Exact Diagonalization and Lanczos Method

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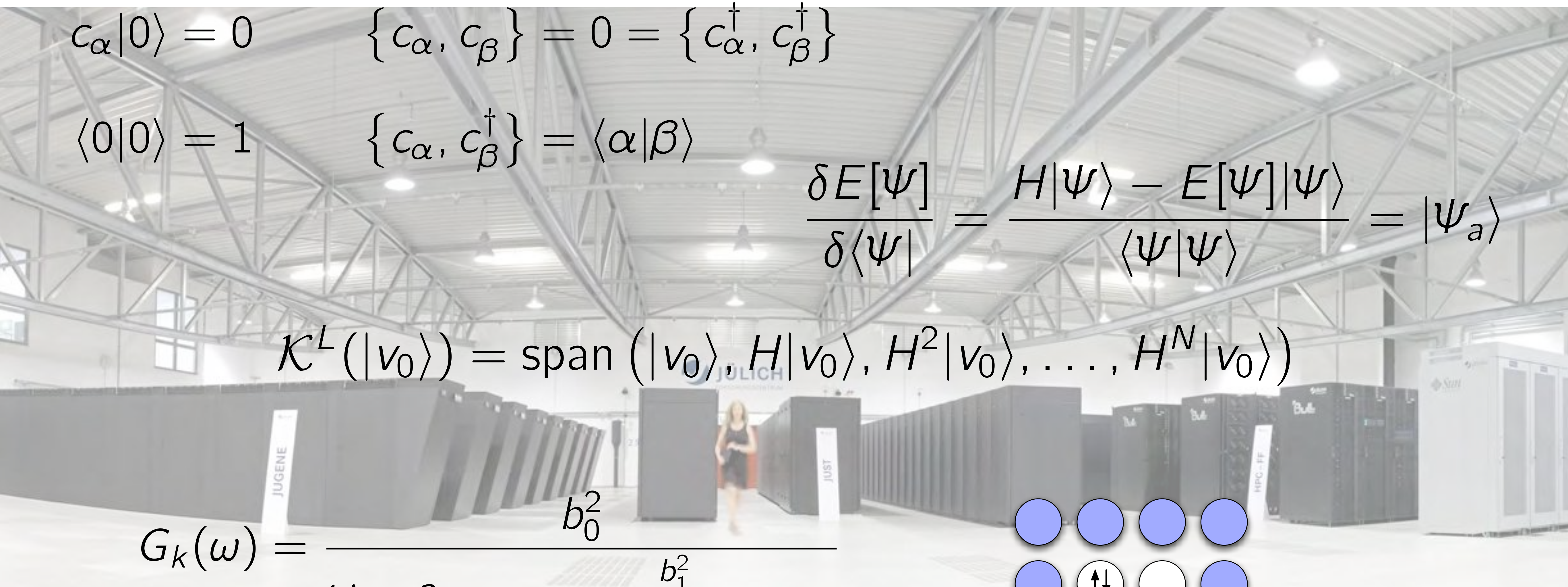


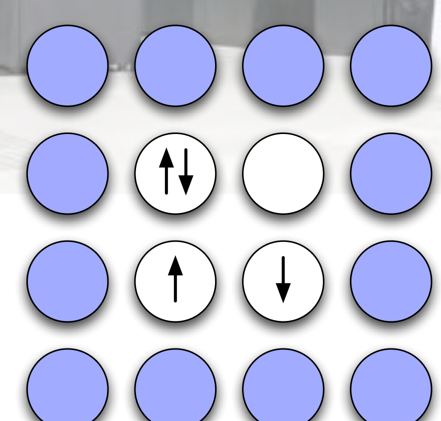
$$c_\alpha|0\rangle = 0 \qquad \left\{c_\alpha, c_\beta\right\} = 0 = \left\{c_\alpha^\dagger, c_\beta^\dagger\right\}$$

$$\langle 0|0\rangle = 1 \qquad \left\{c_\alpha, c_\beta^\dagger\right\} = \langle\alpha|\beta\rangle$$

$$\frac{\delta E[\Psi]}{\delta\langle\Psi|} = \frac{H|\Psi\rangle - E[\Psi]|\Psi\rangle}{\langle\Psi|\Psi\rangle} = |\Psi_a\rangle$$

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

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



The Theory of Everything

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We discuss recent developments in our understanding of matter, broadly construed, and their implications for contemporary research in fundamental physics.

The Theory of Everything is a term for the ultimate theory of the universe—a set of equations capable of describing all phenomena that have been observed, or that will ever be observed (1). It is the modern incarnation of the reductionist ideal of the ancient Greeks, an approach to the natural world that has been fabulously successful in bettering the lot of mankind and continues in many people's minds to be the central paradigm of physics. A special case of this idea, and also a beautiful instance of it, is the equation of conventional nonrelativistic quantum mechanics, which describes the everyday world of human beings—air, water, rocks, fire, people, and so forth. The details of this equation are less important than the fact that it can be written down simply and is completely specified by a handful of known quantities: the charge and mass of the electron, the charges and masses of the atomic nuclei, and Planck's constant. For experts we write

$$i\hbar \frac{\partial}{\partial t} |\Psi > \; = \mathcal{H} |\Psi > \qquad [1]$$

where

$$\mathcal{H} = - \sum_j^{N_e} \frac{\hbar^2}{2m} \nabla_j^2 - \sum_\alpha^{N_i} \frac{\hbar^2}{2M_\alpha} \nabla_\alpha^2 - \sum_j^{N_e} \sum_\alpha^{N_i} \frac{Z_\alpha e^2}{|\vec{r}_j - \vec{R}_\alpha|} + \sum_{j \ll k}^{N_e} \frac{e^2}{|\vec{r}_j - \vec{r}_k|} + \sum_{\alpha \ll \beta}^{N_j} \frac{Z_\alpha Z_\beta e^2}{|\vec{R}_\alpha - \vec{r}_\beta|}. \qquad [2]$$

we have learned why atoms have the size they do, why chemical bonds have the length and strength they do, why solid matter has the elastic properties it does, why some things are transparent while others reflect or absorb light (6). With a little more experimental input for guidance it is even possible to predict atomic conformations of small molecules, simple chemical reaction rates, structural phase transitions, ferromagnetism, and sometimes even superconducting transition temperatures (7). But the schemes for approximating are not first-principles deductions but are rather art keyed to experiment, and thus tend to be the least reliable precisely when reliability is most needed, i.e., when experimental information is scarce, the physical behavior has no precedent, and the key questions have not yet been identified. There are many notorious failures of alleged *ab initio* computation methods, including the phase diagram of liquid ^{3}He and the entire phenomenonology of high-temperature superconductors (8–10). Predicting protein functionality or the behavior of the human brain from these equations is patently absurd. So the triumph of the reductionism of the Greeks is a pyrrhic victory: We have succeeded in reducing all of ordinary physical behavior to a simple, correct Theory of Everything only to discover that it has revealed exactly nothing about many things of great importance.

In light of this fact it strikes a thinking person as odd that the parameters e, $\hbar$, and m appearing in these equations may be measured accurately in laboratory experiments involving large numbers of particles. The electron charge, for example, may be accurately measured by passing current through an electrochemical cell, plating out metal atoms, and measuring the mass deposited, the separation of the atoms in the crystal being known from x-ray diffraction (11). Simple electrical measurements performed on superconducting rings determine to high accuracy the quantity the quantum of magnetic flux $hc/2e$ (11). A version

Theory of Almost Everything

given Hamiltonian

$$H = -\frac{1}{2}\sum_{j=1}^{N_e}\nabla_j^2 + \sum_{j<k}^{N_e}\frac{1}{|r_j - r_k|} - \sum_{j=1}^{N_e}\sum_{\alpha=1}^{N_i}\frac{Z_\alpha}{|r_j - R_\alpha|} + \sum_{\alpha<\beta}^{N_i}\frac{Z_\alpha Z_\beta}{|R_\alpha - R_\beta|}$$

solve eigenvalue problem

$$H\Psi(x_1,\ldots,x_N) = E\,\Psi(x_1,\ldots,x_N)$$

3N-dimensional pde

electrons indistinguishable

how possible?

no observable $M(x_1,\ldots,x_N)$ can distinguish them
i.e. M symmetric under exchange of coordinates

eigenfunction needs to be antisymmetrized

still eigenfunction?

$$\mathcal{A}\,\Psi(x_1,\ldots,x_N) := \frac{1}{\sqrt{N!}}\sum_P (-1)^P\Psi\left(x_{p(1)},\ldots,x_{p(N)}\right)$$

N! terms

antisymmetrization

$$\mathcal{A}\,\Psi(x_1,\ldots,x_N) := \frac{1}{\sqrt{N!}}\sum_P (-1)^P \Psi\left(x_{p(1)},\ldots,x_{p(N)}\right)$$

N! terms — hard problem in general
easy $O(N^3)$ for product wavefunctions

$$\mathcal{A}\,\varphi_{\alpha_1}(x_1)\cdots\varphi_{\alpha_N}(x_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_{\alpha_1}(x_1) & \varphi_{\alpha_2}(x_1) & \cdots & \varphi_{\alpha_N}(x_1) \\ \varphi_{\alpha_1}(x_2) & \varphi_{\alpha_2}(x_2) & \cdots & \varphi_{\alpha_N}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_{\alpha_1}(x_N) & \varphi_{\alpha_2}(x_N) & \cdots & \varphi_{\alpha_N}(x_N) \end{vmatrix}$$

Slater determinants $\Phi_{\alpha_1,\ldots,\alpha_N}(x_1,\ldots,x_N)$

basis of Slater determinants

complete set of single-electron orbitals

$$\sum_n \overline{\varphi_n(x')}\,\varphi_n(x) = \delta(x'-x)$$

expand N-electron function in 1st variable

$$a(x_1,\ldots,x_N) = \sum_{n_1} \int dx_1'\, \underbrace{a(x_1',\ldots,x_N)\,\overline{\varphi_{n_1}(x_1')}}_{=:a_{n_1}(x_2,\ldots,x_N)}\,\varphi_{n_1}(x_1)$$

and repeat to obtain expansion in product states

antisymmetric: states with $n_i{=}n_j$ vanish, $n_i{\leftrightarrow}n_j$ only differ by sign

basis of Slater determinants

$$\left\{\Phi_{n_1,\ldots,n_N}(x_1,\ldots,x_N)\,\middle|\, n_1 < n_2 < \cdots < n_N\right\}$$

second quantization: motivation

get rid of coordinates and their permutations: Dirac states

Slater determinant $\Phi_{\alpha\beta}(x_1, x_2) = \frac{1}{\sqrt{2}} \left(\varphi_\alpha(x_1)\varphi_\beta(x_2) - \varphi_\beta(x_1)\varphi_\alpha(x_2) \right)$

corresponding Dirac state $|\alpha, \beta\rangle = \frac{1}{\sqrt{2}} \left(|\alpha\rangle|\beta\rangle - |\beta\rangle|\alpha\rangle \right)$

use operators $|\alpha, \beta\rangle = c^\dagger_\beta c^\dagger_\alpha |0\rangle$

position of operators encodes signs

$$c^\dagger_\beta c^\dagger_\alpha |0\rangle = |\alpha, \beta\rangle = -|\beta, \alpha\rangle = -c^\dagger_\alpha c^\dagger_\beta |0\rangle$$

product of operators changes sign under commutation: anti-commutation

anti-commutator $\{A, B\} := A\,B + B\,A$

second quantization: motivation

specify N-electron states using operators

N=0: $|0\rangle$ (vacuum state)

normalization: $\langle 0|0\rangle = 1$

N=1: $|\alpha\rangle = c_\alpha^\dagger|0\rangle$ (creation operator adds one electron)

normalization: $\langle\alpha|\alpha\rangle = \langle 0|c_\alpha c_\alpha^\dagger|0\rangle$

overlap: $\langle\alpha|\beta\rangle = \langle 0|c_\alpha c_\beta^\dagger|0\rangle$

adjoint of creation operator must remove one electron:
annihilation operator

$$c_\alpha|0\rangle = 0 \text{ and } c_\alpha c_\beta^\dagger = \pm c_\beta^\dagger c_\alpha + \langle\alpha|\beta\rangle$$

N=2: $|\alpha,\beta\rangle = c_\beta^\dagger c_\alpha^\dagger|0\rangle$

antisymmetry: $c_\alpha^\dagger c_\beta^\dagger = -c_\beta^\dagger c_\alpha^\dagger$

second quantization: formalism

vacuum state $|0\rangle$

and

set of operators c_α related to single-electron states $\varphi_\alpha(x)$

defined by:

$$c_\alpha|0\rangle = 0 \qquad \left\{c_\alpha, c_\beta\right\} = 0 = \left\{c_\alpha^\dagger, c_\beta^\dagger\right\}$$

$$\langle 0|0\rangle = 1 \qquad \left\{c_\alpha, c_\beta^\dagger\right\} = \langle \alpha|\beta\rangle$$

creators/annihilators operate in Fock space
transform like orbitals!

second quantization: field operators

how to express coordinates?
creation/annihilation operators in real-space basis

$\hat{\Psi}^\dagger(x)$ with $x = (r, \sigma)$ creates electron of spin σ at position r

then $c_\alpha^\dagger = \int dx\, \varphi_\alpha(x) \hat{\Psi}^\dagger(x)$

put electron at x with amplitude $\varphi_a(x)$

$\{\varphi_{\alpha_n}(x)\}$ complete set: $\hat{\Psi}^\dagger(x) = \sum_n \overline{\varphi_{\alpha_n}(x)}\, c_{\alpha_n}^\dagger$

they fulfill the standard anti-commutation relations

$$\left\{\hat{\Psi}(x), \hat{\Psi}(x')\right\} = 0 = \left\{\hat{\Psi}^\dagger(x), \hat{\Psi}^\dagger(x')\right\}$$
$$\left\{\hat{\Psi}(x), \hat{\Psi}^\dagger(x')\right\} = \delta(x - x')$$

second quantization: Slater determinants

$$\Phi_{\alpha_1\alpha_2\ldots\alpha_N}(x_1,x_2,\ldots,x_N) = \frac{1}{\sqrt{N!}}\left\langle 0\,\middle|\,\hat{\Psi}(x_1)\hat{\Psi}(x_2)\ldots\hat{\Psi}(x_N)\,c^\dagger_{\alpha_N}\ldots c^\dagger_{\alpha_2}c^\dagger_{\alpha_1}\,\middle|\,0\right\rangle$$

proof by induction

N=1: $\left\langle 0\,\middle|\,\hat{\Psi}(x_1)\,c^\dagger_{\alpha_1}\,\middle|\,0\right\rangle = \left\langle 0\,\middle|\,\varphi_{\alpha_1}(x_1) - c^\dagger_{\alpha_1}\hat{\Psi}(x_1)\,\middle|\,0\right\rangle = \varphi_{\alpha_1}(x_1)$

using $\quad \{\hat{\Psi}(x), c^\dagger_\alpha\} = \int dx'\,\varphi_\alpha(x')\,\left\{\hat{\Psi}(x),\hat{\Psi}^\dagger(x')\right\} = \varphi_\alpha(x)$

N=2: $\left\langle 0\,\middle|\,\hat{\Psi}(x_1)\hat{\Psi}(x_2)\,c^\dagger_{\alpha_2}c^\dagger_{\alpha_1}\,\middle|\,0\right\rangle$

$$= \left\langle 0\,\middle|\,\hat{\Psi}(x_1)\left(\varphi_{\alpha_2}(x_2) - c^\dagger_{\alpha_2}\hat{\Psi}(x_2)\right)c^\dagger_{\alpha_1}\,\middle|\,0\right\rangle$$

$$= \left\langle 0\,\middle|\,\hat{\Psi}(x_1)c^\dagger_{\alpha_1}\,\middle|\,0\right\rangle\varphi_{\alpha_2}(x_2) - \left\langle 0\,\middle|\,\hat{\Psi}(x_1)c^\dagger_{\alpha_2}\hat{\Psi}(x_2)c^\dagger_{\alpha_1}\,\middle|\,0\right\rangle$$

$$= \varphi_{\alpha_1}(x_1)\varphi_{\alpha_2}(x_2) - \varphi_{\alpha_2}(x_1)\varphi_{\alpha_1}(x_2)$$

second quantization: Slater determinants

general N: commute $\Psi(x_N)$ to the right

$$\left\langle 0 \left| \hat\Psi(x_1)\ldots\hat\Psi(x_{N-1})\hat\Psi(x_N)\, c^\dagger_{\alpha_N} c^\dagger_{\alpha_{N-1}} \ldots c^\dagger_{\alpha_1} \right| 0 \right\rangle =$$

$$\begin{aligned}
&+ \left\langle 0 \left| \hat\Psi(x_1)\ldots\hat\Psi(x_{N-1})\, c^\dagger_{\alpha_{N-1}} \ldots c^\dagger_{\alpha_1} \right| 0 \right\rangle \varphi_{\alpha_N}(x_N) \\
&- \left\langle 0 \left| \hat\Psi(x_1)\ldots\hat\Psi(x_{N-1}) \textstyle\prod_{n\neq N-1} c^\dagger_{\alpha_n} \right| 0 \right\rangle \varphi_{\alpha_{N-1}}(x_N) \\
&\vdots \\
&(-1)^{N-1} \left\langle 0 \left| \hat\Psi(x_1)\ldots\hat\Psi(x_{N-1})\, c^\dagger_{\alpha_N} \ldots c^\dagger_{\alpha_2} \right| 0 \right\rangle \varphi_{\alpha_1}(x_N)
\end{aligned}$$

Laplace expansion in terms of $N-1$ dim determinants wrt last line of

$$= \begin{vmatrix}
\varphi_{\alpha_1}(x_1) & \varphi_{\alpha_2}(x_1) & \cdots & \varphi_{\alpha_N}(x_1) \\
\varphi_{\alpha_1}(x_2) & \varphi_{\alpha_2}(x_2) & \cdots & \varphi_{\alpha_N}(x_2) \\
\vdots & \vdots & \ddots & \vdots \\
\varphi_{\alpha_1}(x_N) & \varphi_{\alpha_2}(x_N) & \cdots & \varphi_{\alpha_N}(x_N)
\end{vmatrix}$$

second quantization: Dirac notation

separate coordinates from orbitals

$$\Phi_{\alpha_1\alpha_2\ldots\alpha_N}(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \left\langle 0 \,\middle|\, \hat{\Psi}(x_1)\hat{\Psi}(x_2)\cdots\hat{\Psi}(x_N)\; c^\dagger_{\alpha_N}\cdots c^\dagger_{\alpha_2} c^\dagger_{\alpha_1} \,\middle|\, 0 \right\rangle$$

analogous to Dirac notation

$$\varphi_\alpha(x) = \langle x|\alpha\rangle$$

product states $\prod_{n=1}^{N} c^\dagger_{\alpha_n}|0\rangle$ are many-body generalization of Dirac states

evaluate matrix elements …

second quantization: expectation values

expectation value of N-body operator wrt N-electron Slater determinants

$$\int dx_1 \cdots dx_N \, \overline{\Phi_{\beta_1\cdots\beta_N}(x_1,\cdots,x_N)} \, M(x_1,\cdots,x_N) \, \Phi_{\alpha_1\cdots\alpha_N}(x_1,\cdots,x_N)$$

$$= \int d\boldsymbol{x} \, \frac{1}{\sqrt{N!}} \langle 0| \prod c_{\beta_i} \prod \hat{\Psi}^\dagger(x_n) |0\rangle \, M(\boldsymbol{x}) \, \frac{1}{\sqrt{N!}} \langle 0| \prod \hat{\Psi}(x_n) \prod c^\dagger_{\alpha_j} |0\rangle$$

$$= \langle 0| \prod c_{\beta_i} \underbrace{\frac{1}{N!} \int d\boldsymbol{x} \prod \hat{\Psi}^\dagger(x_n) \, M(\boldsymbol{x}) \, \prod \hat{\Psi}(x_n)}_{=:\hat{M}} \prod c^\dagger_{\alpha_j} |0\rangle$$

$|0\rangle\langle 0| = \mathbb{1}$ on 0-electron space

$$\hat{M} = \frac{1}{N!} \int dx_1 \cdots dx_N \, \hat{\Psi}^\dagger(x_N) \cdots \hat{\Psi}^\dagger(x_1) \, M(x_1,\cdots,x_N) \, \hat{\Psi}(x_1) \cdots \hat{\Psi}(x_N)$$

only valid for N-electron states!

second quantization: zero-body operator

zero-body operator $M_0(x_1,\ldots x_N) = 1$ independent of particle coordinates

second quantized form for operating on N-electron states:

$$\hat{M}_0 = \frac{1}{N!}\int dx_1\,dx_2\cdots x_N\,\hat{\Psi}^\dagger(x_N)\cdots\hat{\Psi}^\dagger(x_2)\hat{\Psi}^\dagger(x_1)\,\hat{\Psi}(x_1)\hat{\Psi}(x_2)\cdots\hat{\Psi}(x_N)$$

$$= \frac{1}{N!}\int dx_2\cdots x_N\,\hat{\Psi}^\dagger(x_N)\cdots\hat{\Psi}^\dagger(x_2)\quad \hat{N}\quad \hat{\Psi}(x_2)\cdots\hat{\Psi}(x_N)$$

$$= \frac{1}{N!}\int dx_2\cdots x_N\,\hat{\Psi}^\dagger(x_N)\cdots\hat{\Psi}^\dagger(x_2)\quad 1\quad \hat{\Psi}(x_2)\cdots\hat{\Psi}(x_N)$$

only(!) when operating on N-electron state

$$\vdots$$

$$= \frac{1}{N!}\,1\cdot 2\,\cdots\,N = 1$$

using $\hat{N} := \int dx\,\hat{\Psi}^\dagger(x)\hat{\Psi}(x)$ with $\left[\hat{N},\, c_n^\dagger\right] = c_n^\dagger$

result independent of N

overlap of Slater determinants

$$\int dx\,\overline{\Phi_{\alpha_n}(x)}\,\Phi_{\beta_m}(x) = \langle 0|c_{\alpha_1}\cdots c_{\alpha_N}\; c_{\beta_N}^\dagger\cdots c_{\beta_1}^\dagger|0\rangle$$

second quantization: one-body operators

one-body operator $M(x_1, \ldots, x_N) = \sum_j M_1(x_j)$

$$\hat{M}_1 = \frac{1}{N!} \int dx_1 \cdots dx_N \, \hat{\Psi}^\dagger(x_N) \cdots \hat{\Psi}^\dagger(x_1) \sum_j M_1(x_j) \, \hat{\Psi}(x_1) \cdots \hat{\Psi}(x_N)$$

$$= \frac{1}{N!} \sum_j \int dx_j \, \hat{\Psi}^\dagger(x_j) \, M_1(x_j) \, (N-1)! \, \hat{\Psi}(x_j)$$

$$= \frac{1}{N} \sum_j \int dx_j \, \hat{\Psi}^\dagger(x_j) \, M_1(x_j) \, \hat{\Psi}(x_j)$$

$$= \int dx \;\; \hat{\Psi}^\dagger(x) \;\; M_1(x) \;\; \hat{\Psi}(x)$$

result independent of N

expand in complete orthonormal set of orbitals

$$\hat{M}_1 = \sum_{n,m} \int dx \, \overline{\varphi_{\alpha_n}(x)} \, M(x) \, \varphi_{\alpha_m}(x) \;\; c^\dagger_{\alpha_n} c_{\alpha_m} = \sum_{n,m} \langle \alpha_n | M_1 | \alpha_m \rangle \;\; c^\dagger_{\alpha_n} c_{\alpha_m}$$

transforms as 1-body operator

second quantization: two-body operators

two-body operator $M(x_1,\ldots,x_N) = \sum_{i<j} M_2(x_i,x_j)$

$$\hat{M}_2 = \frac{1}{N!}\int dx_1\cdots dx_N\,\hat{\Psi}^\dagger(x_N)\cdots\hat{\Psi}^\dagger(x_1)\sum_{i<j} M_2(x_i,x_j)\,\hat{\Psi}(x_1)\cdots\hat{\Psi}(x_N)$$

$$= \frac{1}{N!}\sum_{i<j}\int dx_i dx_j\,\hat{\Psi}^\dagger(x_j)\hat{\Psi}^\dagger(x_i)\,M_2(x_i,x_j)\,(N-2)!\,\hat{\Psi}(x_i)\hat{\Psi}(x_j)$$

$$= \frac{1}{N(N-1)}\sum_{i<j}\int dx_i dx_j\,\hat{\Psi}^\dagger(x_j)\hat{\Psi}^\dagger(x_i)\,M_2(x_i,x_j)\,\hat{\Psi}(x_i)\hat{\Psi}(x_j)$$

$$= \frac{1}{2}\int dx\,dx'\,\hat{\Psi}^\dagger(x')\,\hat{\Psi}^\dagger(x)\;M_2(x,x')\;\hat{\Psi}(x)\,\hat{\Psi}(x')$$

result independent of N

expand in complete orthonormal set of orbitals

$$\hat{M}_2 = \frac{1}{2}\sum_{n,n',m,m'}\int dx dx'\,\overline{\varphi_{\alpha_{n'}}(x')\varphi_{\alpha_n}(x)}\,M_2(x,x')\,\varphi_{\alpha_m}(x)\varphi_{\alpha_{m'}}(x')\;c^\dagger_{\alpha_{n'}}c^\dagger_{\alpha_n}c_{\alpha_m}c_{\alpha_{m'}}$$

$$= \frac{1}{2}\sum_{n,n',m,m'}\langle\alpha_n\alpha_{n'}|M_2|\alpha_m\alpha_{m'}\rangle\;c^\dagger_{\alpha_{n'}}c^\dagger_{\alpha_n}c_{\alpha_m}c_{\alpha_{m'}}$$

2-body matrix

$$\hat{M}_2 = \frac{1}{2} \sum_{n,n',m,m'} \underbrace{\langle \alpha_n \alpha_{n'} | M_2 | \alpha_m \alpha_{m'} \rangle}_{=: M_{nn',mm'}} c^\dagger_{\alpha_{n'}} c^\dagger_{\alpha_n} c_{\alpha_m} c_{\alpha_{m'}}$$

4-index tensor

no contribution for
n=*n'* or *m*=*m'*
sign-change for
n↔*n'* or *m*↔*m'*

collect terms with same operator content

$$\hat{M}_2 = \sum_{n<n',m<m'} \underbrace{\left(M_{nn',mm'} - M_{nn',m'm} \right)}_{=: \breve{M}_{nn',mm'}} c^\dagger_{\alpha_{n'}} c^\dagger_{\alpha_n} c_{\alpha_m} c_{\alpha_{m'}}$$

two-body matrix
of dim $N_{orb}(N_{orb}-1)/2$

together with N_{orb}^2 hopping terms
completely specifies Hamiltonian

Exact Diagonalization

variational principle and Schrödinger equation

energy expectation value $E[\psi] = \dfrac{\langle\psi|H|\psi\rangle}{\langle\Psi|\Psi\rangle}$

variation

$$E[\Psi+\delta\Psi] = E[\Psi] + \frac{\langle\delta\Psi|H|\Psi\rangle + \langle\Psi|H|\delta\Psi\rangle}{\langle\Psi|\Psi\rangle} - \langle\Psi|H|\Psi\rangle\,\frac{\langle\delta\Psi|\Psi\rangle + \langle\Psi|\delta\Psi\rangle}{\langle\Psi|\Psi\rangle^2} + \mathcal{O}^2$$

variational equation: $0 = \dfrac{\delta E[\Psi]}{\delta\Psi} = \dfrac{H|\Psi\rangle - \overbrace{\langle\Psi|H|\Psi\rangle}^{=E[\Psi]}\,|\Psi\rangle}{\langle\Psi|\Psi\rangle} + \text{H.c.}$

equivalent to time-independent Schrödinger equation

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

variational principle

expand $|\Psi\rangle \neq 0$ in eigenfunctions

$$E[\Psi] = \frac{\sum\langle\Psi|\Psi_m\rangle\langle\Psi_m|H|\Psi_n\rangle\langle\Psi_n|\Psi\rangle}{\sum\langle\Psi|\Psi_m\rangle\langle\Psi_m|\Psi_n\rangle\langle\Psi_n|\Psi\rangle} = \frac{\sum E_n\left|\langle\Psi_n|\Psi\rangle\right|^2}{\sum\left|\langle\Psi_n|\Psi\rangle\right|^2} \geq \frac{\sum E_0\left|\langle\Psi_n|\Psi\rangle\right|^2}{\sum\left|\langle\Psi_n|\Psi\rangle\right|^2} = E_0$$

assume eigenvalues sorted $E_0 \leq E_1 \leq \ldots$

$$E[\Psi_{\perp_n}] \geq E_n \quad \text{if } \langle\Psi_i|\Psi_{\perp_n}\rangle = 0 \text{ for } i = 0, \ldots, n-1.$$

variational principle for excited states

in practice only useful when orthogonality to (unknown) states ensured, e.g., by symmetry

expand in Slater basis

rewrite $H|\Psi_n\rangle = E_n|\Psi_n\rangle$

choose (orthonormal) orbital basis $\{\, \varphi_k \mid k \,\}$ and corresponding

basis of Slater determinants $\{\, \phi_{k1,\ldots,kN} \mid k_1 < \ldots < k_N \,\}$

$$|\Psi\rangle = \sum_{k_1<\cdots<k_N} a_{k_1,\ldots,k_N} \, |\Phi_{k_1,\ldots,k_N}\rangle = \sum_i a_i \, |\Phi_i\rangle = |\boldsymbol{\Phi}\rangle \, \boldsymbol{a}$$

expand Schrödinger equation in Slater basis

$$E \, \langle\Phi_i|\Psi\rangle = \langle\Phi_i|H|\Psi\rangle = \sum_j \langle\Phi_i|H|\Phi_j\rangle\langle\Phi_j|\Psi\rangle$$

matrix eigenvalue problem

$$\boldsymbol{H}\boldsymbol{a} = \langle\boldsymbol{\Phi}|\hat{H}|\boldsymbol{\Phi}\rangle\boldsymbol{a} = \begin{pmatrix} \langle\Phi_1|\hat{H}|\Phi_1\rangle & \langle\Phi_1|\hat{H}|\Phi_2\rangle & \cdots \\ \langle\Phi_2|\hat{H}|\Phi_1\rangle & \langle\Phi_2|\hat{H}|\Phi_2\rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = E \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = \; E\boldsymbol{a}$$

variational principle

restrict to finite Slater basis $|\tilde{\mathbf{\Phi}}\rangle := \big(|\Phi_1\rangle, \ldots, |\Phi_{\tilde{L}}\rangle\big)$

$$\langle\tilde{\mathbf{\Phi}}|\hat{H}|\tilde{\mathbf{\Phi}}\rangle\tilde{\boldsymbol{a}}_n = \tilde{\boldsymbol{H}}\tilde{\boldsymbol{a}}_n = \tilde{E}_n\tilde{\boldsymbol{a}}_n \quad \rightsquigarrow \quad |\tilde{\Psi}_n\rangle := |\tilde{\mathbf{\Phi}}\rangle\,\tilde{\boldsymbol{a}}_n$$

solve with LAPACK

variational principle: $E_n \leq \tilde{E}_n$ for $n \in \{0, \ldots, \tilde{L}-1\}$

construct $|\tilde{\Psi}\rangle = \sum_{i=0}^{n} c_i\,|\tilde{\Psi}_i\rangle \neq 0$ with $\langle\Psi_i|\tilde{\Psi}\rangle = 0$ for $i = 1, \ldots, n-1$

$$\rightsquigarrow \tilde{E}_n \;\geq\; E[\tilde{\Psi}] \;\geq\; E_n$$

art: systematically increase basis to achieve convergence

nesting of eigenvalues

consider problem with basis size L as exact problem

variational principle for $-H$: $-E_{L-i} \leq -\tilde{E}_{\tilde{L}-i}$ for $i \in \{1, \ldots, \tilde{L}\}$

$$E_n \leq \tilde{E}_n \leq E_{n+(L-\tilde{L})} \quad \text{for } n \in \{0, \ldots, \tilde{L}-1\}$$

representation of basis

$$|n_{K-1},\dots,n_0\rangle := \prod_{k=0}^{K-1} \left(c_k^\dagger\right)^{n_k} |0\rangle$$

occupation number representation

i	(n_3, n_2, n_1, n_0)	state	I
0	0000		
1	0001		
2	0010		
3	0011	$c_1^\dagger c_0^\dagger \vert 0\rangle = \vert\Phi_1\rangle$	1
4	0100		
5	0101	$c_2^\dagger c_0^\dagger \vert 0\rangle = \vert\Phi_2\rangle$	2
6	0110	$c_2^\dagger c_1^\dagger \vert 0\rangle = \vert\Phi_3\rangle$	3
7	0111		
8	1000		
9	1001	$c_3^\dagger c_0^\dagger \vert 0\rangle = \vert\Phi_4\rangle$	4
10	1010	$c_3^\dagger c_1^\dagger \vert 0\rangle = \vert\Phi_5\rangle$	5
11	1011		
12	1100	$c_3^\dagger c_2^\dagger \vert 0\rangle = \vert\Phi_6\rangle$	6
13	1101		
14	1110		
15	1111		

bit-representation of basis states

```
>>> for i in range(2**4):
...   if bin(i).count('1')==2:
...     print(format(i, "04b"))
...
0011
0101
0110
1001
1010
1100
```

matrix elements: Fermi signs

$$\langle \Phi_I | \hat{H} | \Phi_{I'} \rangle = \sum_{n,m} T_{nm} \langle 0 | c_{I_1} \cdots c_{I_N} \; c_n^\dagger c_m \; c_{I'_N}^\dagger \cdots c_{I'_1}^\dagger | 0 \rangle$$
$$+ \sum_{\substack{n'>n \\ m'>m}} \breve{U}_{nn',mm'} \langle 0 | c_{I_1} \cdots c_{I_N} \; c_{n'}^\dagger c_n^\dagger c_m c_{m'} \; c_{I'_N}^\dagger \cdots c_{I'_1}^\dagger | 0 \rangle$$

normal-order and evaluate overlap (determinant)

orthonormal basis:

$$c_6^\dagger c_2 | \Phi_{I(181)} \rangle = c_6^\dagger c_2 \; c_7^\dagger c_5^\dagger c_4^\dagger c_2^\dagger c_0^\dagger | 0 \rangle$$
$$= (-1)^3 c_6^\dagger c_7^\dagger c_5^\dagger c_4^\dagger c_2 c_2^\dagger c_0^\dagger | 0 \rangle$$
$$= (-1)^3 c_6^\dagger c_7^\dagger c_5^\dagger c_4^\dagger \left(1 - c_2^\dagger c_2\right) c_0^\dagger | 0 \rangle$$
$$= (-1)^3 c_6^\dagger c_7^\dagger c_5^\dagger c_4^\dagger \cdot c_0^\dagger | 0 \rangle$$
$$= +| \Phi_{I(241)} \rangle = (-1)^2 c_7^\dagger c_6^\dagger c_5^\dagger c_4^\dagger \cdot c_0^\dagger | 0 \rangle$$

count set bits: `popcnt`

$$1\,0\,1\,1\,0\,1\,0\,1 \quad = \quad (-1)^c \; 1\,1\,1\,1\,0\,0\,0\,1$$

many-body problem

dimension of Hilbert space

ways of putting N electrons in K orbitals: $K\,(K-1)\,(K-2)\cdots(K-(N-1)) = K!/(K-N)!$

order in which electrons are put does not matter: $N!$

$$\dim \mathcal{H}_K^{(N)} = \frac{K!}{N!(K-N)!} = \binom{K}{N}$$

use symmetry to reduce dimension

e.g., spin conserved

$$\dim \mathcal{H}_{2K}^{(N_\uparrow,N_\downarrow)} = \binom{K}{N_\uparrow} \times \binom{K}{N_\downarrow}$$

```
>>> def binom(K,N):
...   if N==0:
...     return 1
...   else:
...     return (K-N+1)*binom(K,N-1)/N
...
>>> binom(24,12)**2
7312459672336
>>> binom(24,12)**2*8/2**30
54482
```

M	$N_\uparrow$	$N_\downarrow$	dimension of Hilbert space
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
14	7	7	11 778 624
16	8	8	165 636 900
18	9	9	2 363 904 400
20	10	10	34 134 779 536
22	11	11	497 634 306 624
24	12	12	7 312 459 672 336

sparseness

$$\langle \Phi_I | \hat{H} | \Phi_{I'} \rangle = \sum_{n,m} T_{nm} \langle 0 | c_{I_1} \cdots c_{I_N} \; c_n^\dagger c_m \; c_{I'_N}^\dagger \cdots c_{I'_1}^\dagger | 0 \rangle$$
$$+ \sum_{\substack{n'>n \\ m'>m}} \breve{U}_{nn',mm'} \langle 0 | c_{I_1} \cdots c_{I_N} \; c_{n'}^\dagger c_n^\dagger c_m c_{m'} \; c_{I'_N}^\dagger \cdots c_{I'_1}^\dagger | 0 \rangle$$

almost all matrix elements are zero, except

diagonal elements	1011001010	
single hop	1011100010	$N \times (K-N)$
pair-hop	1001100011	$N(N-1)/2 \times (K-N)(K-N-1)/2$

even more sparse for TB (short-range hopping)
and local Coulomb (Hubbard) interaction

matrix-vector products are *very* fast

Lanczos method

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

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

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

steepest descent minimization in high-dimensional space
local minima?

minimal eigenvalue: steepest descent

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

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

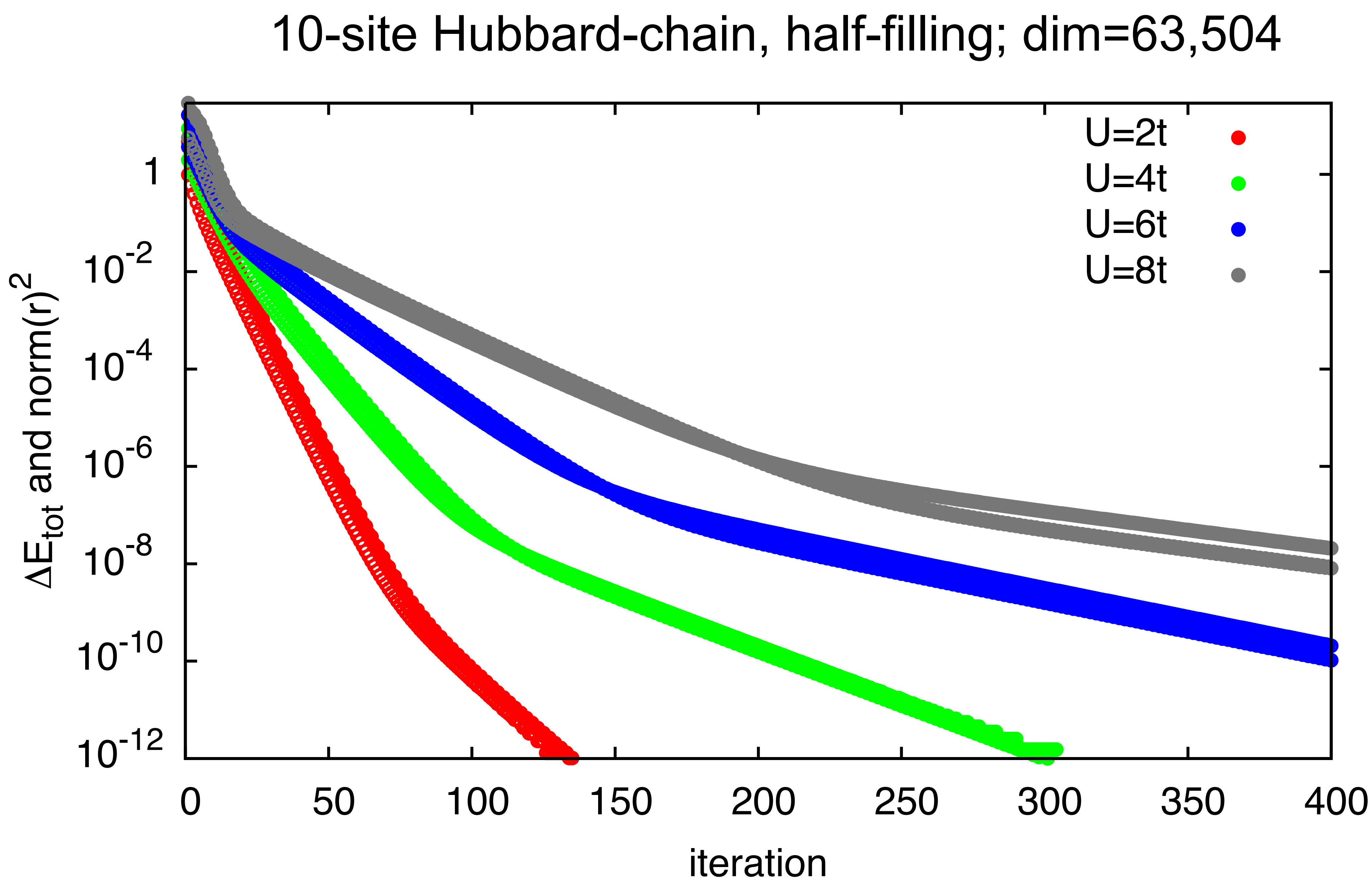
$$H|v_0\rangle = b_1\,|v_1\rangle + a_0\,|v_0\rangle$$

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

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 $(|\Psi_1\rangle, H|\Psi_1\rangle) \in \text{span}\left(|\Psi_0\rangle, H|\Psi_0\rangle, H^2|\Psi_0\rangle\right)$

minimize on span $(|\Psi_2\rangle, H|\Psi_2\rangle) \in \text{span}\left(|\Psi_0\rangle, H|\Psi_0\rangle, H^2|\Psi_0, H^3|\Psi_0\rangle\right)$

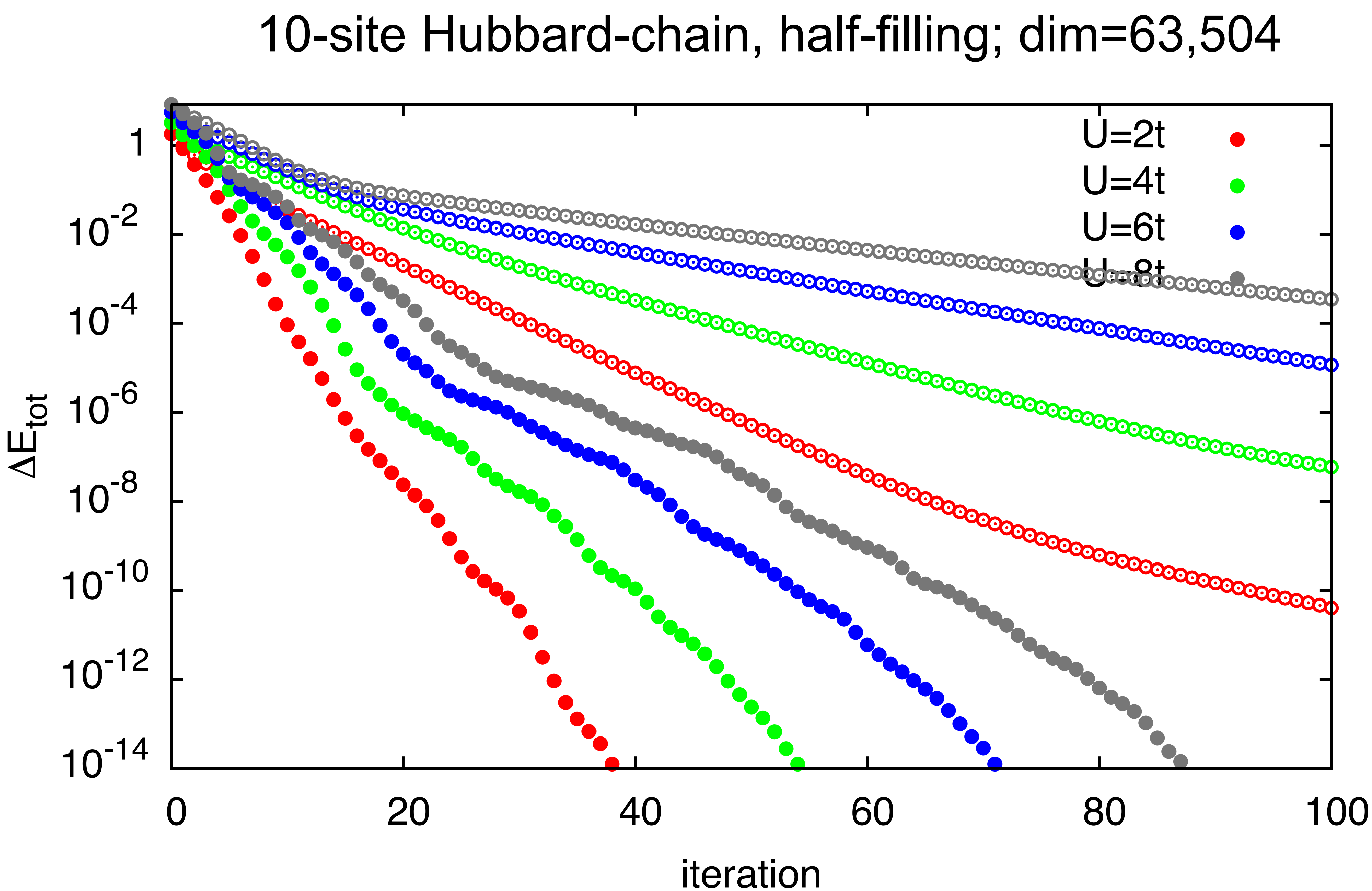
etc.

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 ⇒ 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

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

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

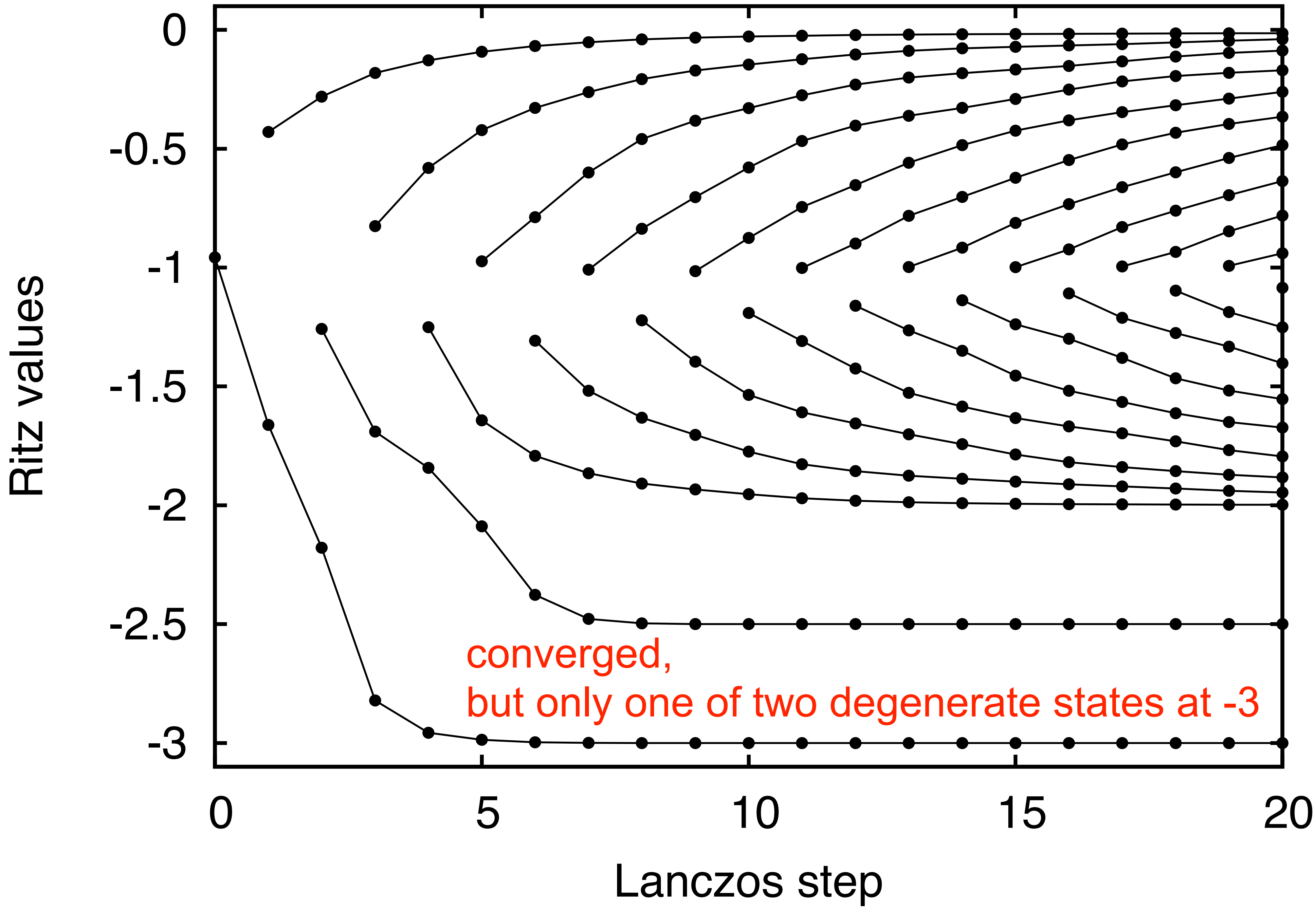
$$
H_{\mathcal{K}^L(|v_0\rangle)} = \begin{pmatrix}
a_0 & b_1 & 0 & 0 & & 0 & 0 \\
b_1 & a_1 & b_2 & 0 & \cdots & 0 & 0 \\
0 & b_2 & a_2 & b_3 & & 0 & 0 \\
0 & 0 & b_3 & a_3 & & 0 & 0 \\
 & \vdots & & & \ddots & \vdots & \\
0 & 0 & 0 & 0 & & a_{L-1} & b_L \\
0 & 0 & 0 & 0 & \cdots & b_L & a_L
\end{pmatrix}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

Lanczos algorithm

`v=init`	
`b0=norm2(v)`	not part of tridiagonal matrix
`scal(1/b0,v)`	`v`= $\lvert v_0\rangle$
`w=0`	
`w=w+H*v`	`w`= $H\lvert v_0\rangle$
`a[0]=dot(v,w)`	
`axpy(-a[0],v,w)`	`w`= $\lvert \tilde{v}_1\rangle = H\lvert v_0\rangle - a_0\lvert v_0\rangle$
`b[1]=norm2(w)`	
`for n=1,2,...`	
`  if abs(b[n])<eps then exit`	invariant subspace
`  scal(1/b[n],w)`	`w`= $\lvert v_n\rangle$
`  scal( -b[n],v)`	`v`= $-b_n\lvert v_{n-1}\rangle$
`  swap(v,w)`	
`  w=w+H*v`	`w`= $H\lvert v_n\rangle - b_n\lvert v_{n-1}\rangle$
`  a[n]=dot(v,w)`	`a[n]`= $\langle v_n\lvert H\rvert v_n\rangle - b_n\langle v_n\vert v_{n-1}\rangle$
`  axpy(-a[n],v,w)`	`w`= $\lvert \tilde{v}_{n+1}\rangle$
`  b[n+1]=norm2(w)`	
`  diag(a[0]..a[n], b[1]..b[n])`	getting a_{n+1} needs another $H\lvert v\rangle$
`  if converged then exit`	
`end`	

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

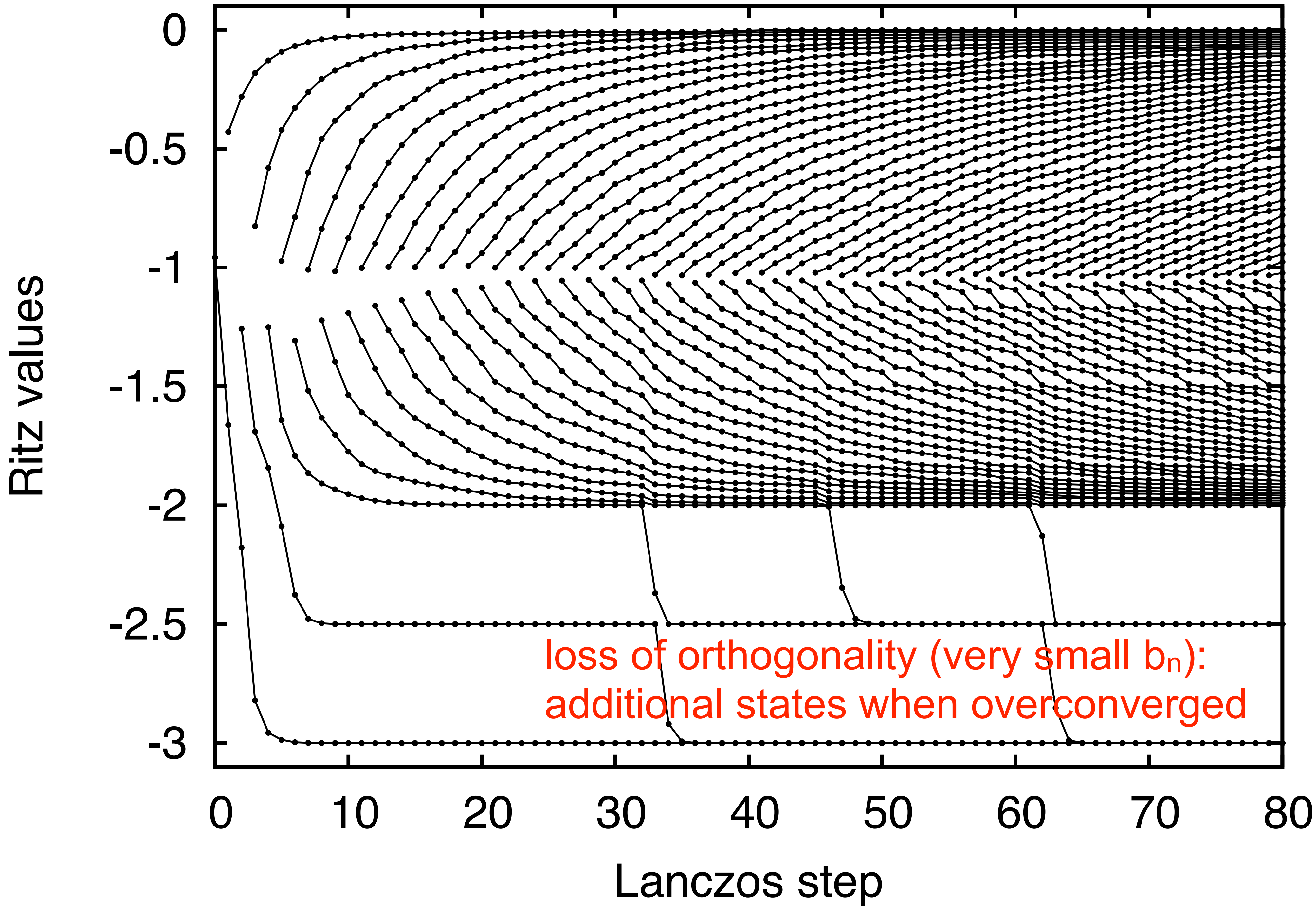
assume $|\varphi_1\rangle$ and $|\varphi_2\rangle$ are degenerate eigenstates with eigenvalue ε, then their expansion in the orthonormal basis of the Krylov space is

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

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

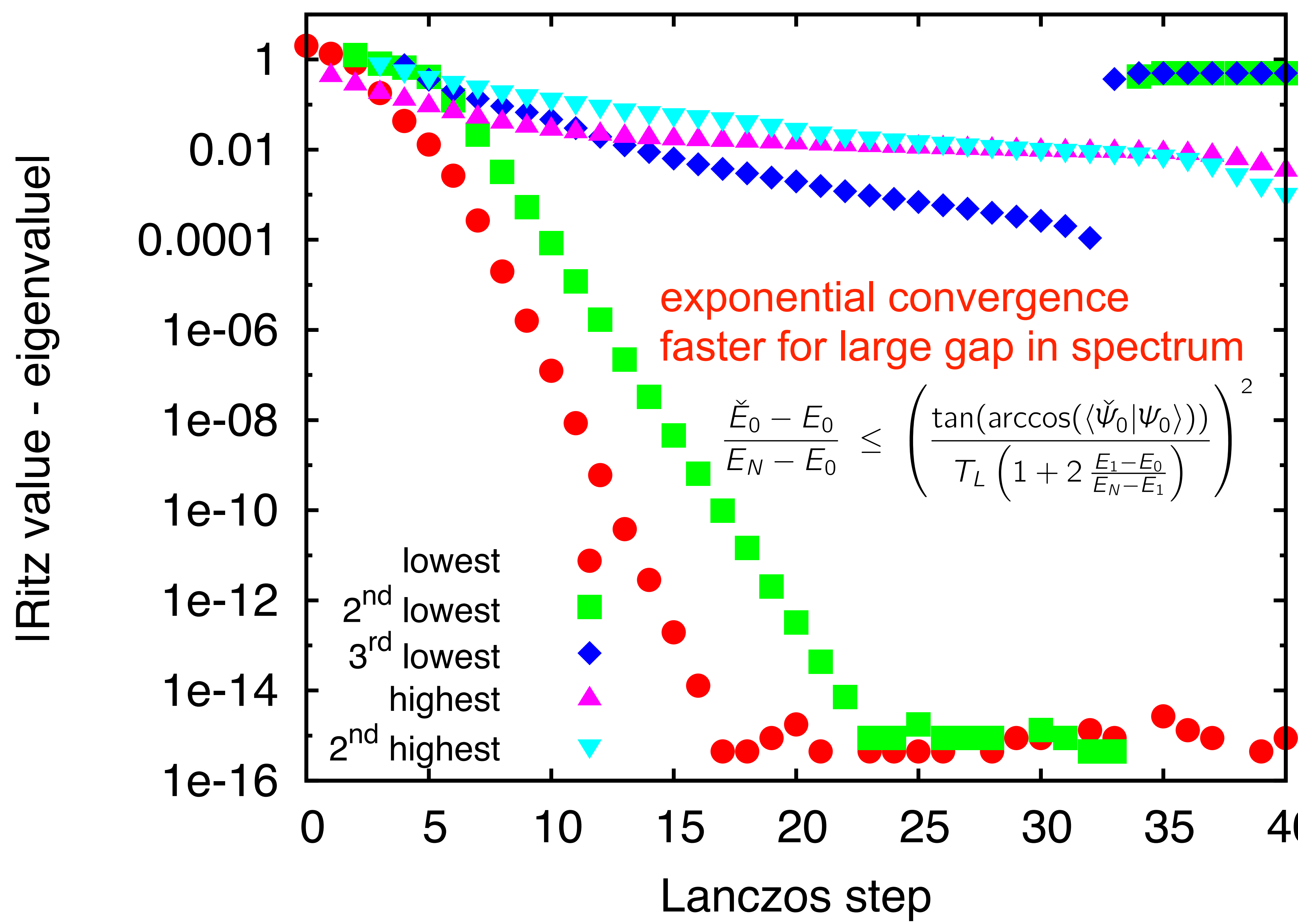
loss of orthogonality

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

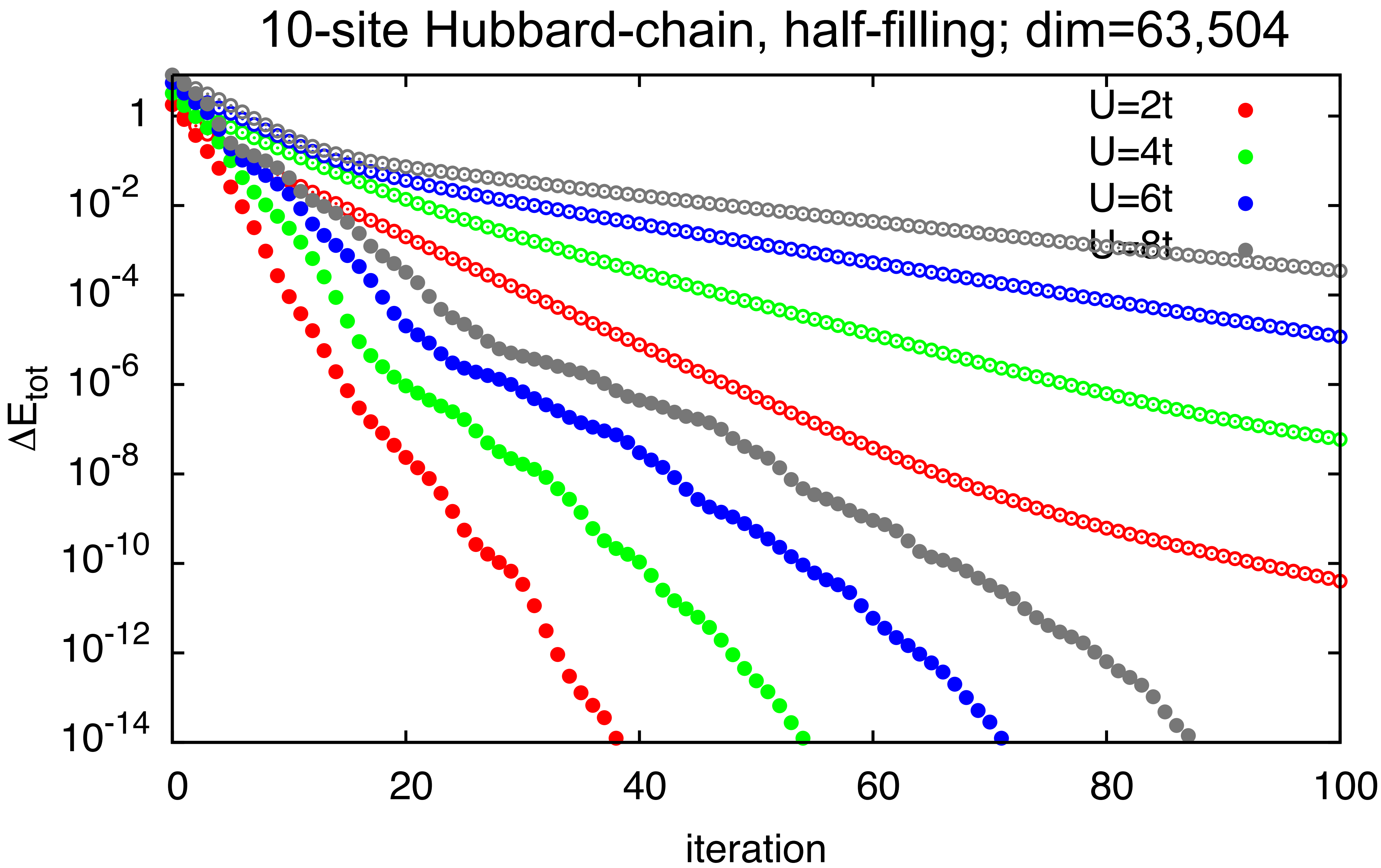


convergence to extremal eigenvalues

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 ⇒ would require very large memory

instead: re-run Lanczos iteration from same $|v_0\rangle$
and accumulate eigenvector on the fly

Green function

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

need entire spectrum !?

Green function

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

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

run Lanczos starting from $|\Psi_c\rangle$ (normalized!)

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

Green function is 0,0 element of inverse matrix

Green 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

invert block-2×2 matrix

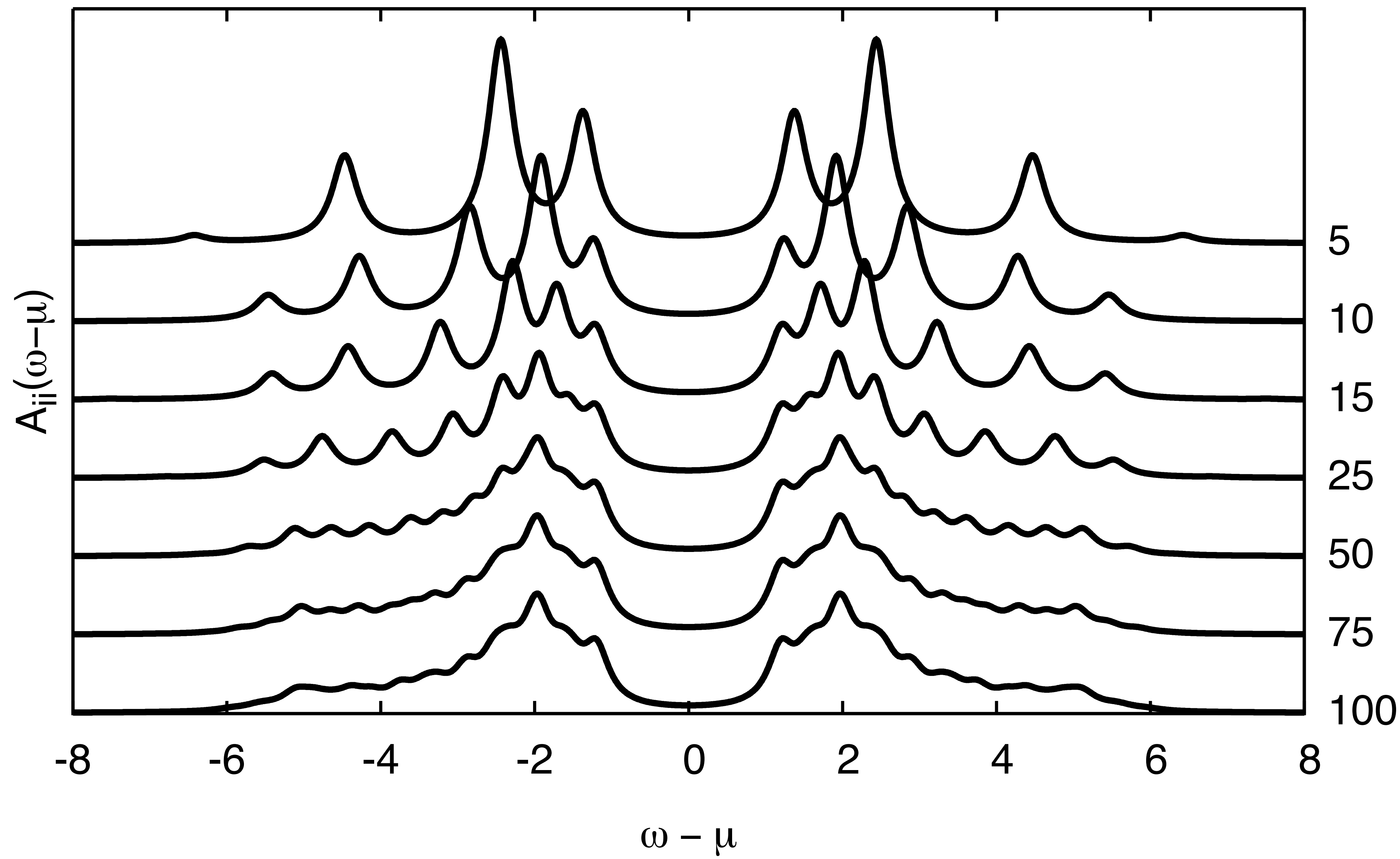
$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \begin{aligned} &A\tilde{A} + B\tilde{C} = 1 && = (A - BD^{-1}C)\tilde{A} \\ &C\tilde{A} + D\tilde{C} = 0 \rightsquigarrow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

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

recursively

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

convergence by moments



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

summary

indistinguishable electrons

$$\begin{vmatrix} \varphi_{\alpha_1}(x_1) & \varphi_{\alpha_2}(x_1) & \cdots & \varphi_{\alpha_N}(x_1) \\ \varphi_{\alpha_1}(x_2) & \varphi_{\alpha_2}(x_2) & \cdots & \varphi_{\alpha_N}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_{\alpha_1}(x_N) & \varphi_{\alpha_2}(x_N) & \cdots & \varphi_{\alpha_N}(x_N) \end{vmatrix}$$

(anti)symmetrization is hard
Slater determinants to the rescue

second quantization

$$= \langle 0 | \hat{\Psi}(x_1) \cdots \hat{\Psi}(x_N)\; c^\dagger_{\alpha_N} \cdots c^\dagger_{\alpha_1} | 0 \rangle$$

$$c_\alpha|0\rangle = 0 \qquad \{c_\alpha, c_\beta\} = 0 = \{c^\dagger_\alpha, c^\dagger_\beta\}$$

$$\langle 0|0\rangle = 1 \qquad \{c_\alpha, c^\dagger_\beta\} = \langle \alpha|\beta\rangle$$

occupation number representation

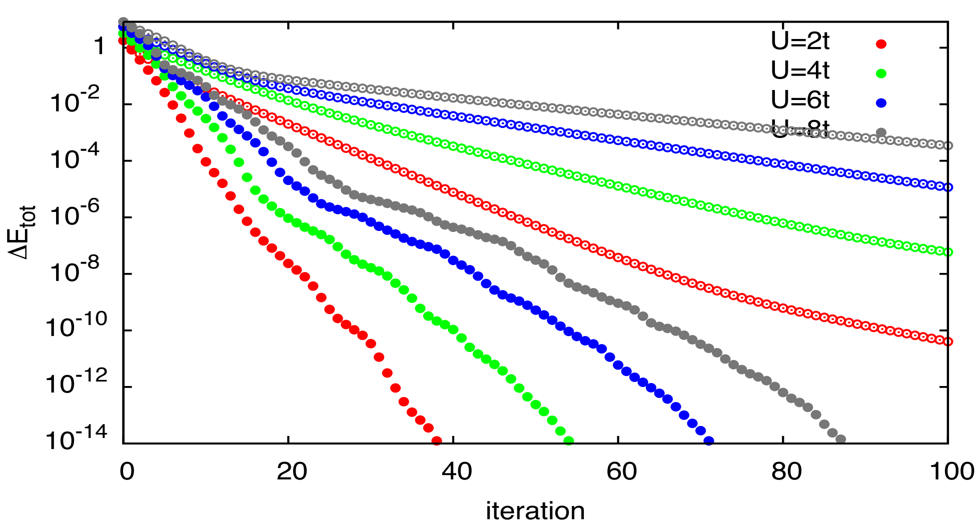
$$|n_{K-1}, \ldots, n_0\rangle := \prod \left(c^\dagger_k\right)^{n_k} |0\rangle$$

bit counting

$$1\,0\,1\,1\,0\,1\,0\,1 \;=\; (-1)^c\; 1\,1\,1\,1\,0\,0\,0\,1$$

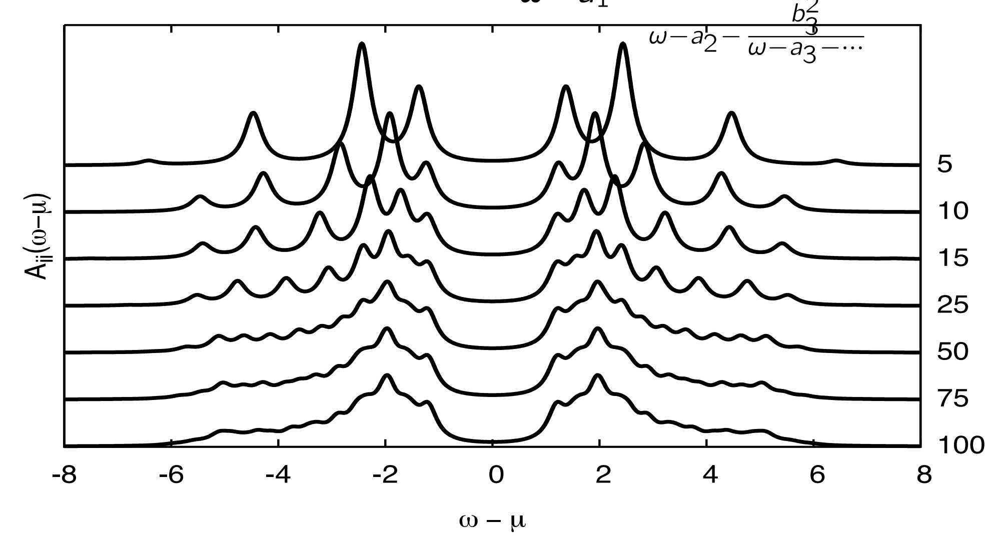
steepest descent ⇒ Krylov space

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



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 matrix-vector product: OpenMP

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

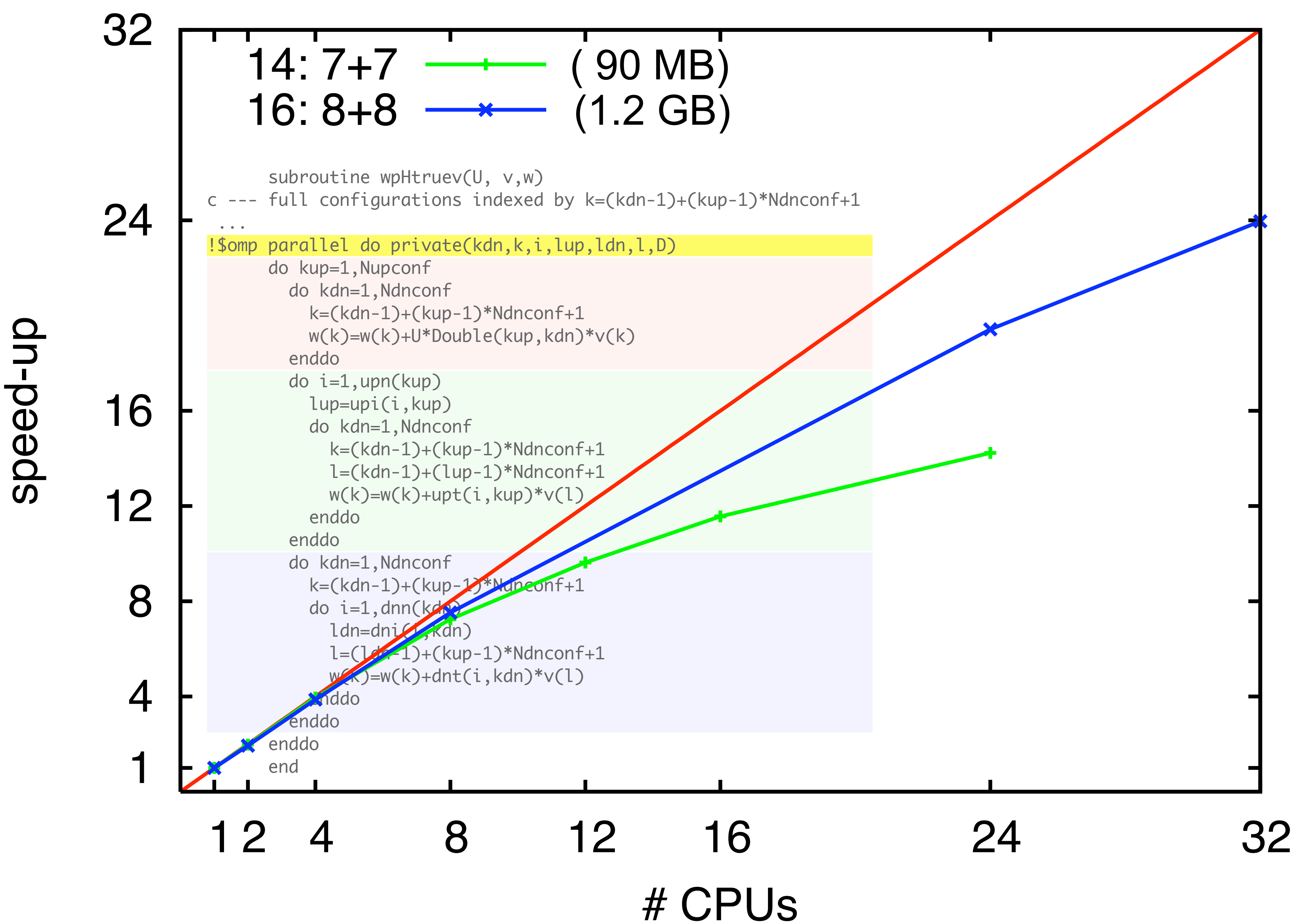
```
      subroutine wpHtruev(U, v,w)
c --- full configurations indexed by k=(kdn-1)+(kup-1)*Ndnconf+1
 ...
!$omp parallel do private(kdn,k,i,lup,ldn,l,D)
      do kup=1,Nupconf
        do kdn=1,Ndnconf
          k=(kdn-1)+(kup-1)*Ndnconf+1
          w(k)=w(k)+U*Double(kup,kdn)*v(k)
        enddo
  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

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

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

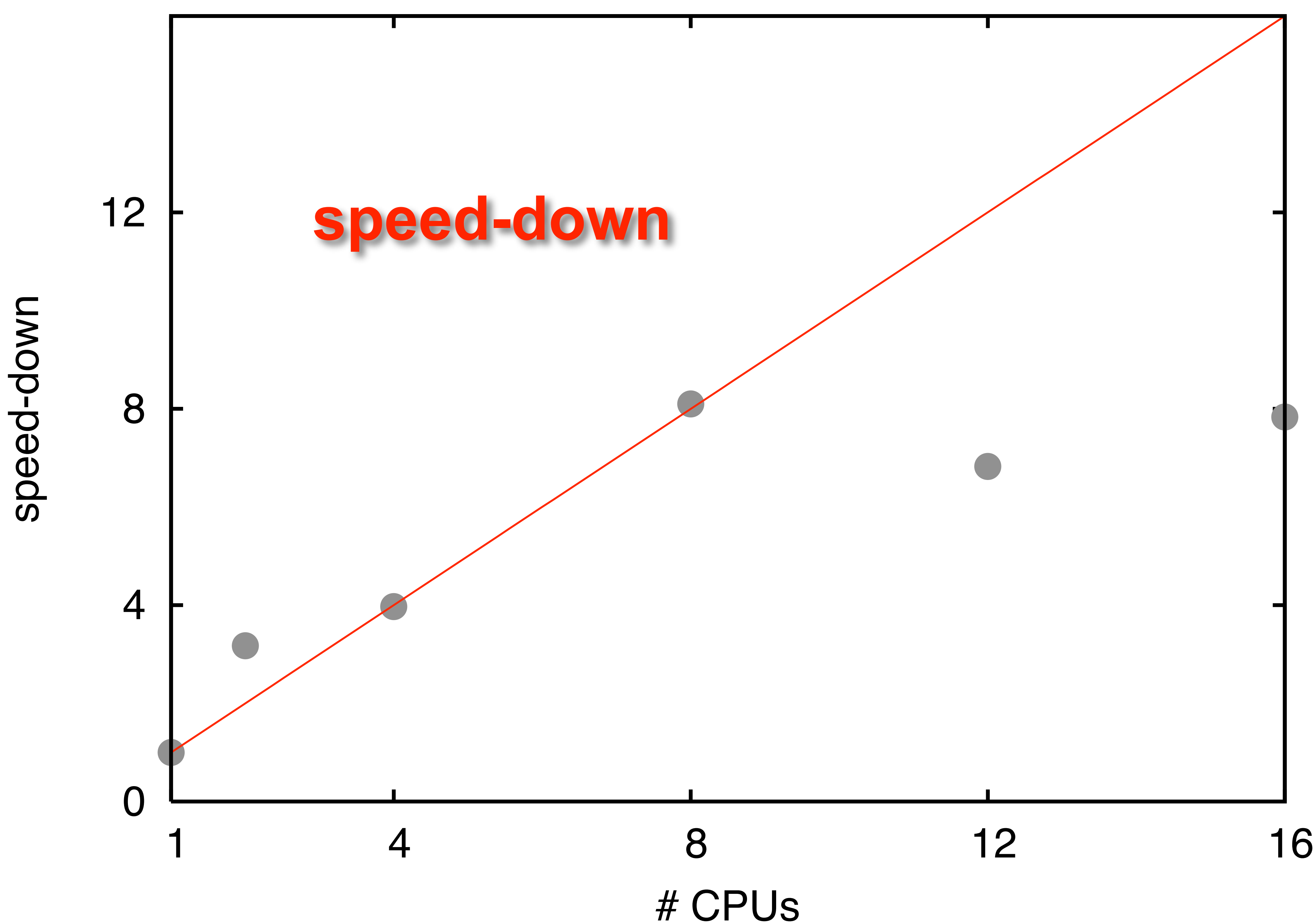
$$\sum_{\langle ij\rangle,\sigma=\downarrow} t_{i,j}\, c^\dagger_{j,\sigma} c_{i,\sigma}$$

OpenMP on Jump



distributed memory

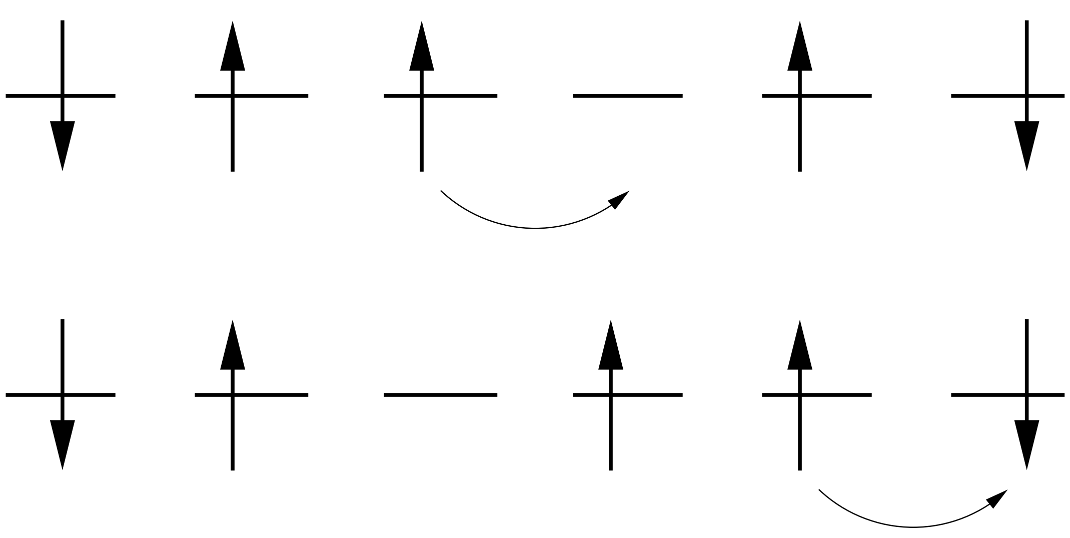
MPI-2: one-sided communication



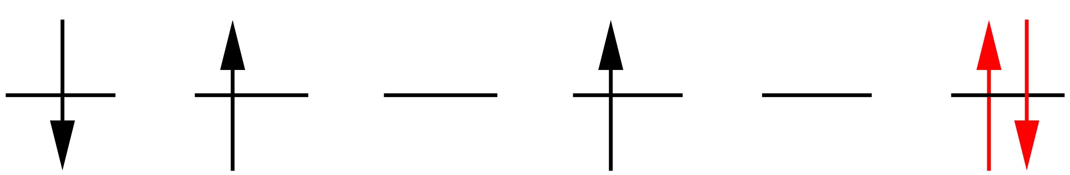
Hubbard model

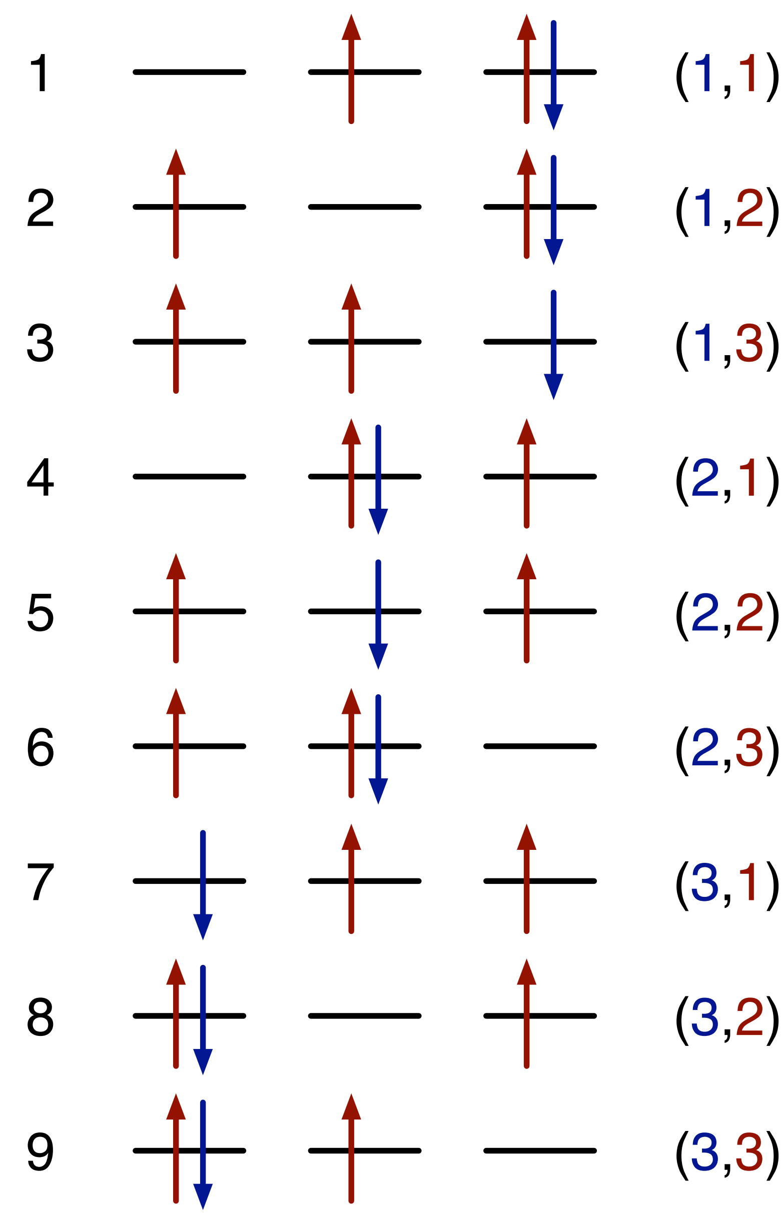
$$H = \sum_{\langle ij \rangle,\sigma} t_{i,j}\, c^{\dagger}_{j,\sigma} c_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

hopping: spin unchanged

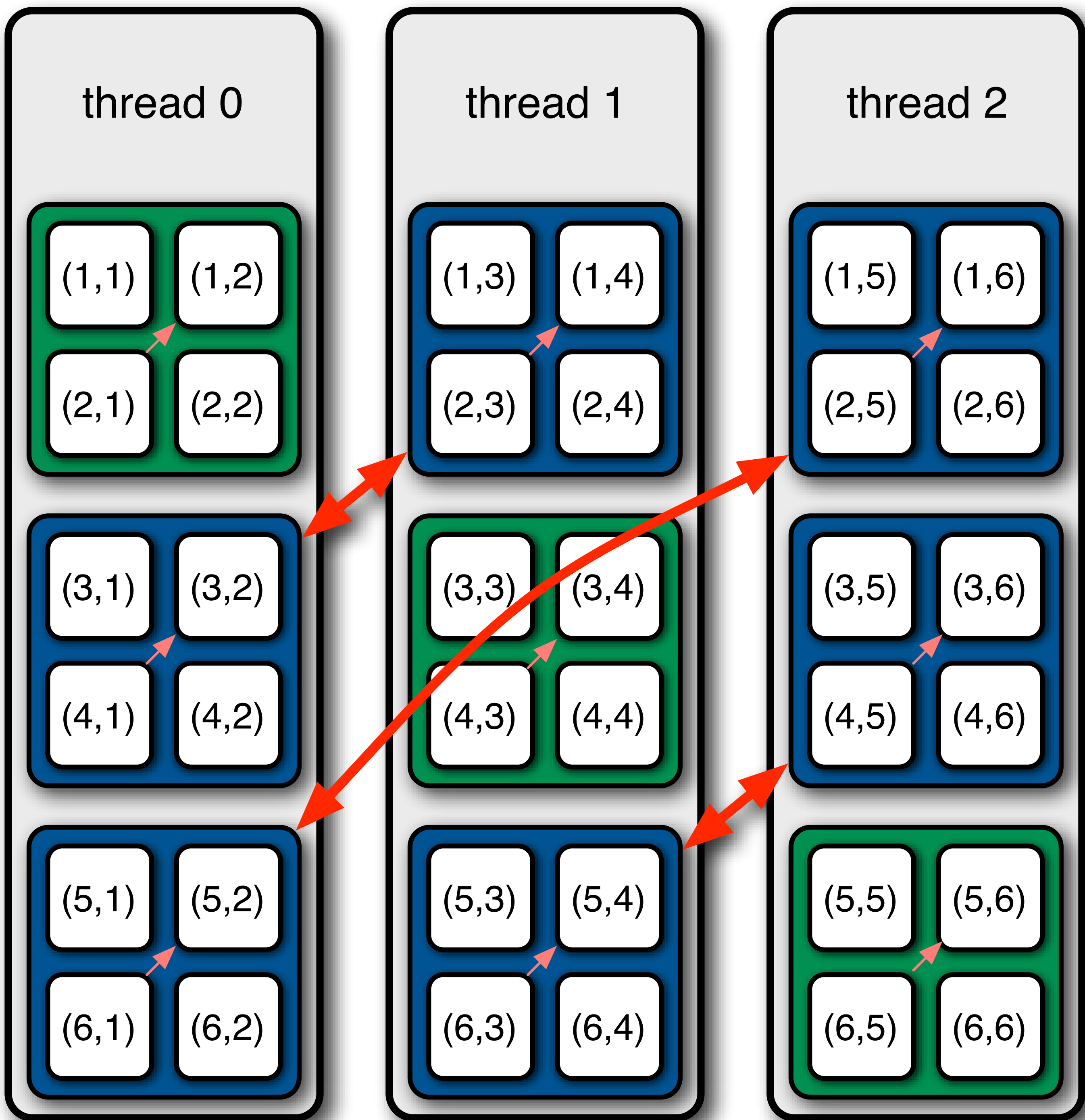


interaction diagonal





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



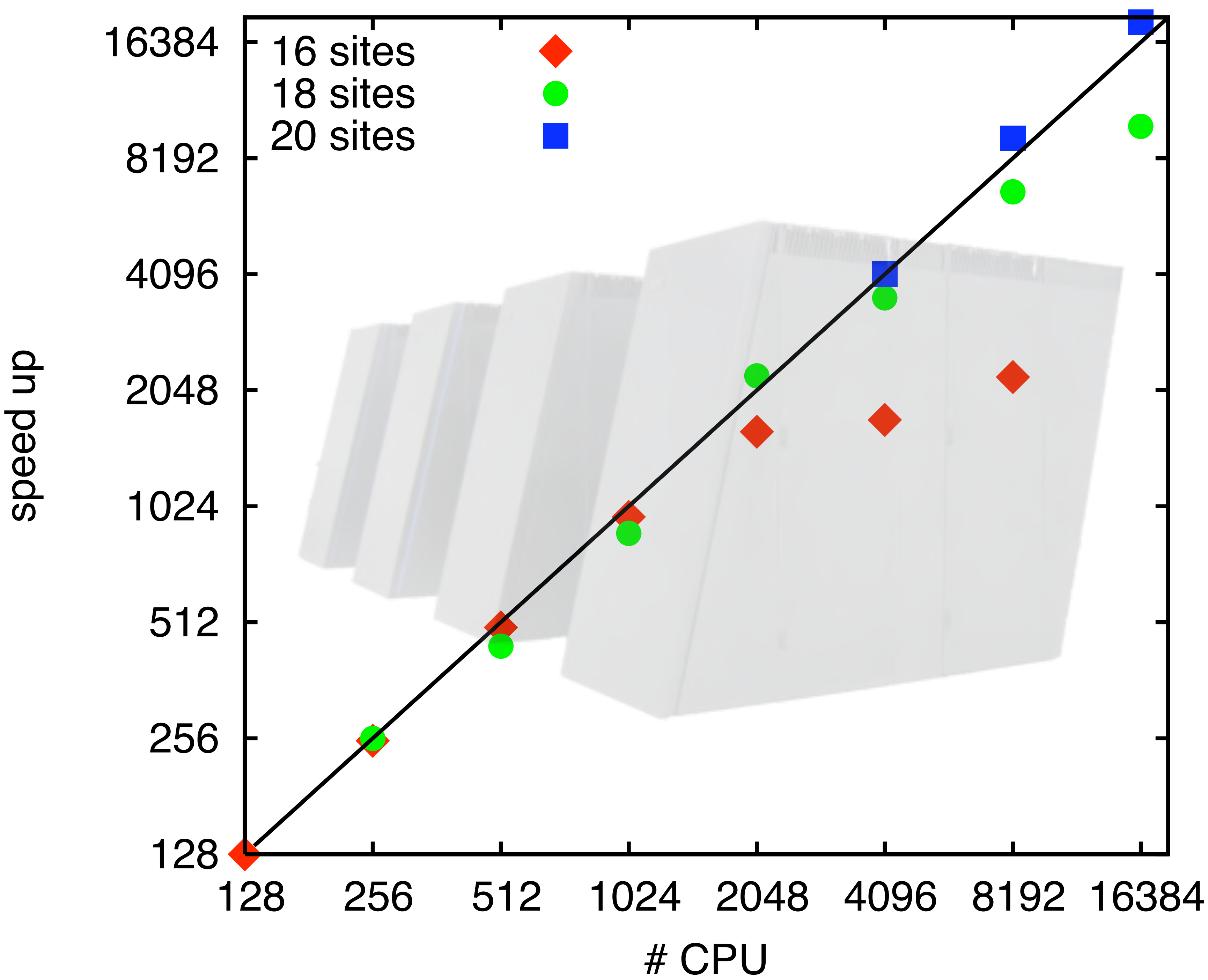
Lanczos-vector as matrix:
$v(i_\downarrow,i_\uparrow)$

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

implementation:

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

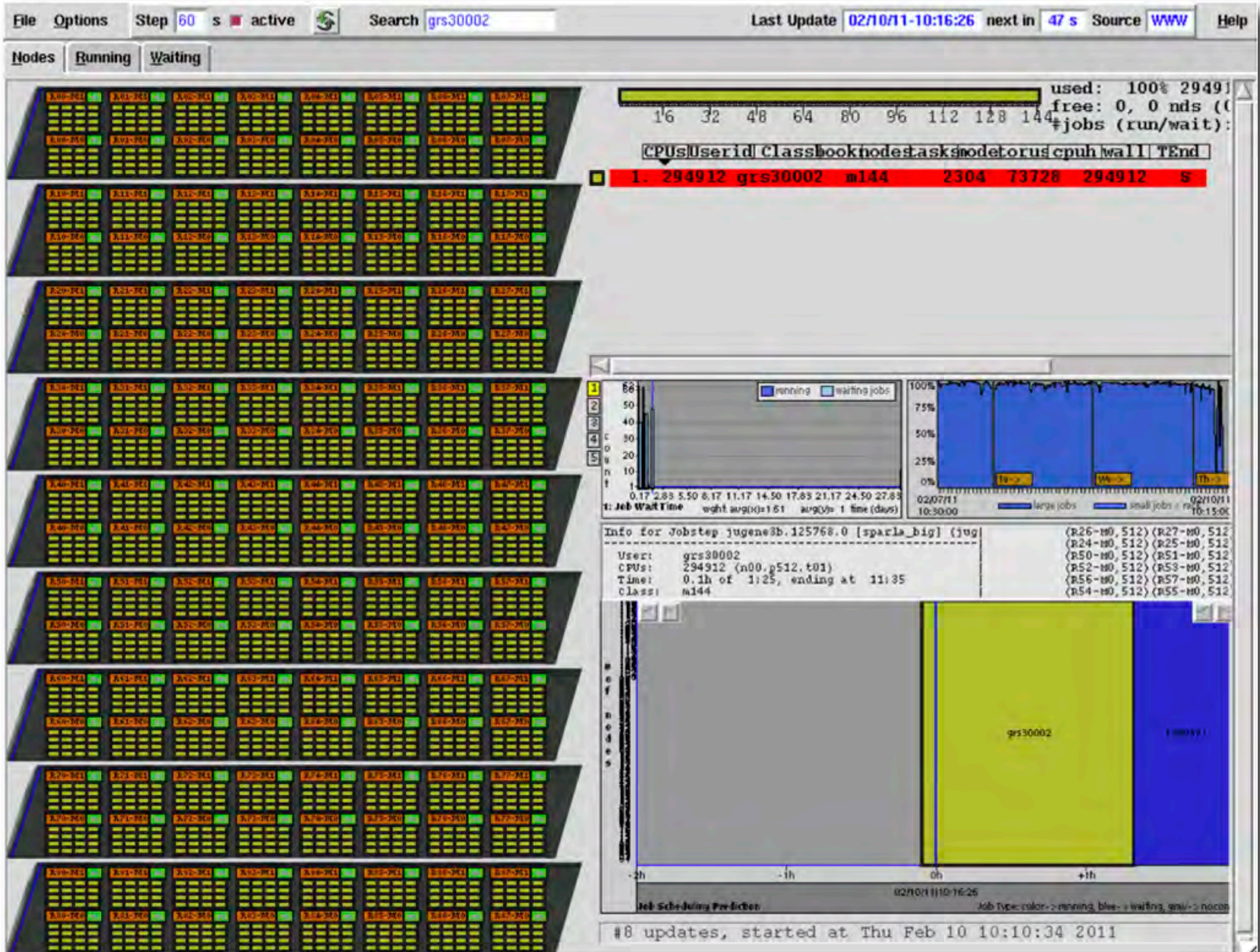
Implementation on IBM BlueGene/P



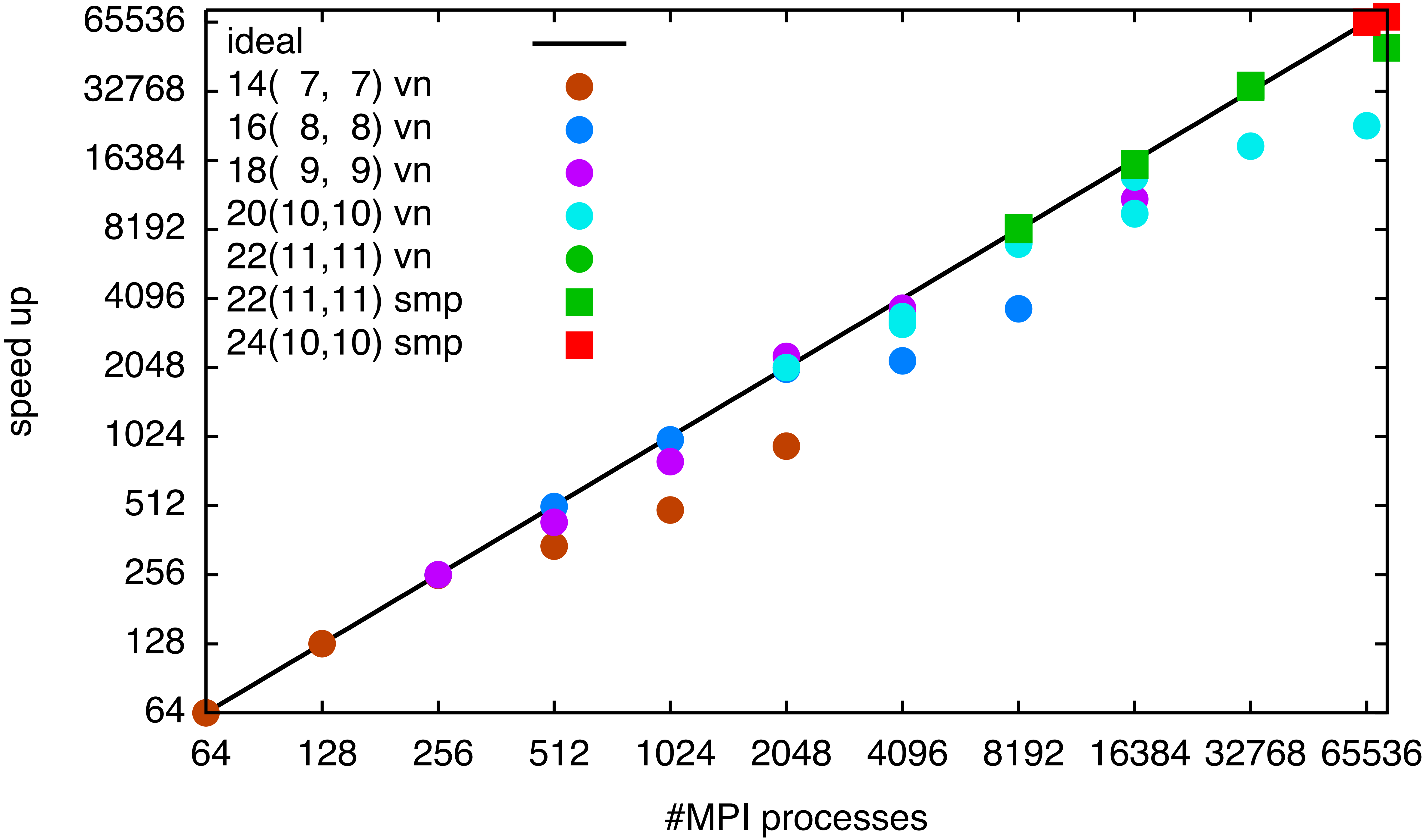
sites	memory
16	1 GB
18	18 GB
20	254 GB

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

performance on full Jugene?



performance on full Jugene!



performance on full Jugene!