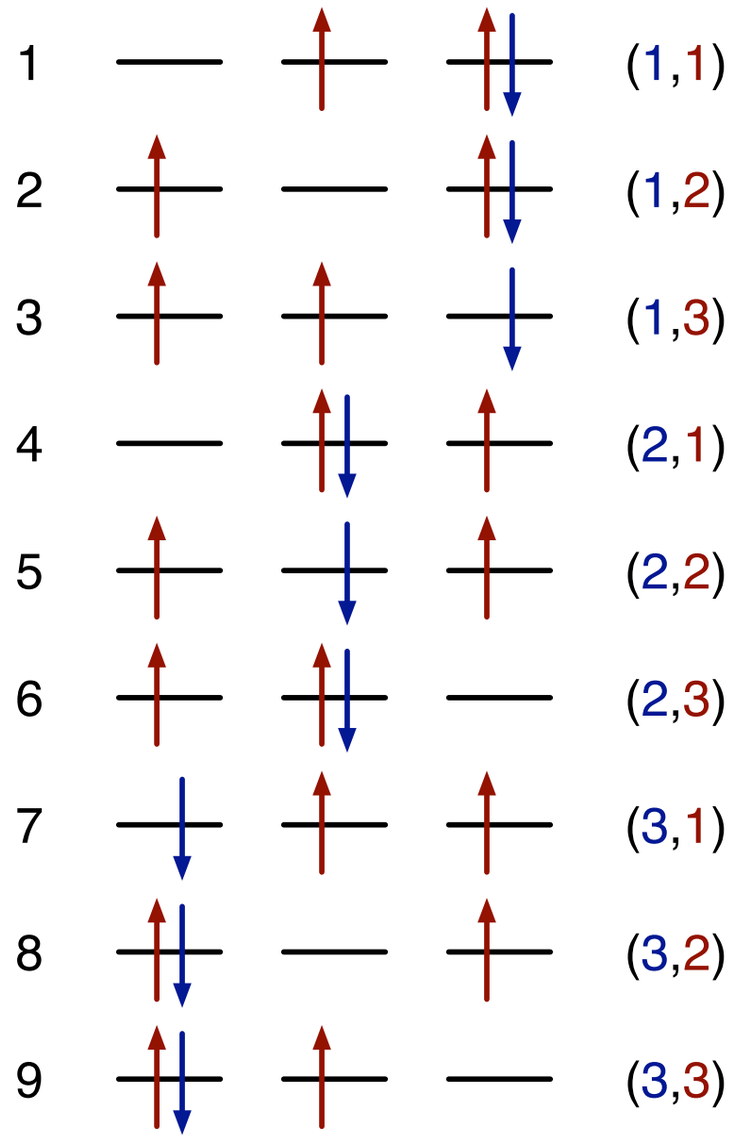
$$H = \sum_{\langle ij \rangle, \sigma} \; t_{i,j} \, c^{\dagger}_{j,\sigma} c_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

hopping: spin unchanged

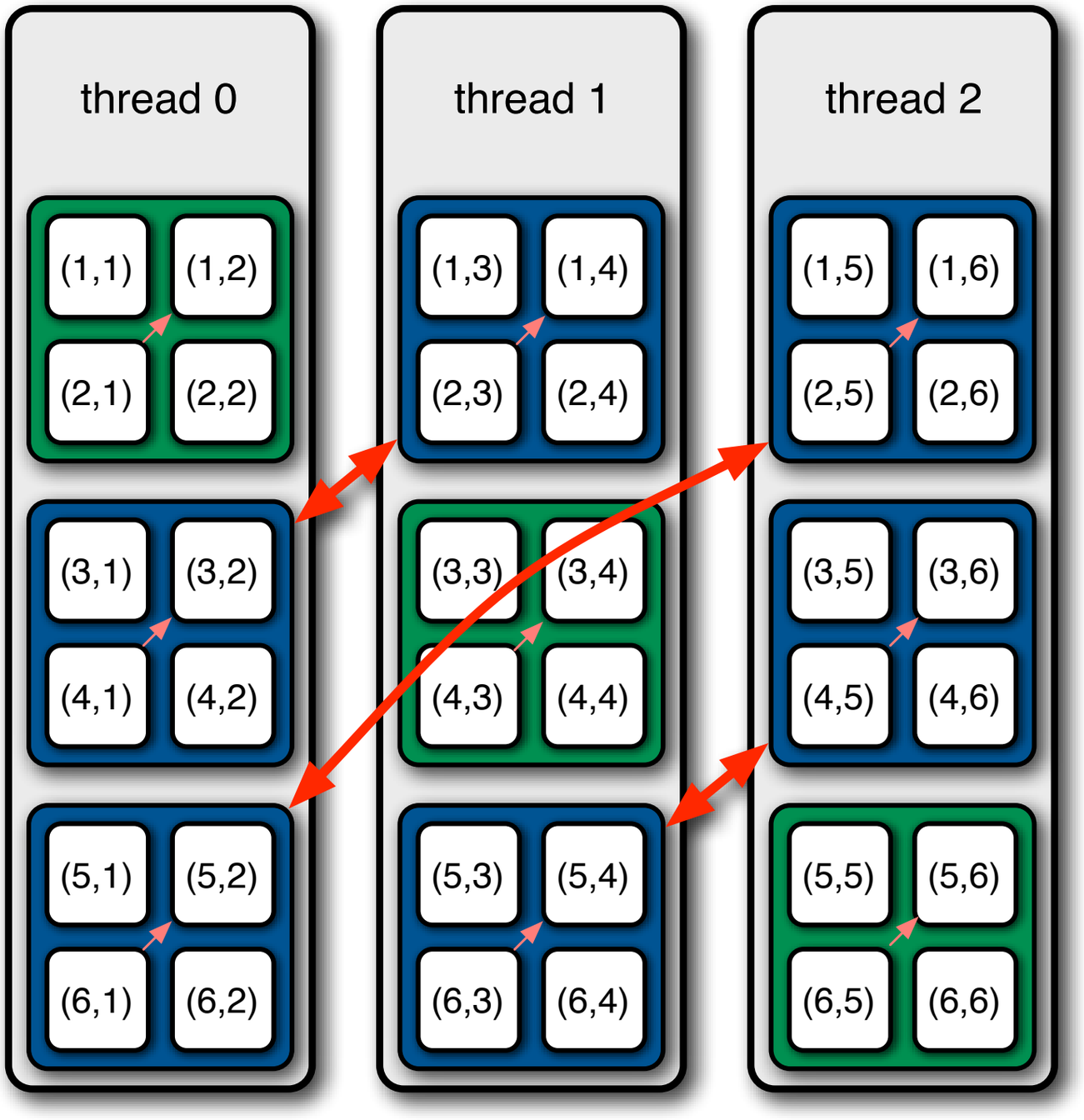


interaction diagonal





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



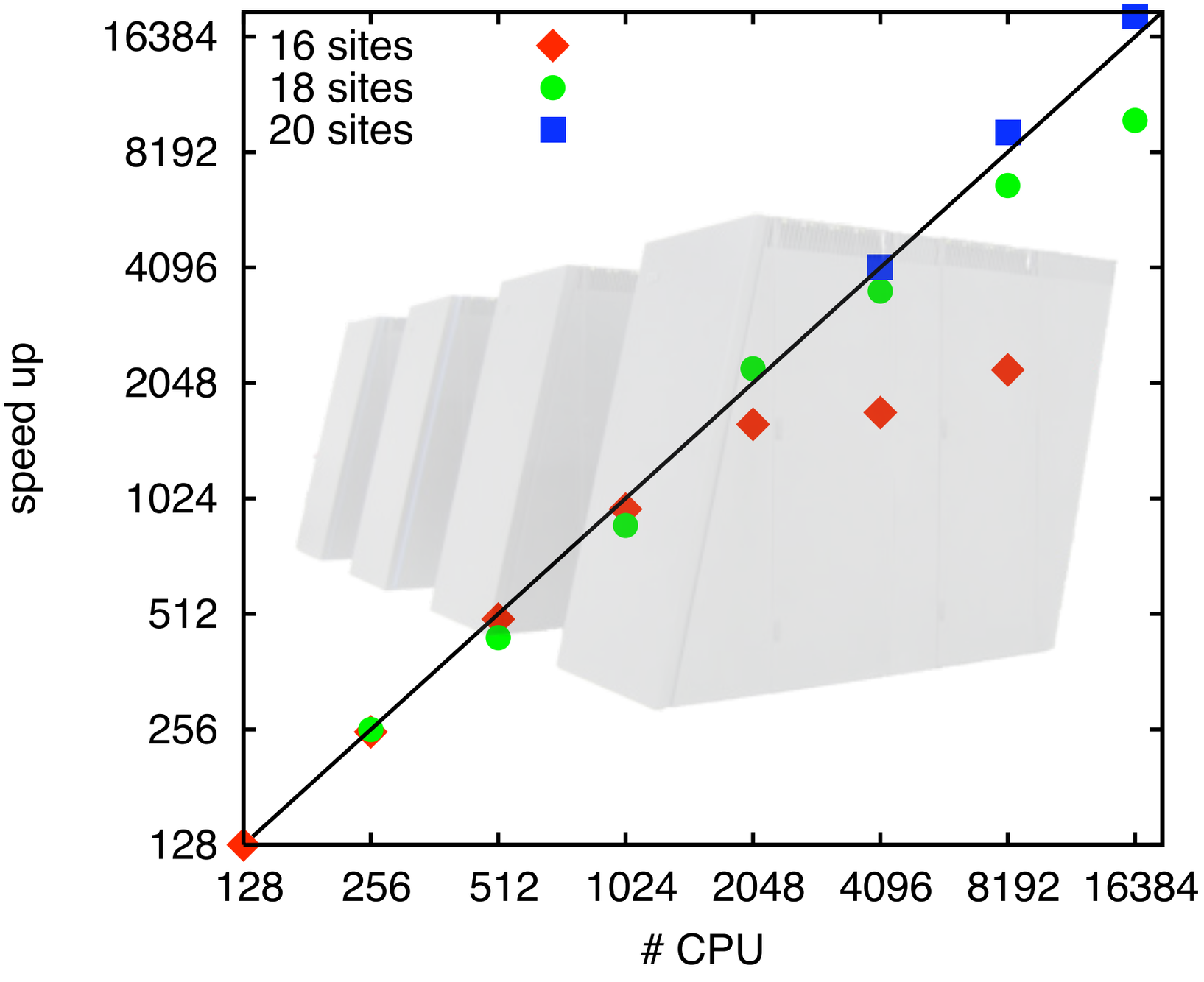
Lanczos-vector as matrix:
$v(i_{\downarrow},i_{\uparrow})$

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

implementation:

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

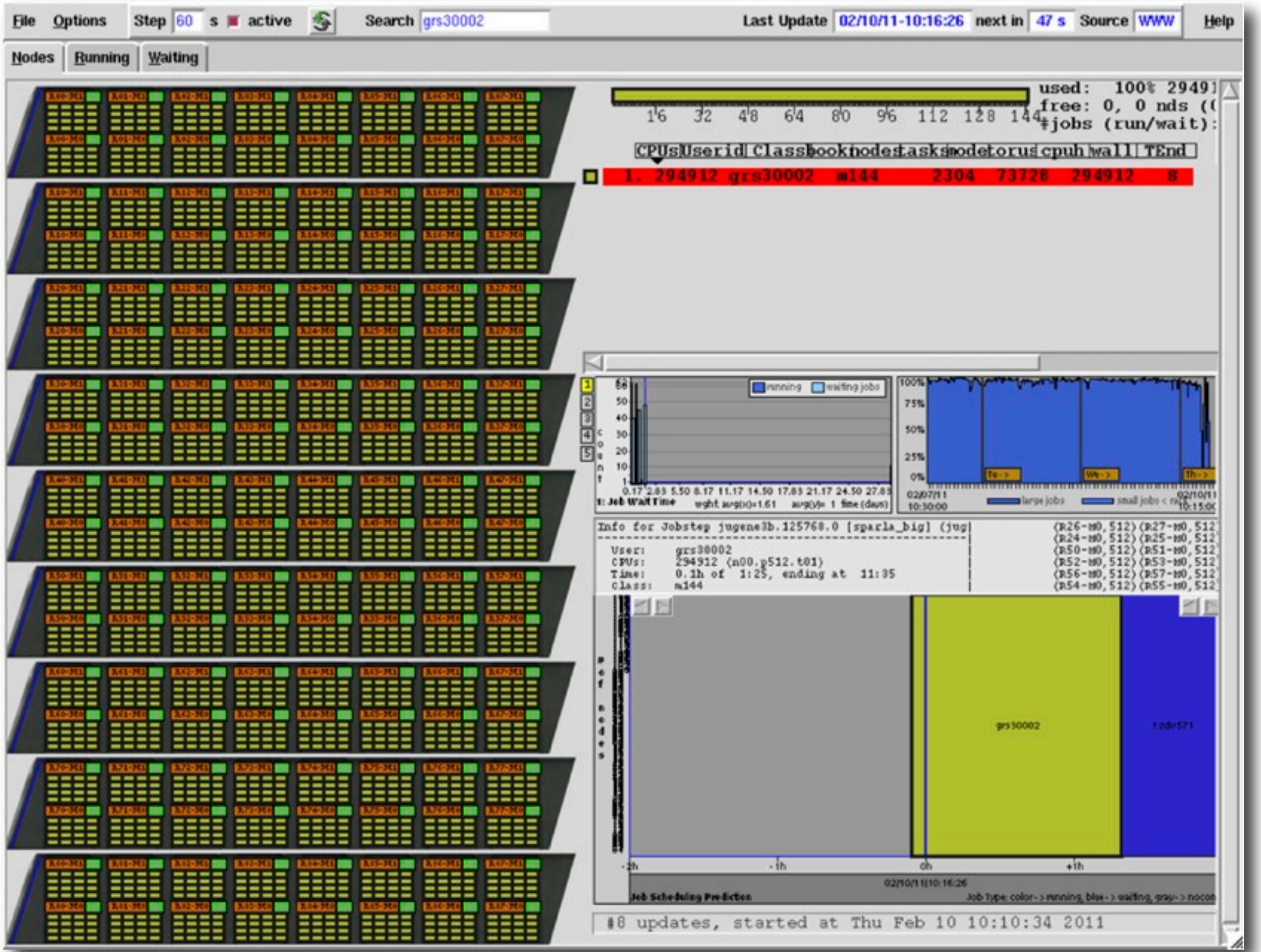
Implementation on IBM BlueGene/P



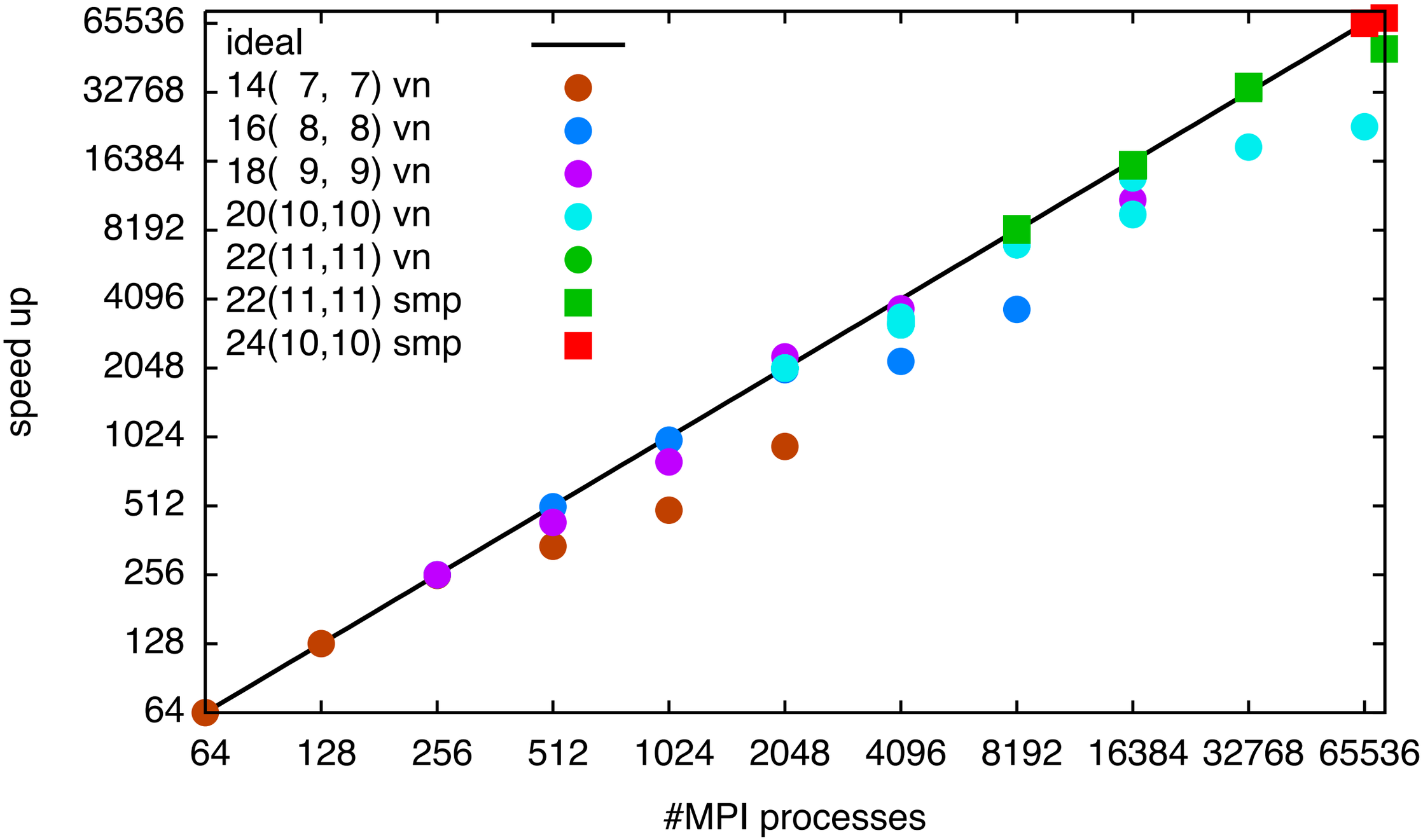
sites	memory
16	1 GB
18	18 GB
20	254 GB

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

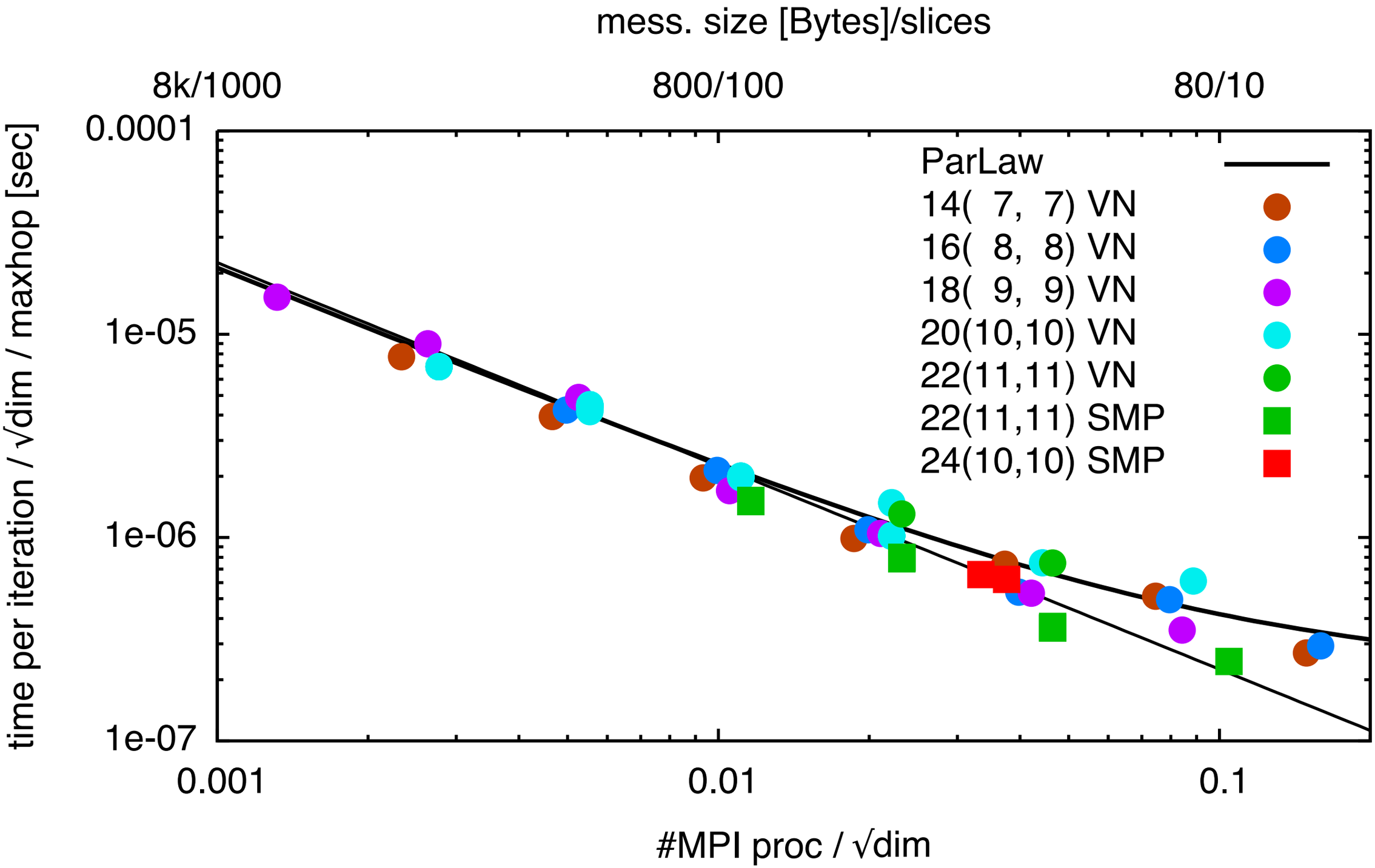
performance on full Jugene?



performance on full Jugene!



performance on full Jugene!



Spin-Systems

pairwise interaction

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

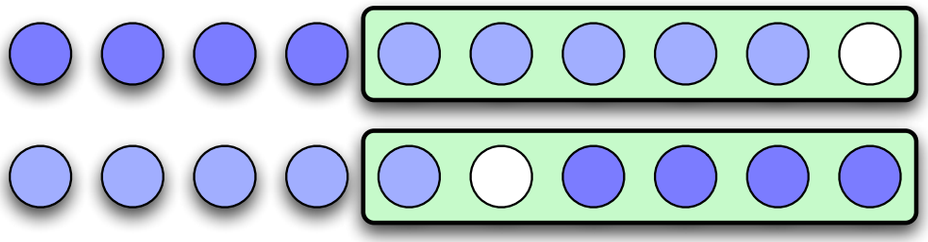
spin configurations

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

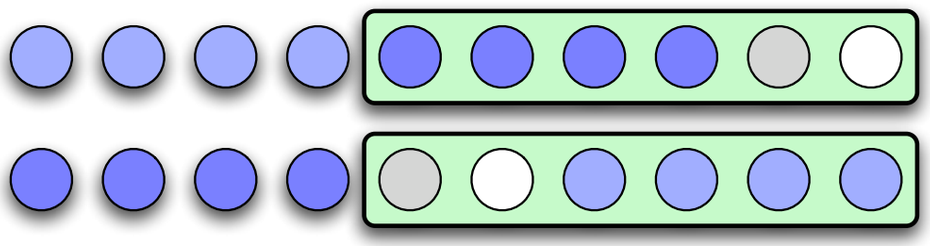
matrix transpose via `MPI_alltoallv` or systolic algorithm

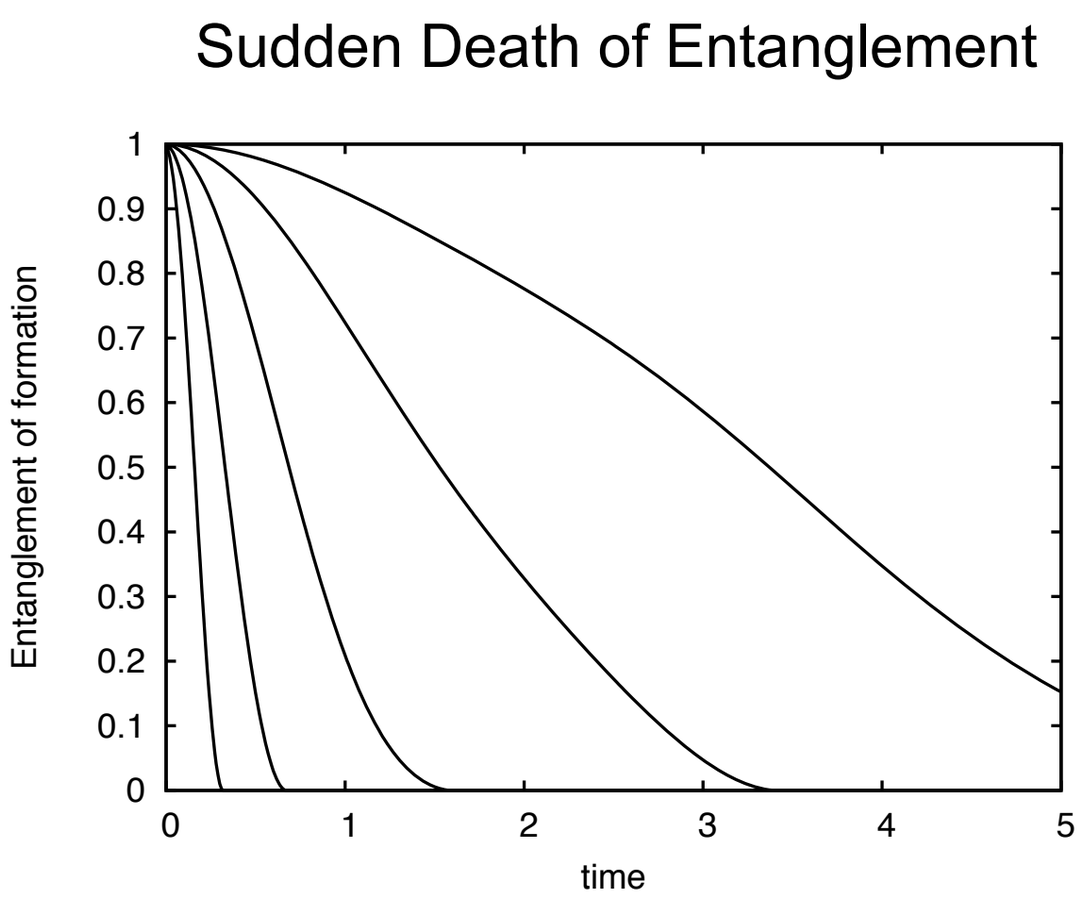
decoherence: single spin

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



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

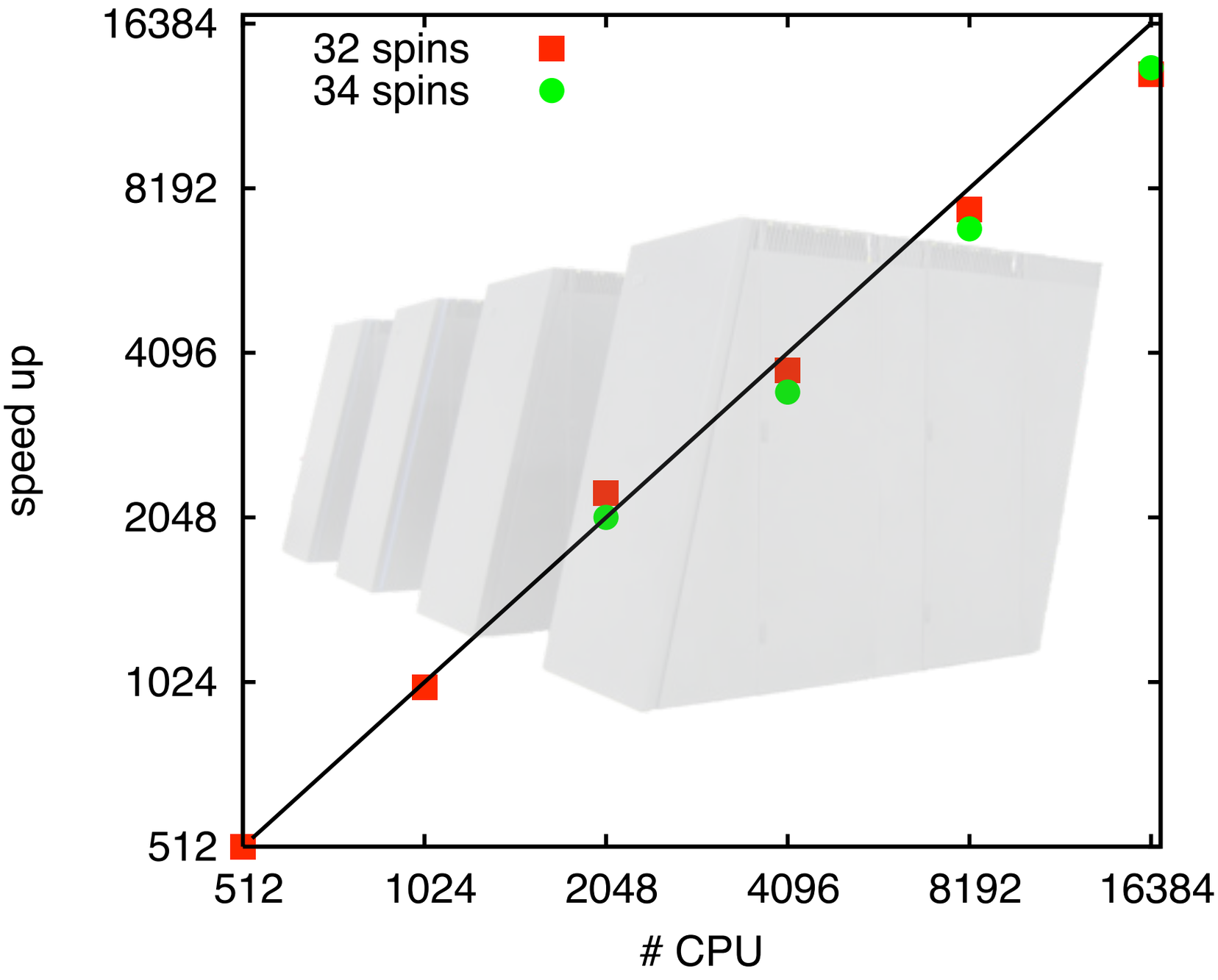
MPI_alltoall

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

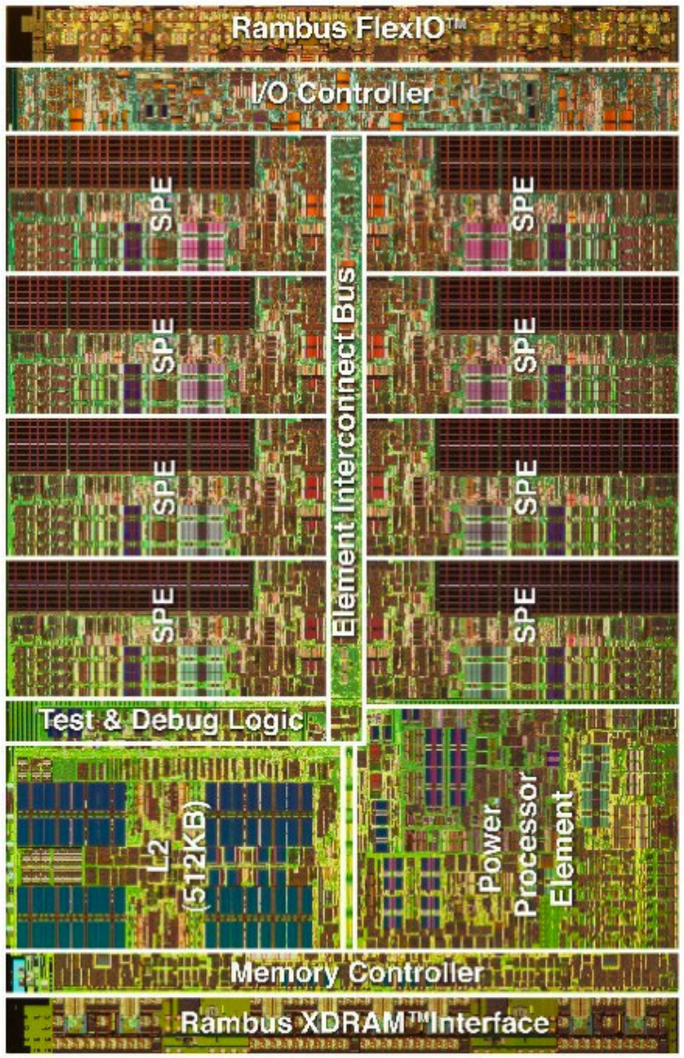
bit reordering: 43 210 ---> 21 034 -> 21 430 (mirror $i_<$)

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

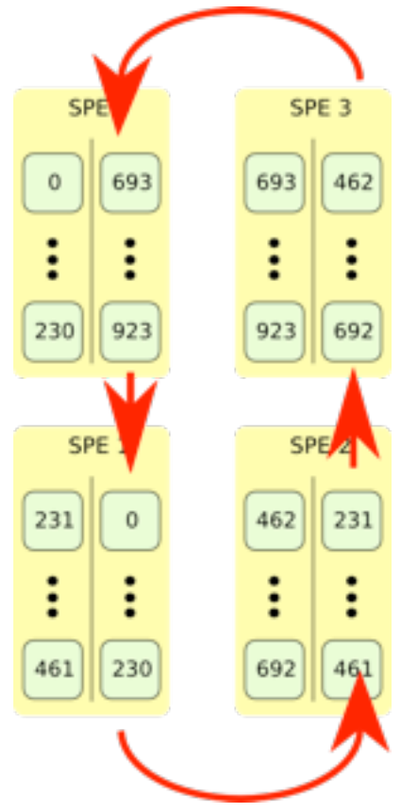
additional partitioning
of local memory

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 optimized bath-parametrization

single-site DMFT

Hubbard model

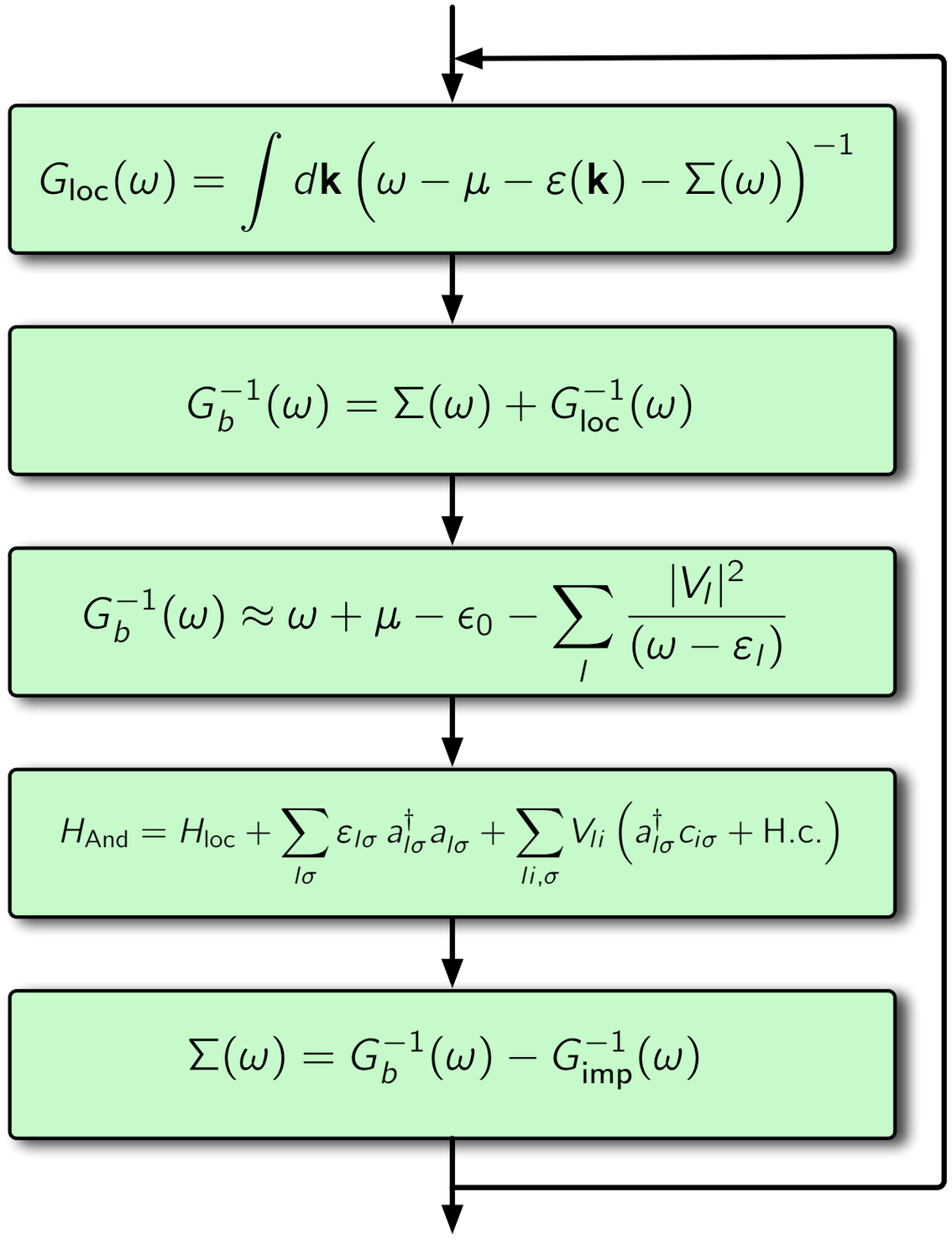
$$H = -\sum_{ij\sigma} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

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?

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

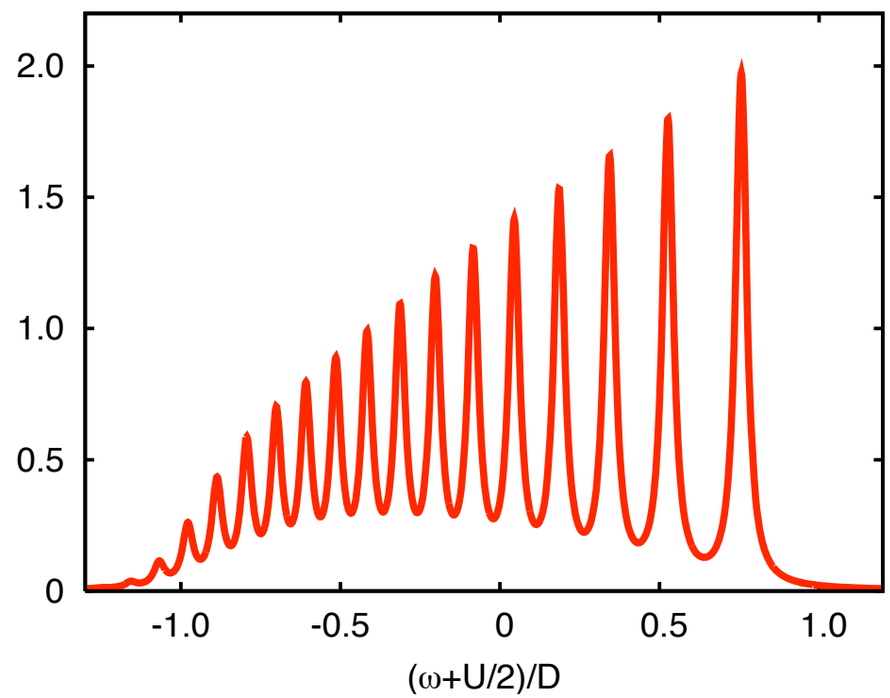
$$H_{\text{And}} = \varepsilon_0 \sum_\sigma n_\sigma + U n_\uparrow n_\downarrow + \sum_\sigma \sum_{l=1}^{N_b} \left(\varepsilon_l n_{l\sigma} + V_l \left(a_{l\sigma}^\dagger c_\sigma + c_\sigma^\dagger a_{l\sigma} \right) \right)$$

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

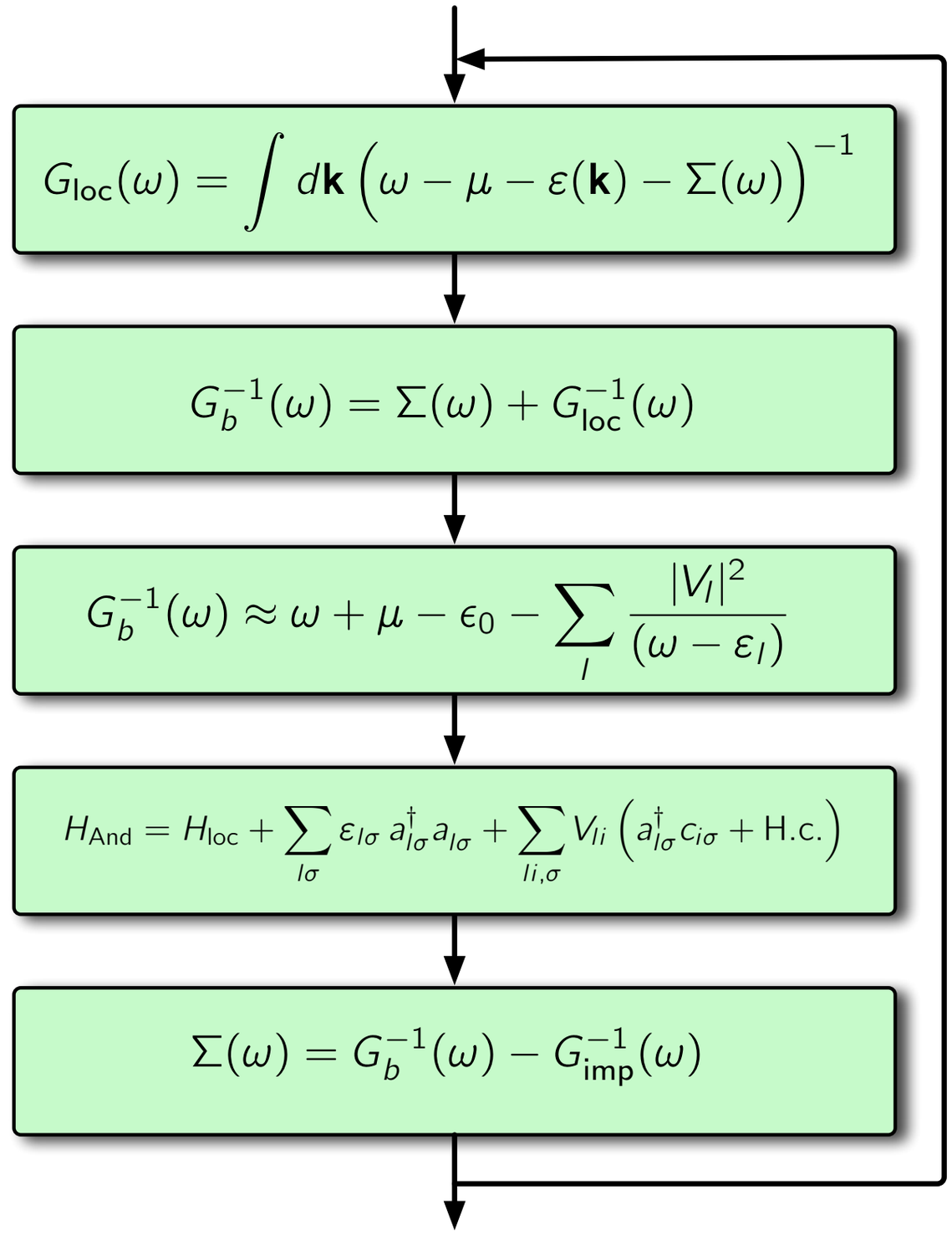
$$H = -\sum_{ij\sigma} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

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: $\int d\mathbf{k}\, H(\mathbf{k}) = \epsilon_0$

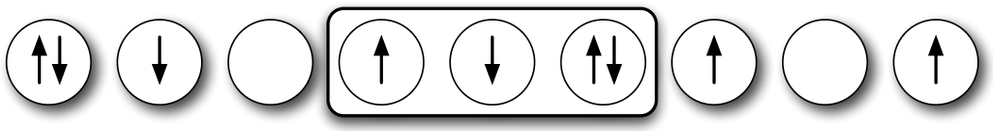
$$H_{\text{loc}} = \epsilon_0 + U\, n_{\uparrow} n_{\downarrow}$$



DMFT for clusters

Hubbard model

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

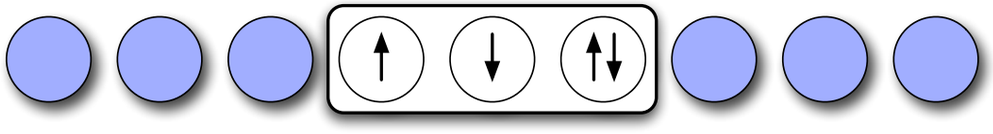


Bloch: $e^{-ik}\ 1\ e^{ik}\ e^{2ik}\ e^{3ik}\ e^{4ik}$

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

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

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



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

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

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

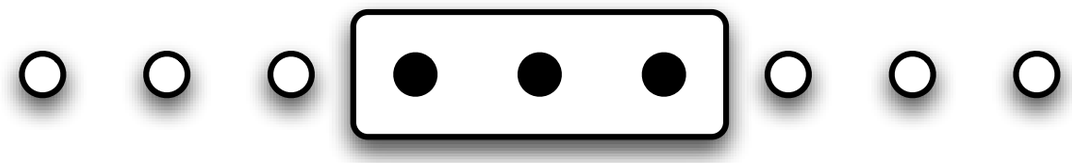
$$H_{\mathrm{And}} = H_{\mathrm{loc}} + \sum_{lm,\sigma} E_{lm,\sigma}\, a^{\dagger}_{l\sigma} a_{m\sigma} + \sum_{li,\sigma} \Gamma_{li} \left(a^{\dagger}_{l\sigma} c_{i\sigma} + \mathrm{H.c.}\right)$$

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

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

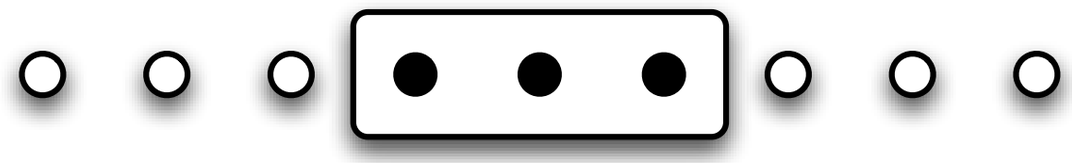
DCA

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

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

translation symmetry
coarse-grained Hamiltonian

CDMFT

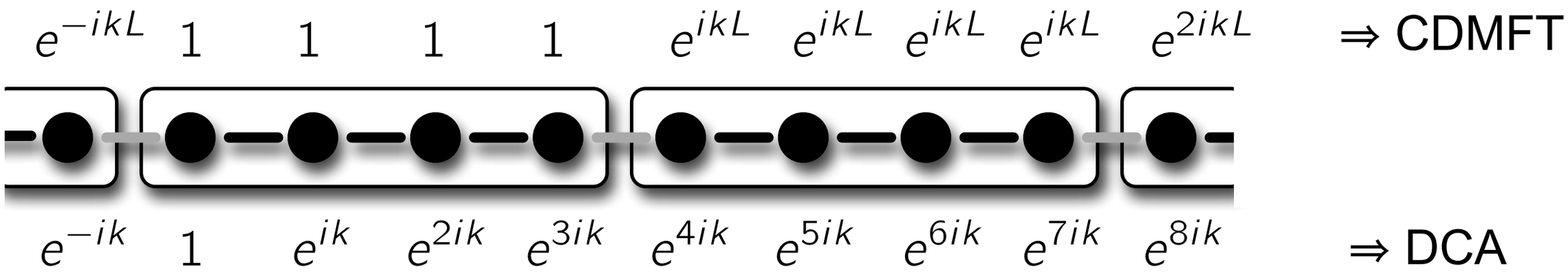


no translation symmetry
original Hamiltonian on cluster

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

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

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**:

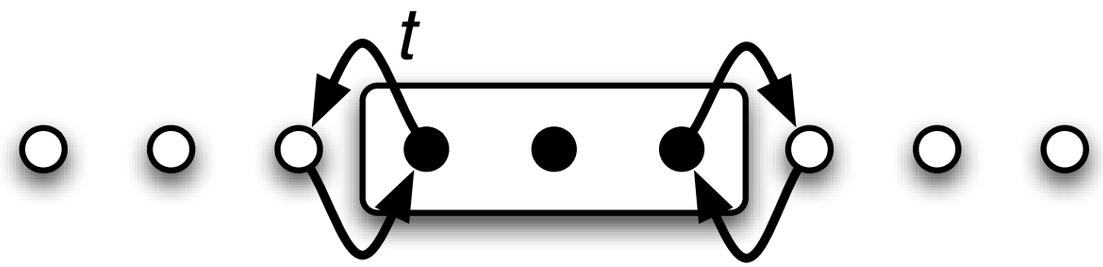
$$\sum_l |V_{l,\mathrm{K}}|^2 = \int d\tilde{\mathbf{k}}\, \varepsilon^2_{\mathrm{K}+\tilde{\mathrm{k}}} - \left(\int d\tilde{\mathbf{k}}\, \varepsilon_{\mathrm{K}+\tilde{\mathrm{k}}} \right)^2$$

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

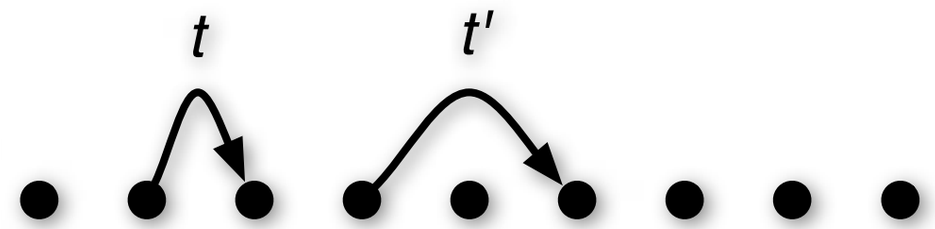
hybridization sum-rules: CDMFT

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

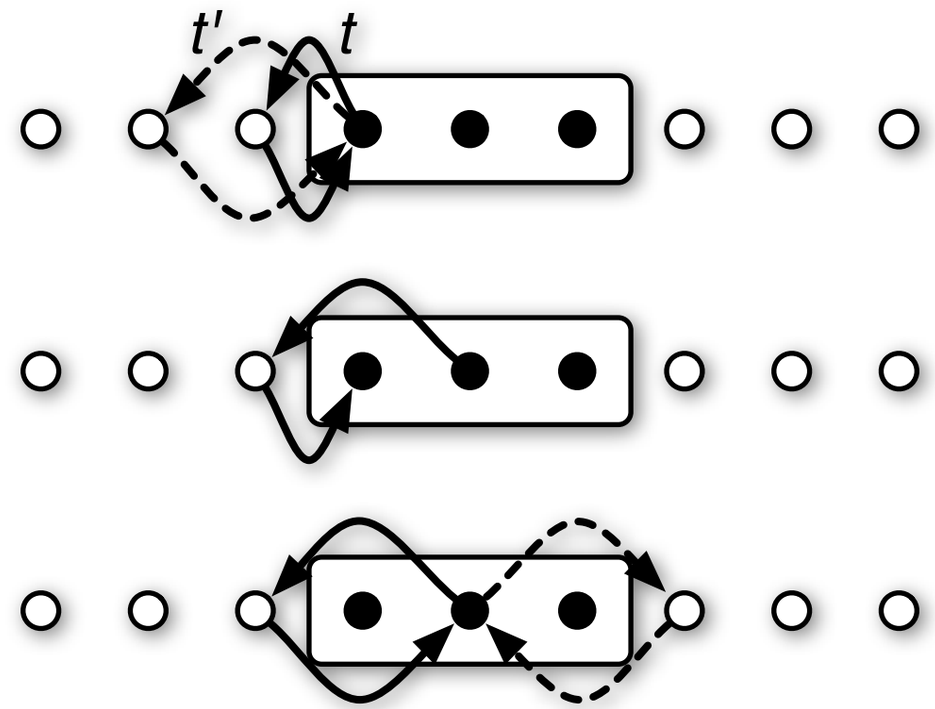
$$\sum_l \mathbf{V}_l \mathbf{V}_l^\dagger = \int d\tilde{\mathbf{k}}\, \mathbf{H}^2(\tilde{\mathbf{k}}) - \left(\int d\tilde{\mathbf{k}}\, \mathbf{H}(\tilde{\mathbf{k}}) \right)^2 = \begin{pmatrix} t^2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & t^2 \end{pmatrix}$$



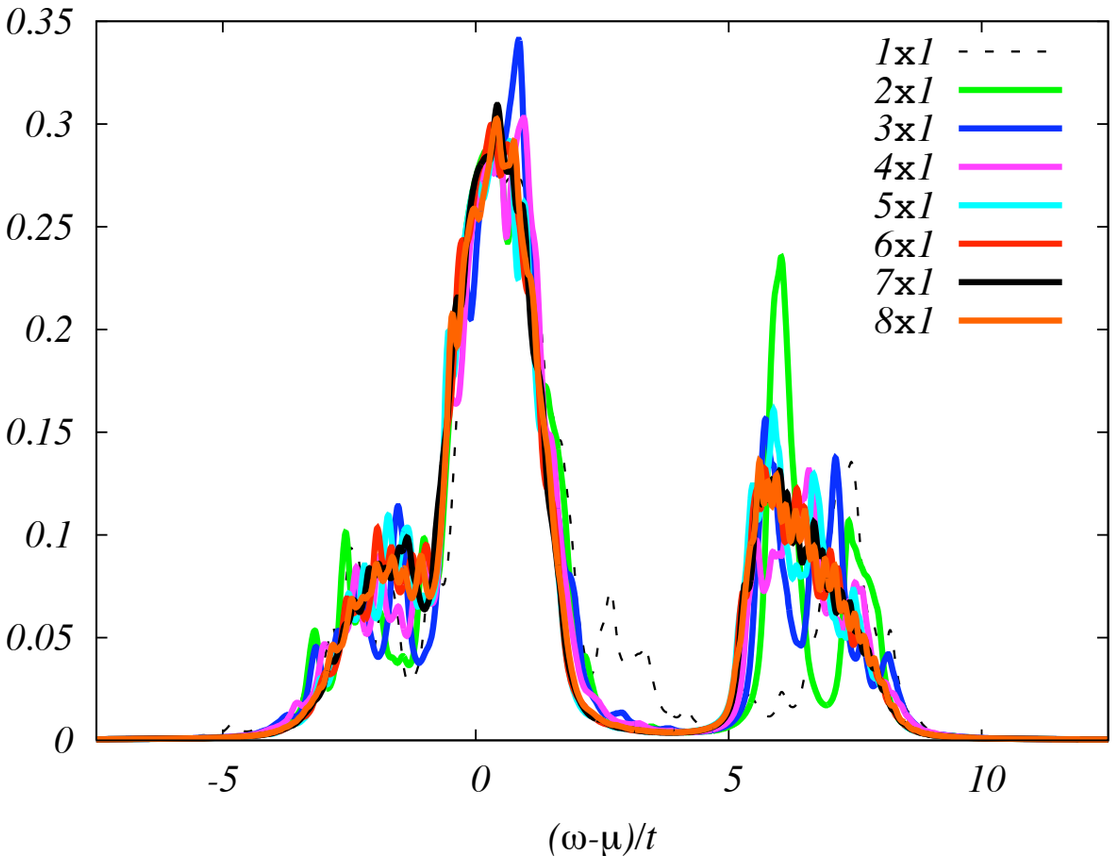
hybridization sum-rules: CDMFT



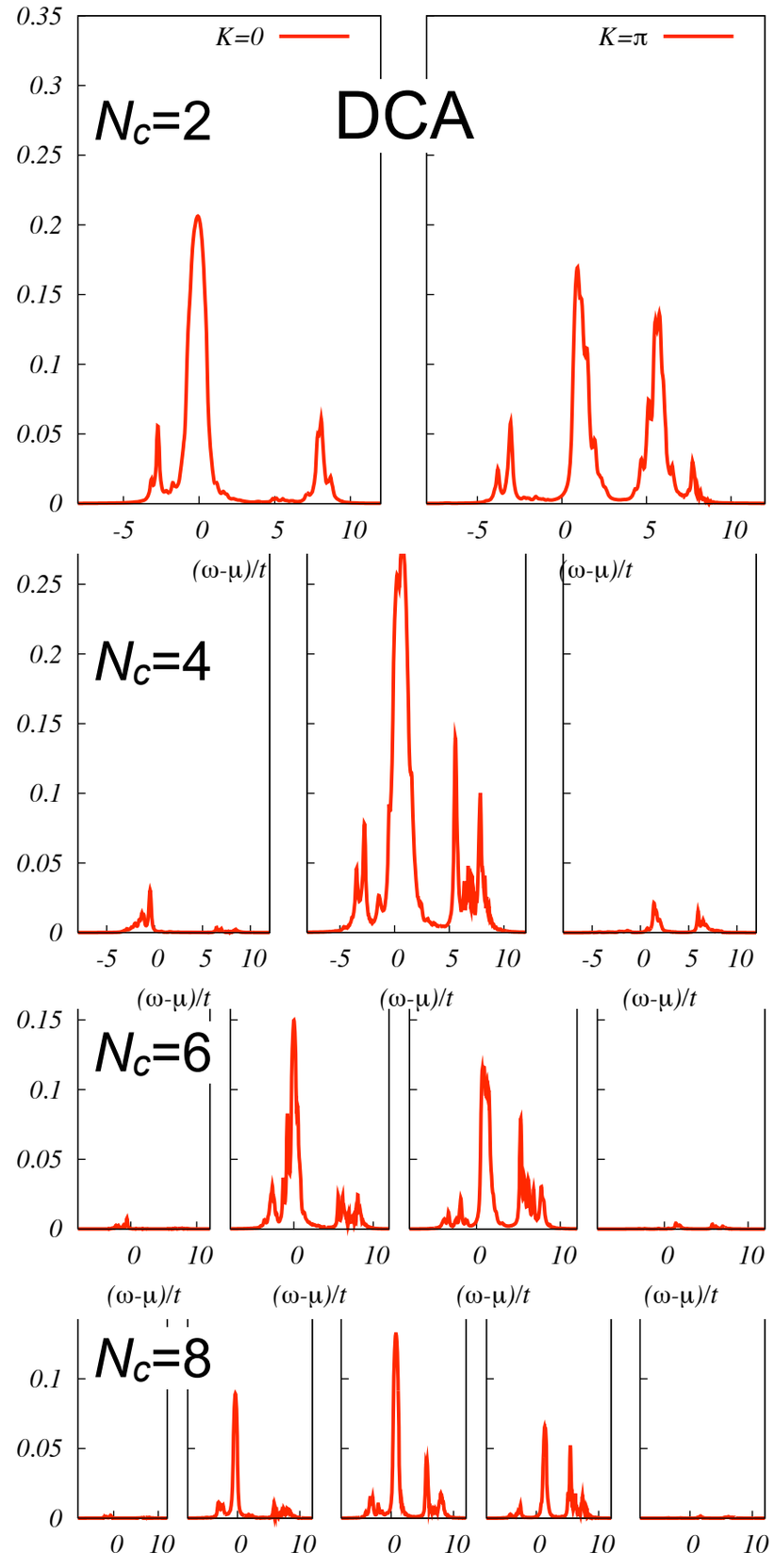
$$\left(\sum_l V_{l,i}\bar{V}_{l,j}\right) = \begin{pmatrix} t^2+t'^2 & t\,t' & 0 \\ t\,t' & 2t'^2 & t\,t' \\ 0 & t\,t' & t^2+t'^2 \end{pmatrix}$$



example: 1-d clusters



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



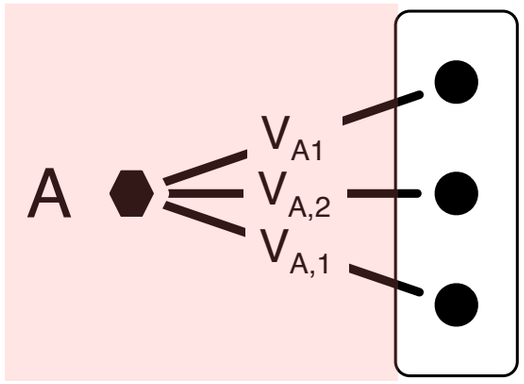
symmetry of bath

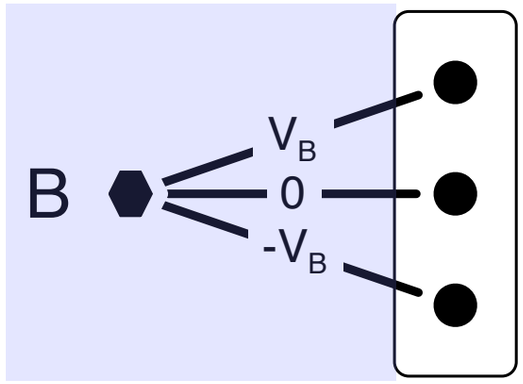
$$\mathbf{W} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{pmatrix}$$

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





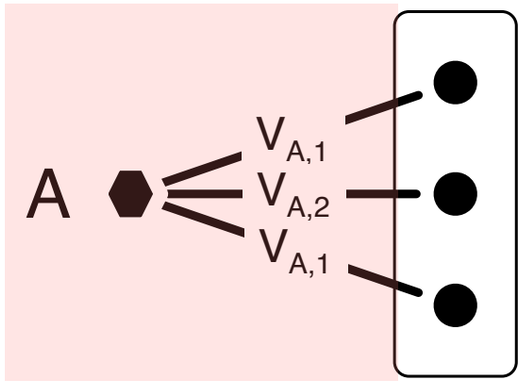
symmetry of bath

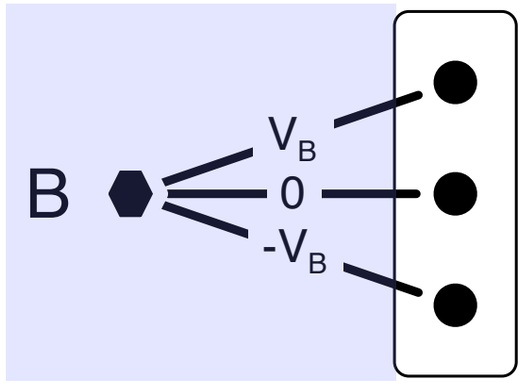
$$\mathbf{W} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -1 \end{pmatrix}$$

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

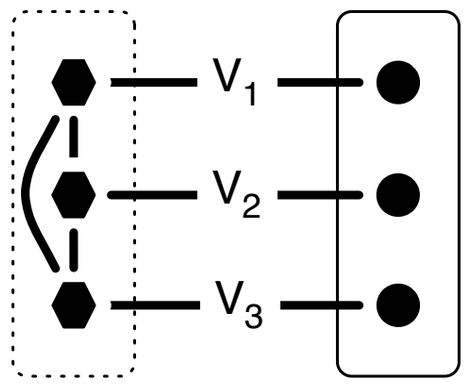
$$\mathbf{W}^\dagger \mathbf{G}_b^{-1} \mathbf{W} = \begin{pmatrix} G_{b,11}^{-1} + G_{b,13}^{-1} & \sqrt{2}\, G_{b,12}^{-1} & 0 \\ \sqrt{2}\, G_{b,21}^{-1} & G_{b,22}^{-1} & 0 \\ 0 & 0 & G_{b,11}^{-1} - G_{b,13}^{-1} \end{pmatrix}$$

block-diagonal





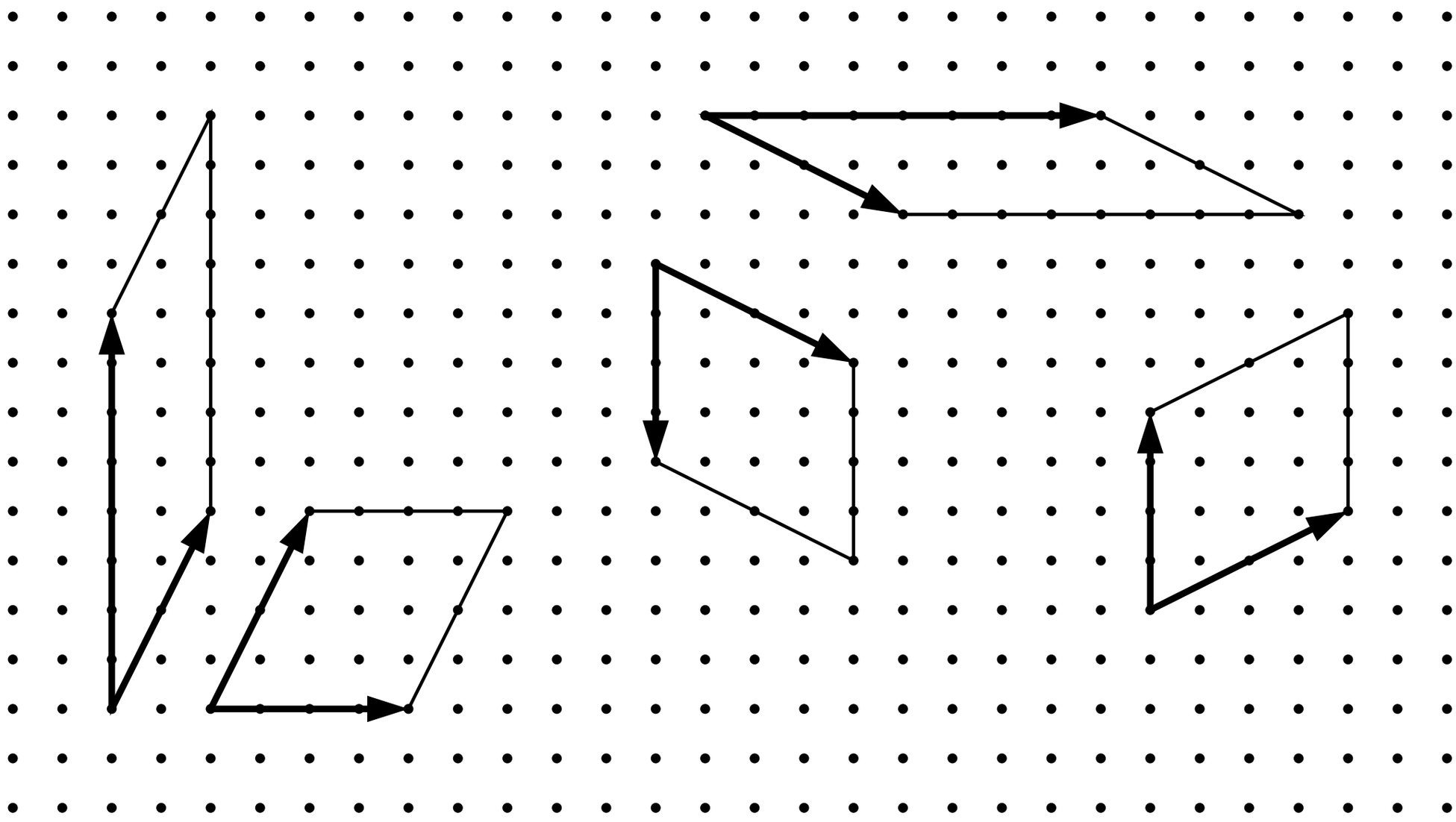
cluster replica: 2A+B



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

supercells

$$\mathbf{C} = \mathbf{A}\,\mathbf{L} \qquad V = \left|\det(\mathbf{C})\right|$$



are they all different?

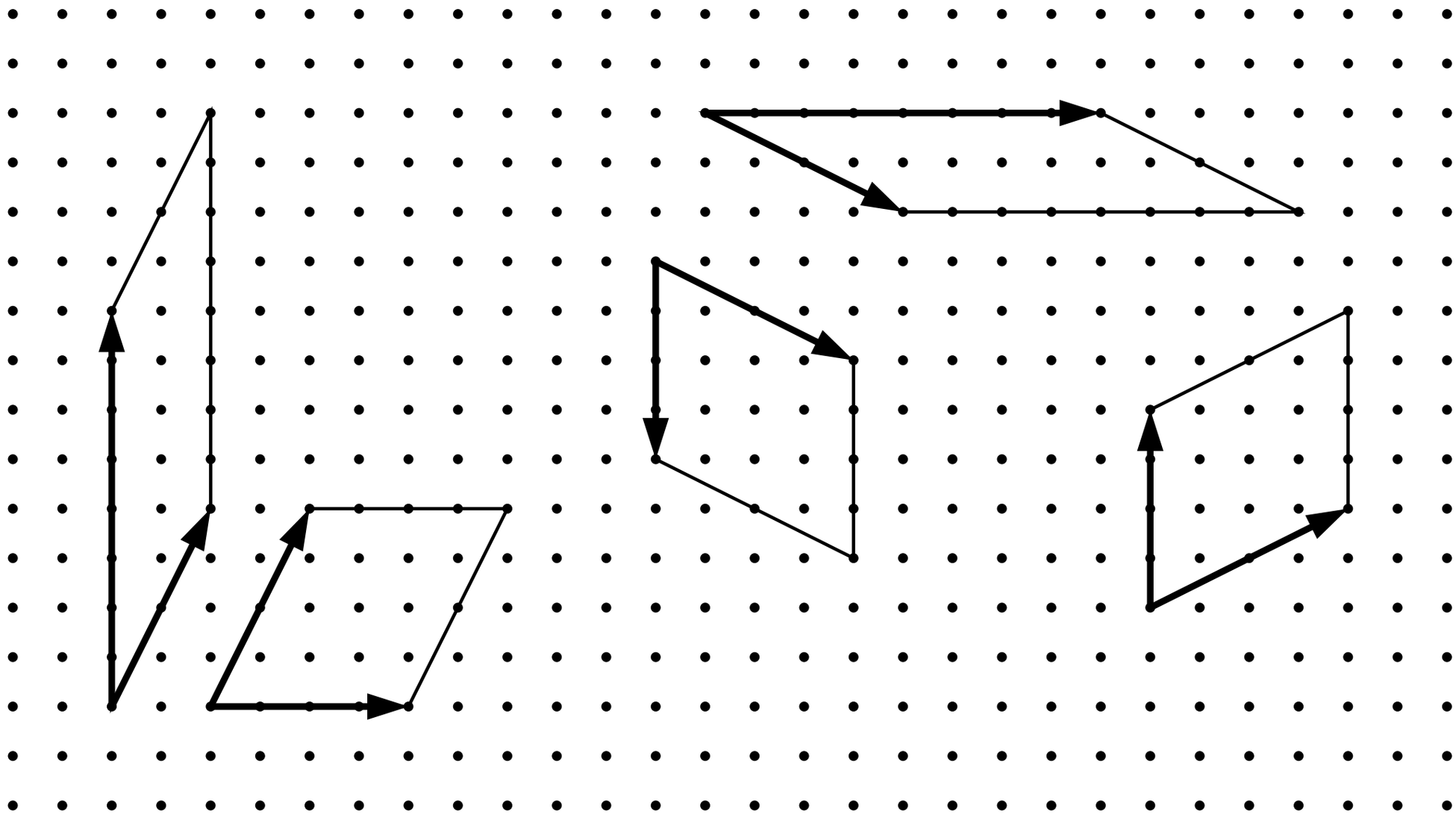
Hermite normal form

$$\mathbf{\Lambda} = \begin{pmatrix} \lambda_{11} & 0 & 0 & \cdots \\ \lambda_{21} & \lambda_{22} & 0 & \\ \lambda_{31} & \lambda_{32} & \lambda_{33} & \\ \vdots & & & \ddots \end{pmatrix} \qquad 0 \le \lambda_{ij} < \lambda_{ii}$$

Euclidean algorithm

$$\gcd(a,b) = \begin{cases} |a| & \text{if } b = 0 \quad \text{(change sign of column)} \\ \gcd(b,a) & \text{if } |a| < |b| \quad \text{(exchange columns)} \\ \gcd(a - \lfloor a/b \rfloor b, b) & \text{otherwise} \quad \text{(add integer multiple of col)} \end{cases}$$

Hermite normal form



$\mathbf{L}: \begin{pmatrix} 2 & 0 \\ 4 & 8 \end{pmatrix}_{\text{HNF}} \quad \begin{pmatrix} 4 & 2 \\ 0 & 4 \end{pmatrix}$ $\quad \begin{pmatrix} 0 & 4 \\ -4 & -2 \end{pmatrix} \quad \begin{pmatrix} 4 & 8 \\ -2 & 0 \end{pmatrix} \quad \begin{pmatrix} 4 & 0 \\ 2 & 4 \end{pmatrix}_{\text{HNF}}$

HNF

symmetry

enumeration & properties of clusters

Betts Criteria

www.cond-mat.de/sims/cluster/

List supercells | HNF reduction | LLL reduction | Align primitive vectors

Number of lattice points N: 8

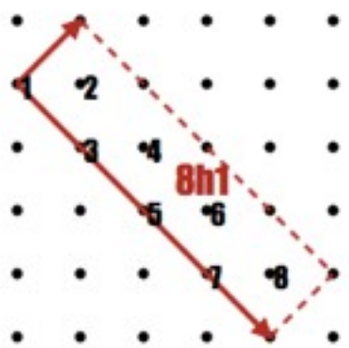
Primitive vectors ($\vec{a}_1$,$\vec{a}_2$): square | 1 0 | 0 1

Betts numbering: ☑ Show number

Betts labeling: ☑ Show label

List all supercells

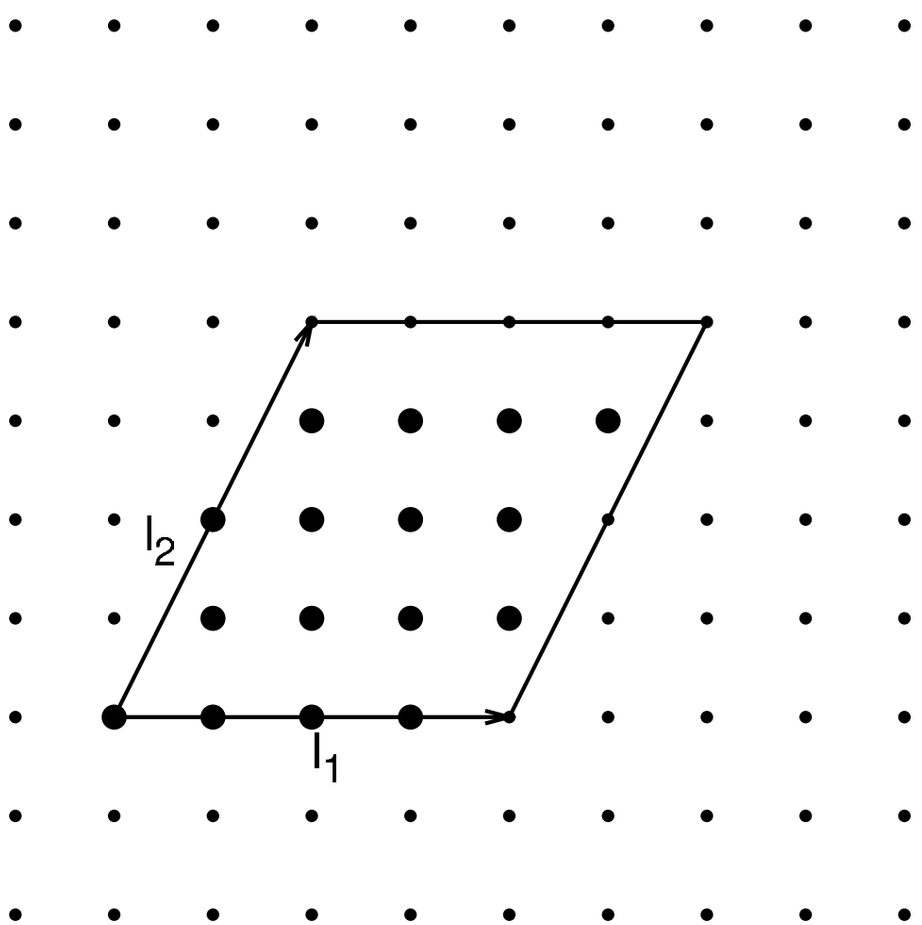
Show all plots

No	Nαk	l_1	l_2	L_1	L_2	√σ ▼	S ▼	J ▼	I_F ▼	I_B ▼	hide all
1	8h0	(8, 0)	(0, 1)	(0, 1)	(8, 0)	0.50	C_{2v}	19	6	-	 hide
2	8h1	(8, 0)	(1, 1)	(1, 1)	(4,-4)	0.69	C_2	9	6	3	

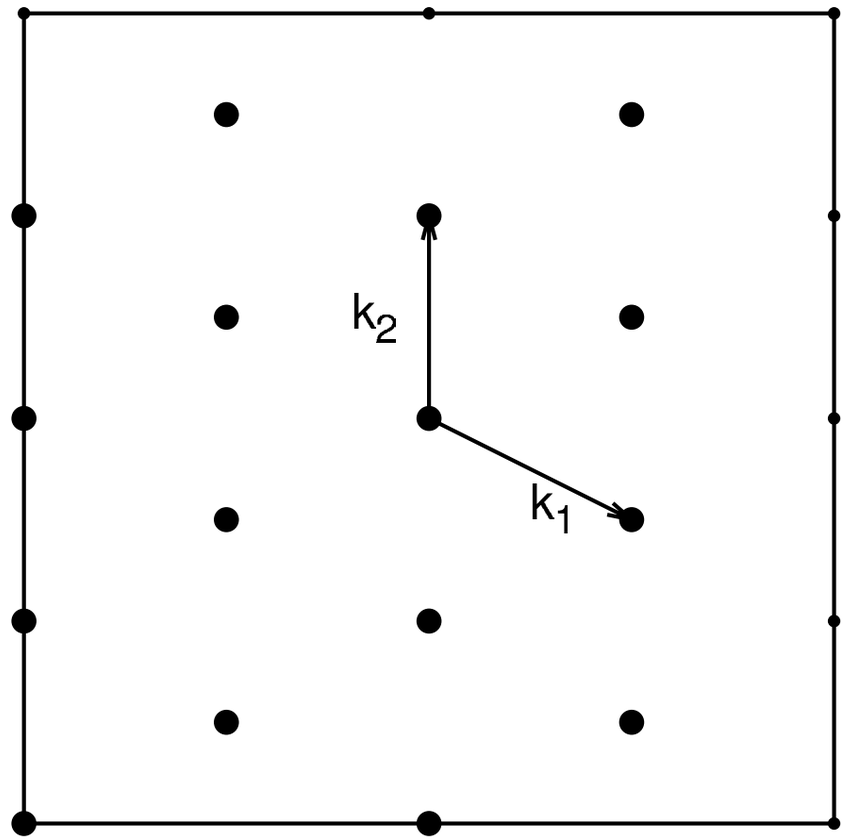
http://www.cond-mat.de/sims/cluster/

supercell: *k*-point sampling

$$\mathbf{K}_{\mathcal{S}} = (2\pi\mathbf{C}^{-1})^T = \mathbf{G}(\mathbf{L}^{-1})^T$$



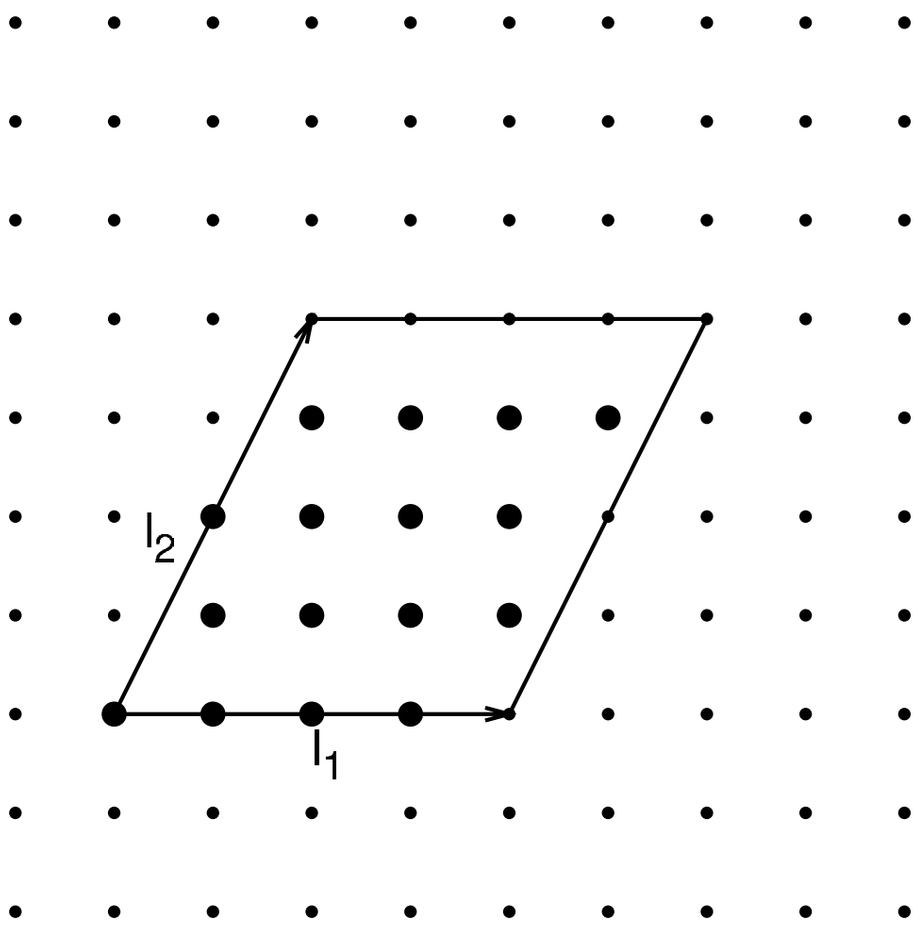
supercell



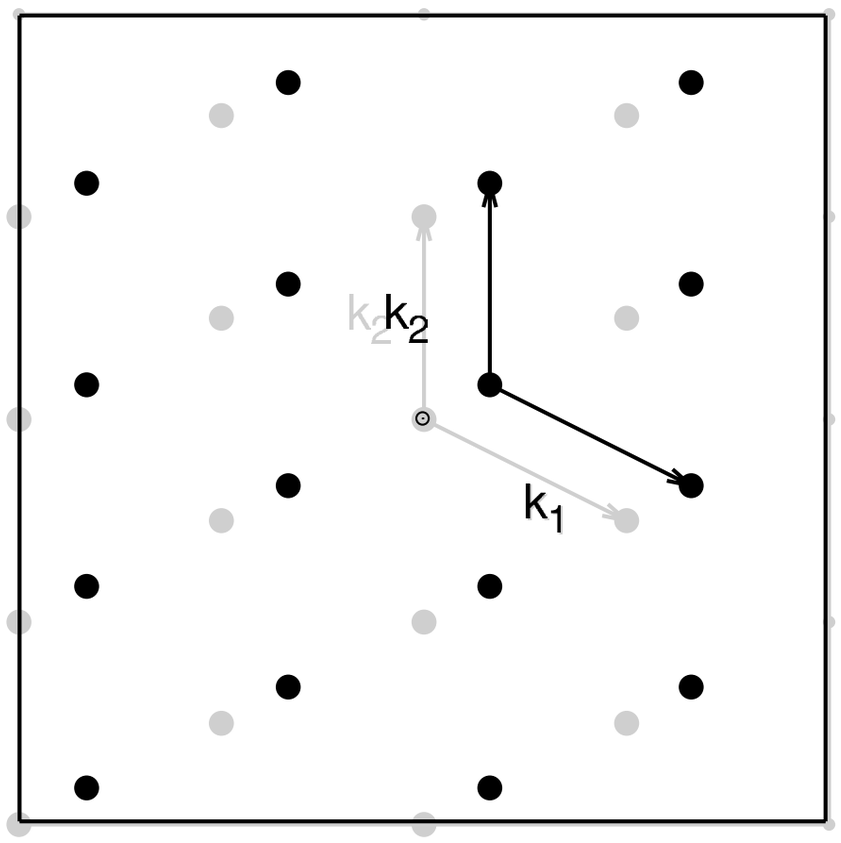
Brillouin zone

supercell: *k*-point sampling

$$\mathbf{K}_{\mathcal{S}} = (2\pi\mathbf{C}^{-1})^T = \mathbf{G}(\mathbf{L}^{-1})^T$$



supercell



Brillouin zone

Monkhorst-Pack grid

particularly suited for Brillouin-zone integrals

$$\mathbf{L} = \begin{pmatrix} n_1 & 0 & 0 \\ 0 & n_2 & 0 \\ 0 & 0 & n_3 \end{pmatrix}$$

$$\tilde{\mathbf{k}} = \sum_i \frac{(n_i - 1)\mathbf{k}_i}{2n_i}$$

PHYSICAL REVIEW B VOLUME 13, NUMBER 12 15 JUNE 1976

Special points for Brillouin-zone integrations*

Hendrik J. Monkhorst and James D. Pack
Department of Physics, University of Utah, Salt Lake City, Utah 84112
(Received 21 January 1976)

A method is given for generating sets of special points in the Brillouin zone which provides an efficient means of integrating periodic functions of the wave vector. The integration can be over the entire Brillouin zone or over specified portions thereof. This method also has applications in spectral and density-of-state calculations. The relationships to the Chadi-Cohen and Gilat-Raubenheimer methods are indicated.

top cited Phys. Rev. papers

Table 1. *Physical Review* Articles with more than 1000 Citations Through June 2003

Publication	# cites	Av. age	Title	Author(s)
PR **140**, A1133 (1965)	3227	26.7	Self-Consistent Equations Including Exchange and Correlation Effects	W. Kohn, L. J. Sham
PR **136**, B864 (1964)	2460	28.7	Inhomogeneous Electron Gas	P. Hohenberg, W. Kohn
PRB **23**, 5048 (1981)	2079	14.4	Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems	J. P. Perdew, A. Zunger
PRL **45**, 566 (1980)	1781	15.4	Ground State of the Electron Gas by a Stochastic Method	D. M. Ceperley, B. J. Alder
PR **108**, 1175 (1957)	1364	20.2	Theory of Superconductivity	J. Bardeen, L. N. Cooper, J. R. Schrieffer
PRL **19**, 1264 (1967)	1306	15.5	A Model of Leptons	S. Weinberg
PRB **12**, 3060 (1975)	1259	18.4	Linear Methods in Band Theory	O. K. Anderson
PR **124**, 1866 (1961)	1178	28.0	Effects of Configuration Interaction of Intensities and Phase Shifts	U. Fano
RMP **57**, 287 (1985)	1055	9.2	Disordered Electronic Systems	P. A. Lee, T. V. Ramakrishnan
RMP **54**, 437 (1982)	1045	10.8	Electronic Properties of Two-Dimensional Systems	T. Ando, A. B. Fowler, F. Stern
PRB **13**, 5188 (1976)	1023	20.8	Special Points for Brillouin-Zone Integrations	H. J. Monkhorst, J. D. Pack

PR, Physical Review; PRB, Physical Review B; PRL, Physical Review Letters; RMP, Reviews of Modern Physics.

S. Redner: *Citation Statistics from 110 years of Physical Review*
Physics Today June 2005, p. 49

top cited Phys. Rev. papers

Table 1. *Physical Review* Articles with more than 1000 Citations Through June 2003

Publication	# cites	Av. age	Title	Author(s)
PR **140**, A1133 (1965)	3227	26.7	Self-Consistent Equations Including Exchange and Correlation Effects	W. Kohn, L. J. Sham
PR **136**, B864 (1964)	2460	28.7	Inhomogeneous Electron Gas	P. Hohenberg, W. Kohn
PRB **23**, 5048 (1981)	2079	14.4	Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems	J. P. Perdew, A. Zunger
PRL **45**, 566 (1980)	1781	15.4	Ground State of the Electron Gas by a Stochastic Method	D. M. Ceperley, B. J. Alder
PR **108**, 1175 (1957)	1364	20.2	Theory of Superconductivity	J. Bardeen, L. N. Cooper, J. R. Schrieffer
PRL **19**, 1264 (1967)	1306	15.5	A Model of Leptons	S. Weinberg
PRB **12**, 3060 (1975)	1259	18.4	Linear Methods in Band Theory	O. K. Anderson
PR **124**, 186				
RMP **57**, 28				
RMP **54**, 43				
PRB **13**, 518				
PR, Physical				

top 10 cited Phys Rev papers (July 2007)

	article			cites	title	author(s)
1	PR	140	A1133	(1965)	4930	Self Consistent Equations..	W. Kohn & L. J. Sham
2	PR	136	B864	(1965)	3564	Inhomogeneous Electron Gas..	P. Hohenberg & W. Kohn
3	PRB	23	5048	(1981)	3007	Self-Interaction Correction to..	J. P. Perdew & A. Zunger
4	PRL	45	566	(1980)	2514	Ground State of the Electron..	D. M. Ceperley & B. J. Alder
5	PRL	77	3865	(1996)	2478	Generalized Gradient Approx...	Perdew, Burke, Ernzerhof
6	PRB	13	5188	(1976)	2277	Special Points for Brillouin..	H. J. Monkhorst & J. D. Pack
7	PRB	54	11169	(1996)	1933	Efficient Iterative Schemes....	G. Kresse & J. Furthmuller
8	PRB	43	1993	(1991)	1776	Efficient Pseudopotentials for	N. Troullier & J.L. Martins
9	PRB	41	7892	(1990)	1749	Soft Self-Consistent Pseudopotentials...	D. Vanderbilt
10	PR	108	1175	(1957)	1650	Theory of Superconductivity	Bardeen, Cooper, Schrieffer

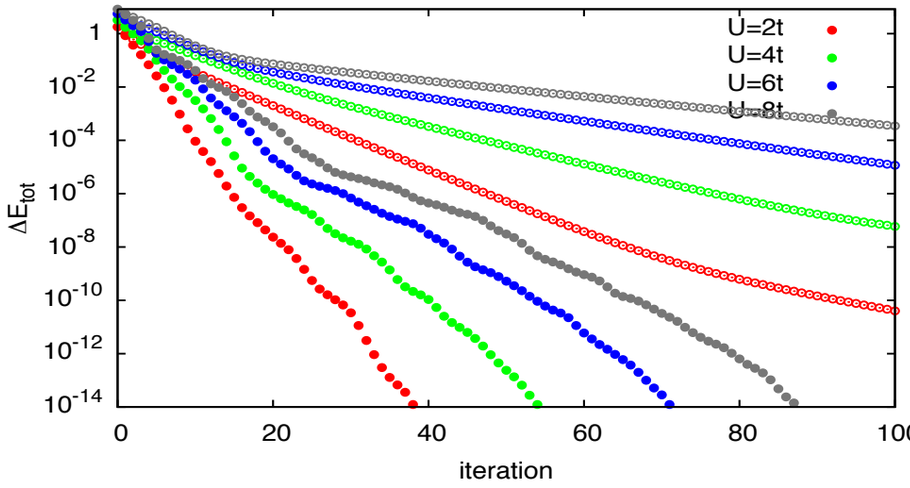
S. Rec
Physic

S. Redner: *A Physicist's Perspective on Citation Analysis*
Trends in Research Measurement Metrics, Washington DC, Oct 2010
http://physics.bu.edu/~redner/talks/citations-10.pdf

summary

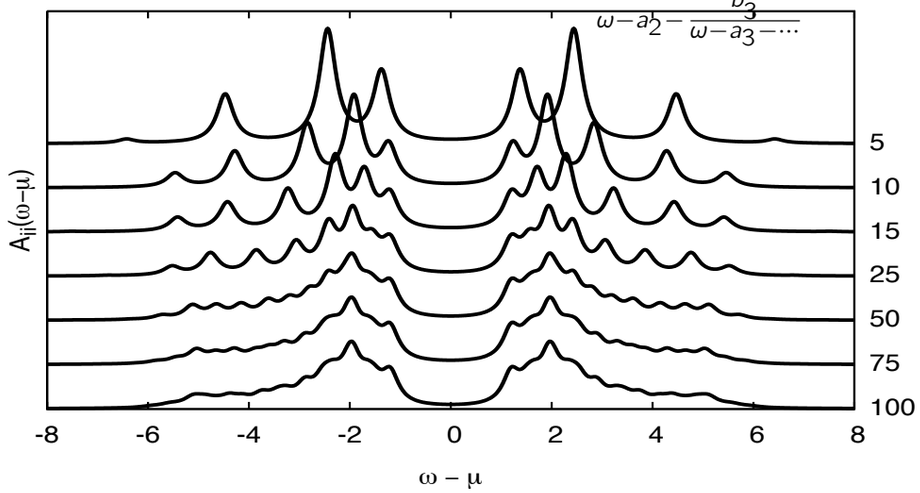
steepest descent ⇒ Krylov space

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

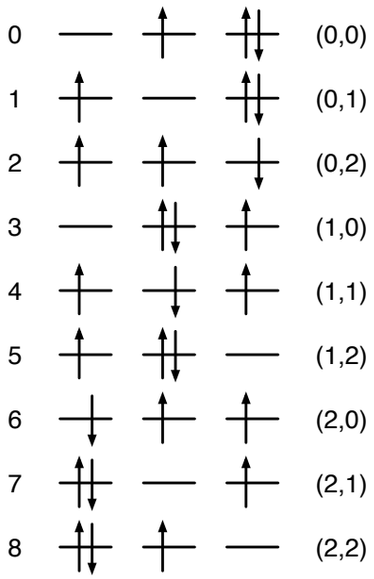


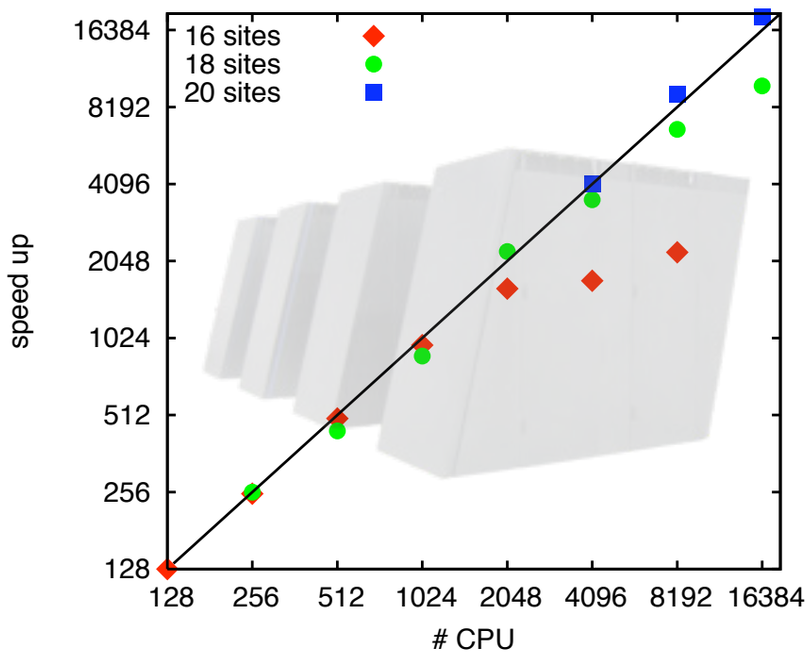
spectral function: moments

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

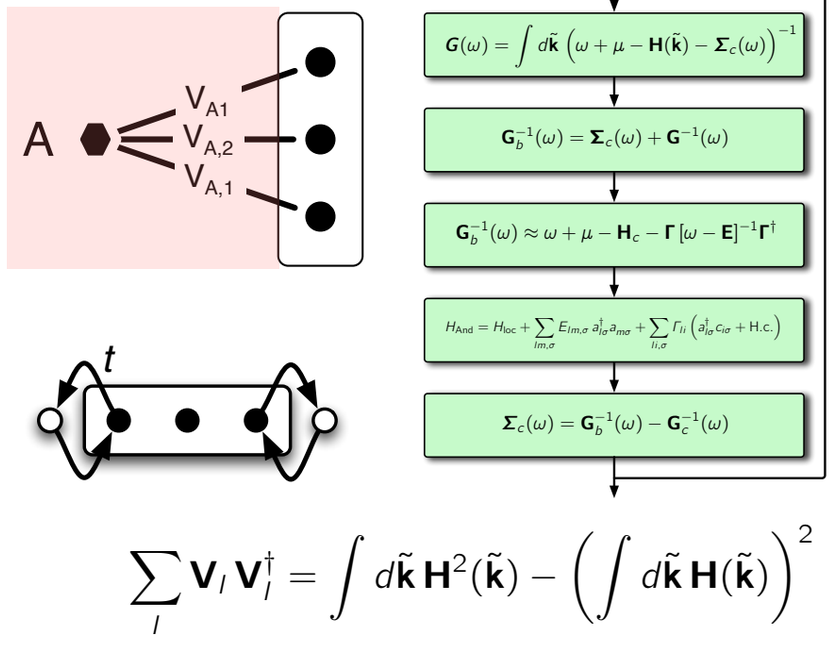


sparse Hamiltonian in Wannier representation





bath parametrization



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