Exact Diagonalization and Lanczos Method

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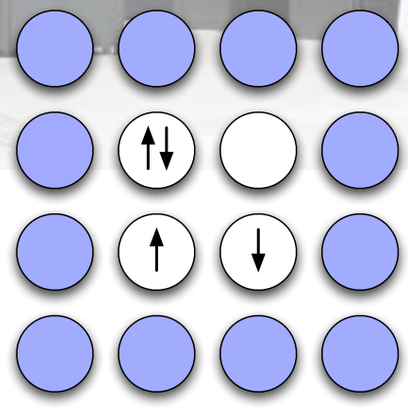
$$c_\alpha|0\rangle = 0 \qquad \left\{c_\alpha, c_\beta\right\} = 0 = \left\{c_\alpha^\dagger, c_\beta^\dagger\right\}$$

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

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

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

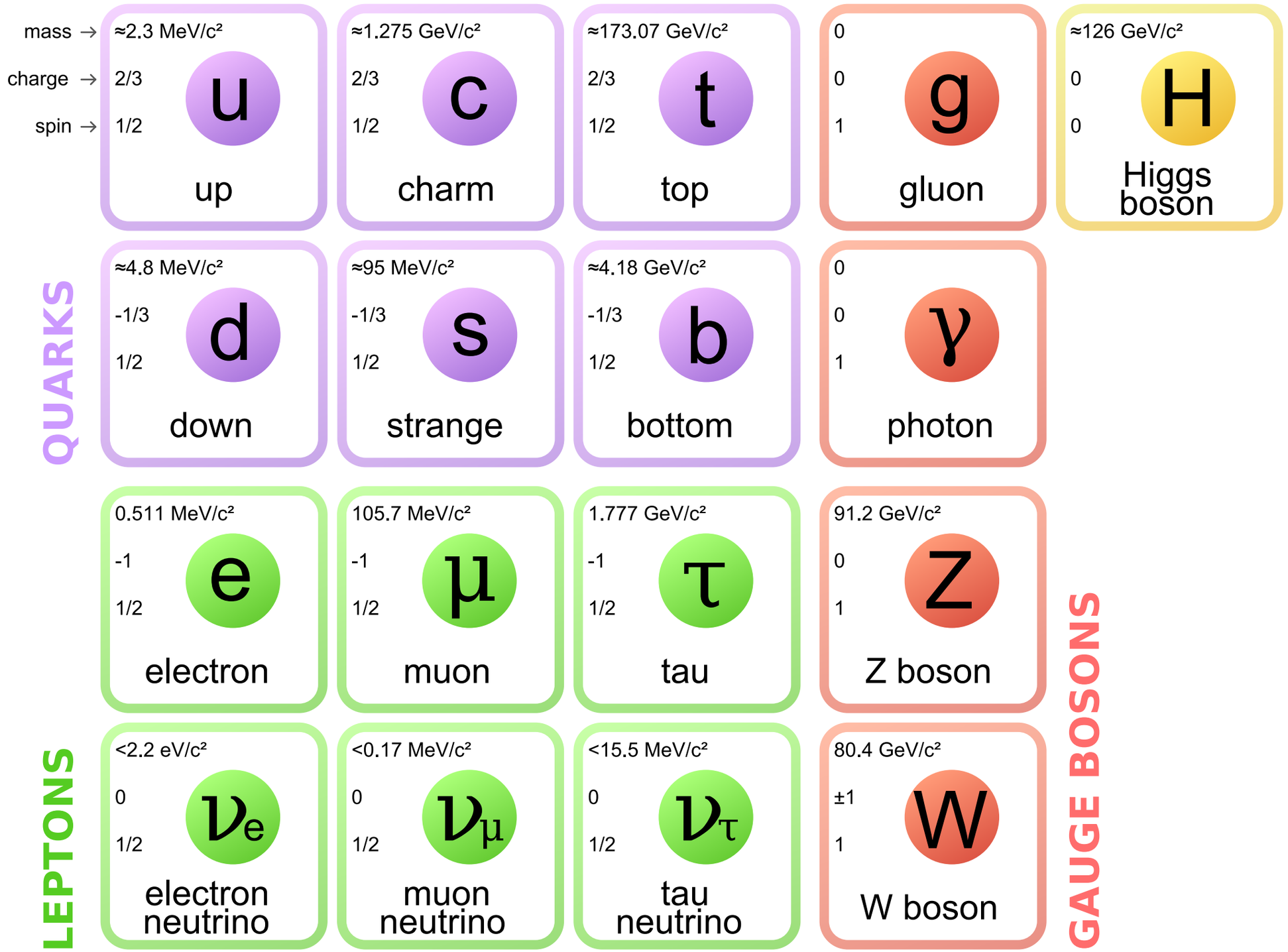
$$G_k(\omega) = \cfrac{b_0^2}{\omega - a_0 - \cfrac{b_1^2}{\omega - a_1 - \cfrac{b_2^2}{\omega - a_2 - \cfrac{b_3^2}{\omega - a_3 - \cdots}}}}$$



Identical Twins

Diane Arbus:
Identical Twins,
Roselle, NJ, 1967

Standard Model: Elementary Particles



en.wikipedia.org/wiki/Standard_Model

indistinguishability and statistics

N-particle systems described by wave-function with
N particle degrees of freedom (tensor space):

$\Psi(x_1, ..., x_N)$

introduces **labeling** of particles

indistinguishable particles: no observable exists to distinguish them
in particular no observable can depend on labeling of particles

probability density is an observable

consider permutations *P* of particle labels

$$P\psi(x_1, x_2) = \psi(x_2, x_1) \text{ with } |\psi(x_1, x_2)|^2 = |\psi(x_2, x_1)|^2$$

$$\rightsquigarrow \; P\psi(x_1, x_2) = e^{i\phi}\psi(x_1, x_2)$$

when $P^2 = \mathrm{Id} \Rightarrow e^{i\phi} = \pm 1$ (Ψ (anti)symmetric under permutation)

antisymmetric: $\Psi(x_1, x_2 \to x_1) = 0$ (Pauli principle)

antisymmetrization

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

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

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

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

second quantization: motivation

labeling of coordinates of identical particles is artificial
get rid of coordinates?

Dirac formalism
separate coordinates from states

$$\varphi(x) = \langle x|\varphi\rangle$$

absorb coordinates in operators

$$\int dx\, \overline{\varphi_n(x)} M(x) \varphi_m(x) = \int dx\, \langle \varphi_n|x\rangle M(x) \langle x|\varphi_m\rangle =: \langle \varphi_n|\hat{M}|\varphi_m\rangle$$

coordinate-free formalism

second quantization: coordinates

vacuum state $|0\rangle$

and

set of operators operators $\hat{\Psi}(x)$

defined by:

$$\hat{\psi}(x)|0\rangle = 0 \qquad \{\hat{\psi}(x), \hat{\psi}(x')\} = 0 = \{\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x')\}$$

$$\langle 0|0\rangle = 1 \qquad \{\hat{\psi}(x), \hat{\psi}^\dagger(x')\} = \delta(x-x')$$

anticommutator: $\{A, B\} := AB + BA$

density operator: $\hat{N} := \int dx'\, \hat{\Psi}^\dagger(x')\hat{\Psi}(x')$

$$\hat{N}\,\hat{\Psi}(x) = -\int dx'\, \hat{\Psi}^\dagger(x')\hat{\Psi}(x)\hat{\Psi}(x') = \int dx' \Big(\hat{\Psi}(x)\hat{\Psi}^\dagger(x') - \delta(x-x')\Big)\hat{\Psi}(x') = \hat{\Psi}(x)\big(\hat{N}-1\big)$$

second quantization: states

creation operator $\quad c_\alpha^\dagger := \int dx\, \varphi_\alpha(x)\, \hat{\psi}^\dagger(x)$

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

$$\{c_\alpha,\ c_\beta^\dagger\} = \int dx'\, \overline{\varphi_\alpha(x')}\, \{\hat{\psi}(x'),\ c_\beta^\dagger\} = \int dx'\, \overline{\varphi_\alpha(x')}\varphi_\beta(x') = \langle\alpha|\beta\rangle$$

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

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

second quantization: Slater determinants

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

proof by induction

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

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

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

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

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

second quantization: Slater determinants

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

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

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

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

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

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 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 $M(x_1,\ldots x_N) = 1$ independent of particle coordinates

second quantized form for operating on N-electron states:

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

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

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

only(!) when operating on N-electron state

$$\vdots$$

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

result independent of N

second quantization: one-body operators

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

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

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

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

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

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 $\quad M(x_1,\ldots,x_N)=\sum_{i<j} M_2(x_i,x_j)$

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

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

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

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

result independent of N

expand in complete orthonormal set of orbitals

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

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

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
$n \leftrightarrow n'$ or $m \leftrightarrow m'$

no self-interaction

exchange terms

collect terms with same operator content

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

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 $|\tilde{\mathbf{\Phi}}\rangle := \left(|\Phi_1\rangle, \ldots, |\Phi_{\tilde{L}}\rangle\right)$

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

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 $i = 0, \ldots, n-1$

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

art: systematically increase basis to achieve convergence

representation of basis

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

occupation number representation

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

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

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

steepest descent minimization in high-dimensional space
local minima?

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

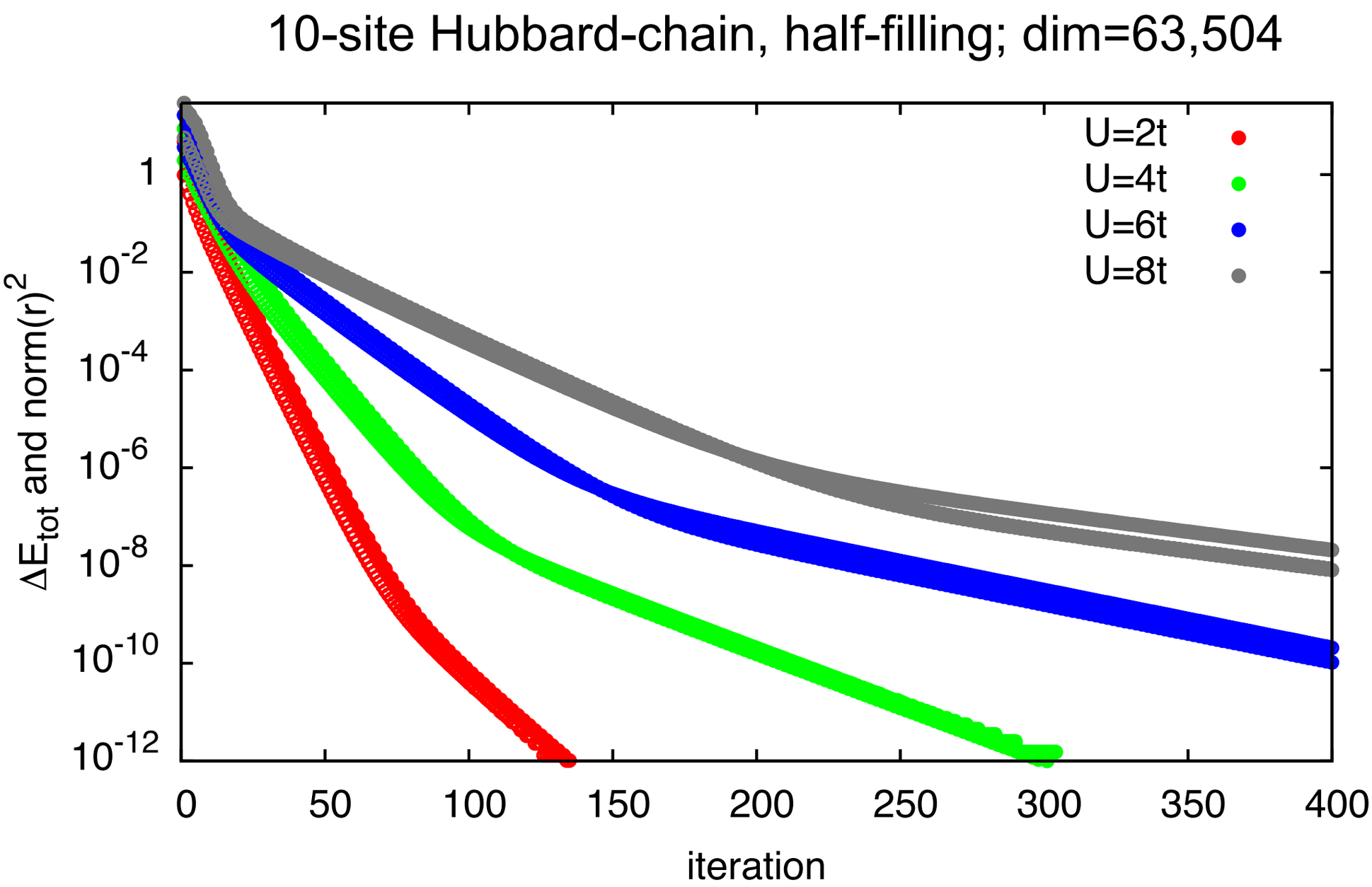
$$H|v_0\rangle = b_1\,|v_1\rangle + a_0\,|v_0\rangle$$

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

diagonalize to find lowest eigenvector

iterate!

convergence



Lanczos idea

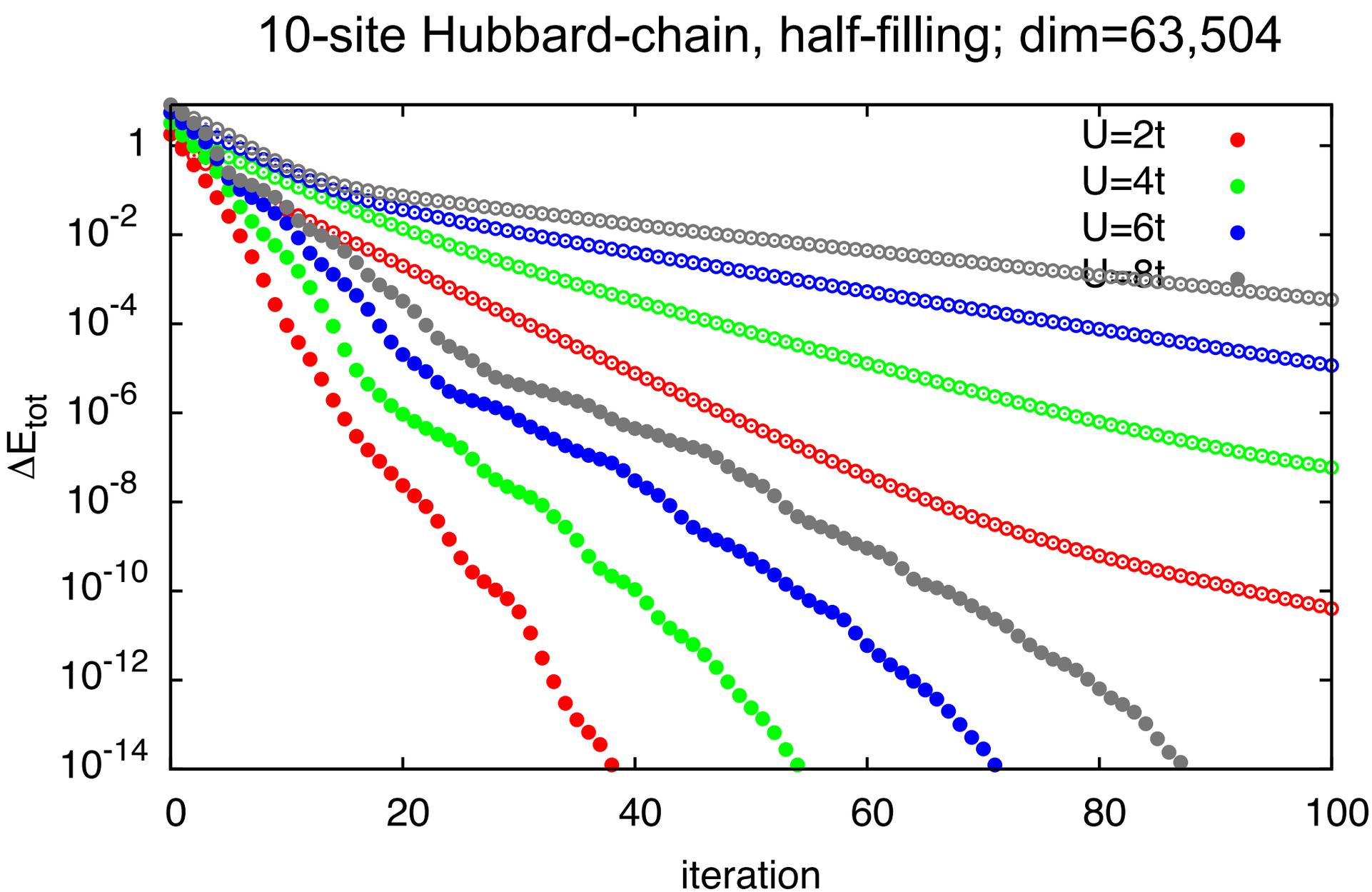
minimize on span $(|\psi_0\rangle, H|\psi_0\rangle)$ to obtain $|\psi_1\rangle$
minimize on span $(|\psi_1\rangle, H|\psi_1\rangle) \in$ span $\left(|\psi_0\rangle, H|\psi_0\rangle, H^2|\psi_0\rangle\right)$
minimize on span $(|\psi_2\rangle, H|\psi_2\rangle) \in$ span $\left(|\psi_0\rangle, H|\psi_0\rangle, H^2|\psi_0, H^3|\psi_0\rangle\right)$
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: $a_n := \langle v_n|H|v_n\rangle \qquad b_n := \sqrt{\langle \tilde{v}_n|\tilde{v}_n\rangle}$

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

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

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

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

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

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

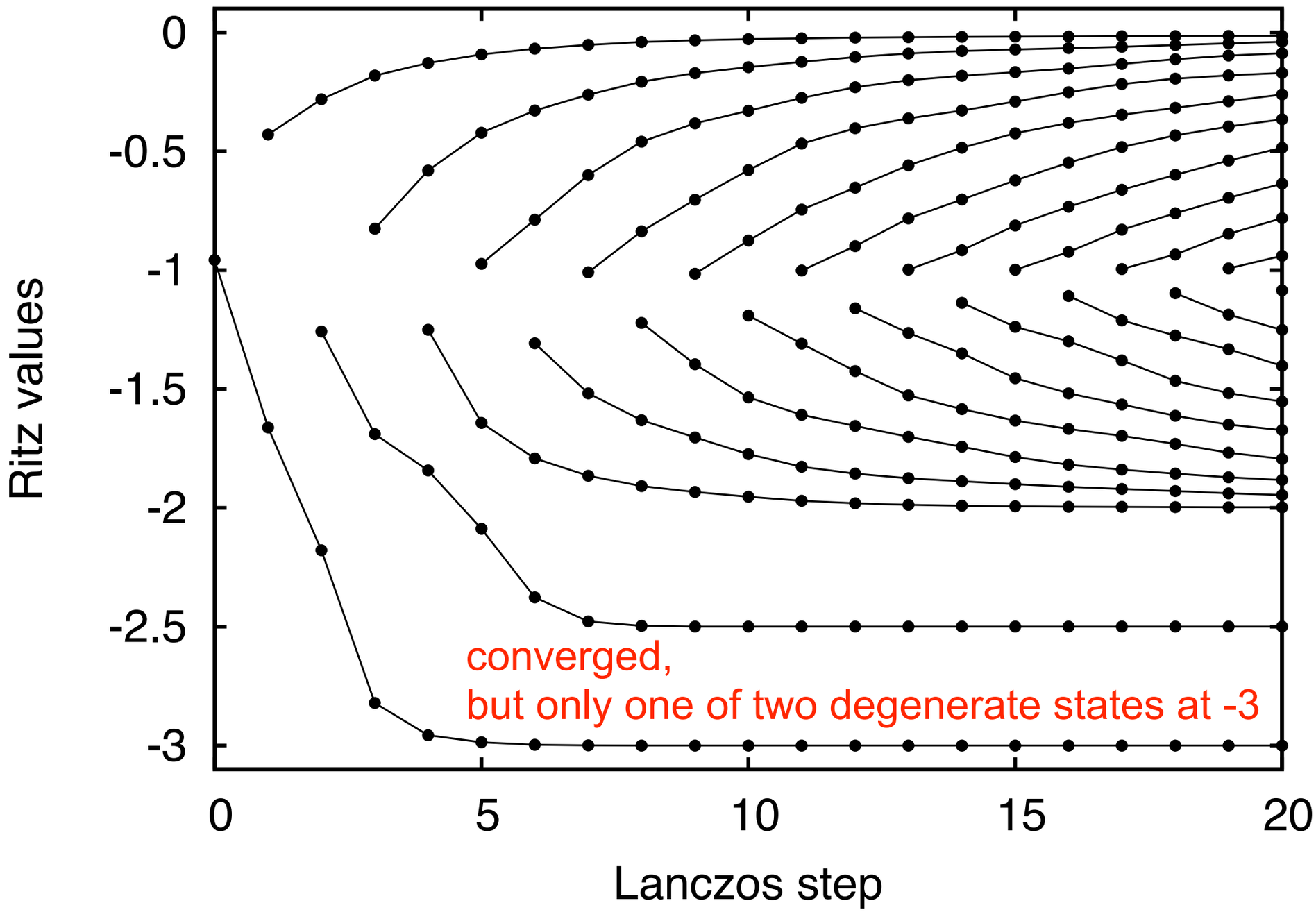
$\mathtt{a[n]} = \langle v_n|H|v_n\rangle - b_n\langle v_n|v_{n-1}\rangle$

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

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

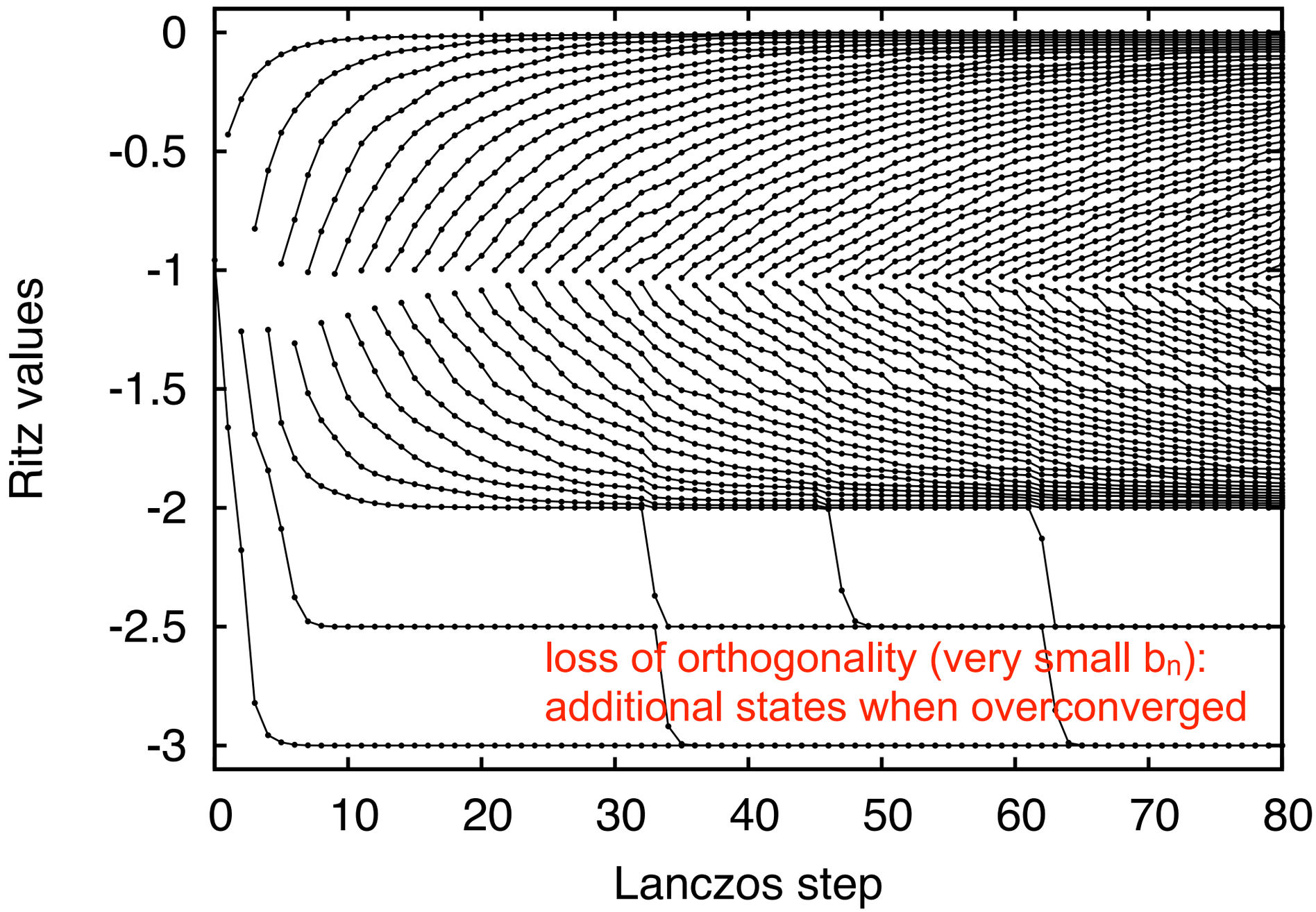
spectrum of tridiagonal matrix

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



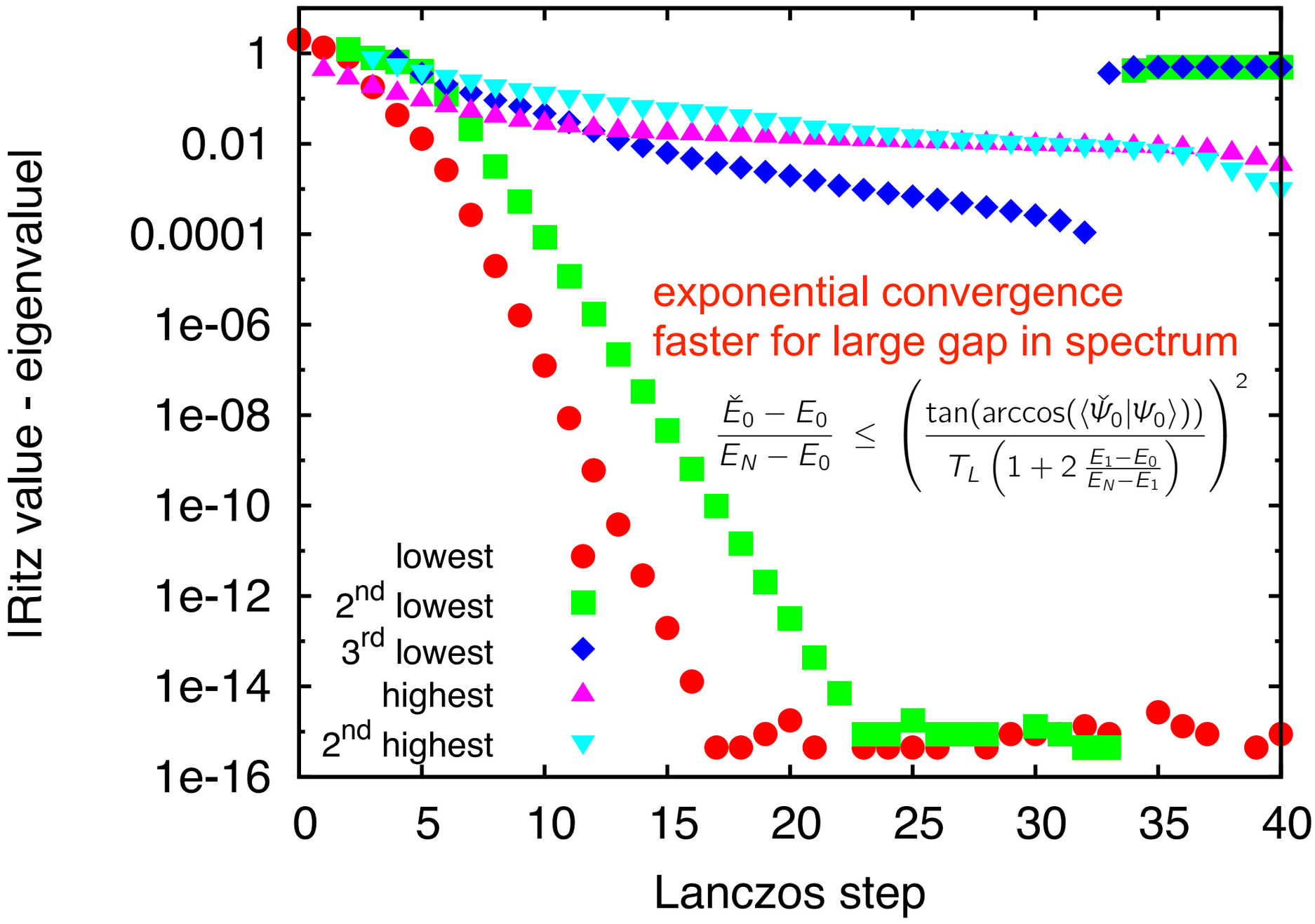
loss of orthogonality

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

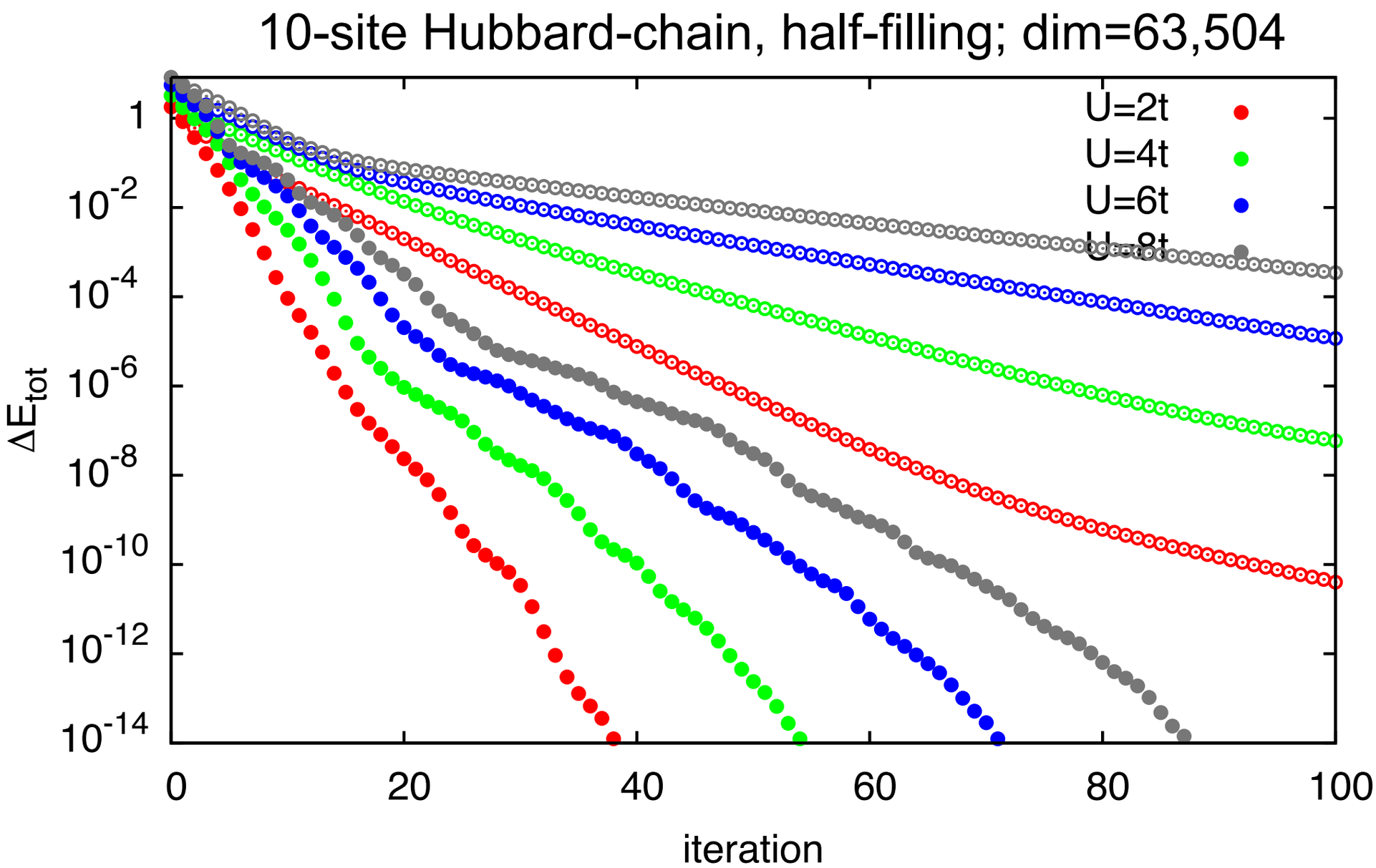


convergence to extremal eigenvalues

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

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

$$A\tilde{A} + B\tilde{C} = 1 \qquad = (A - BD^{-1}C)\tilde{A}$$

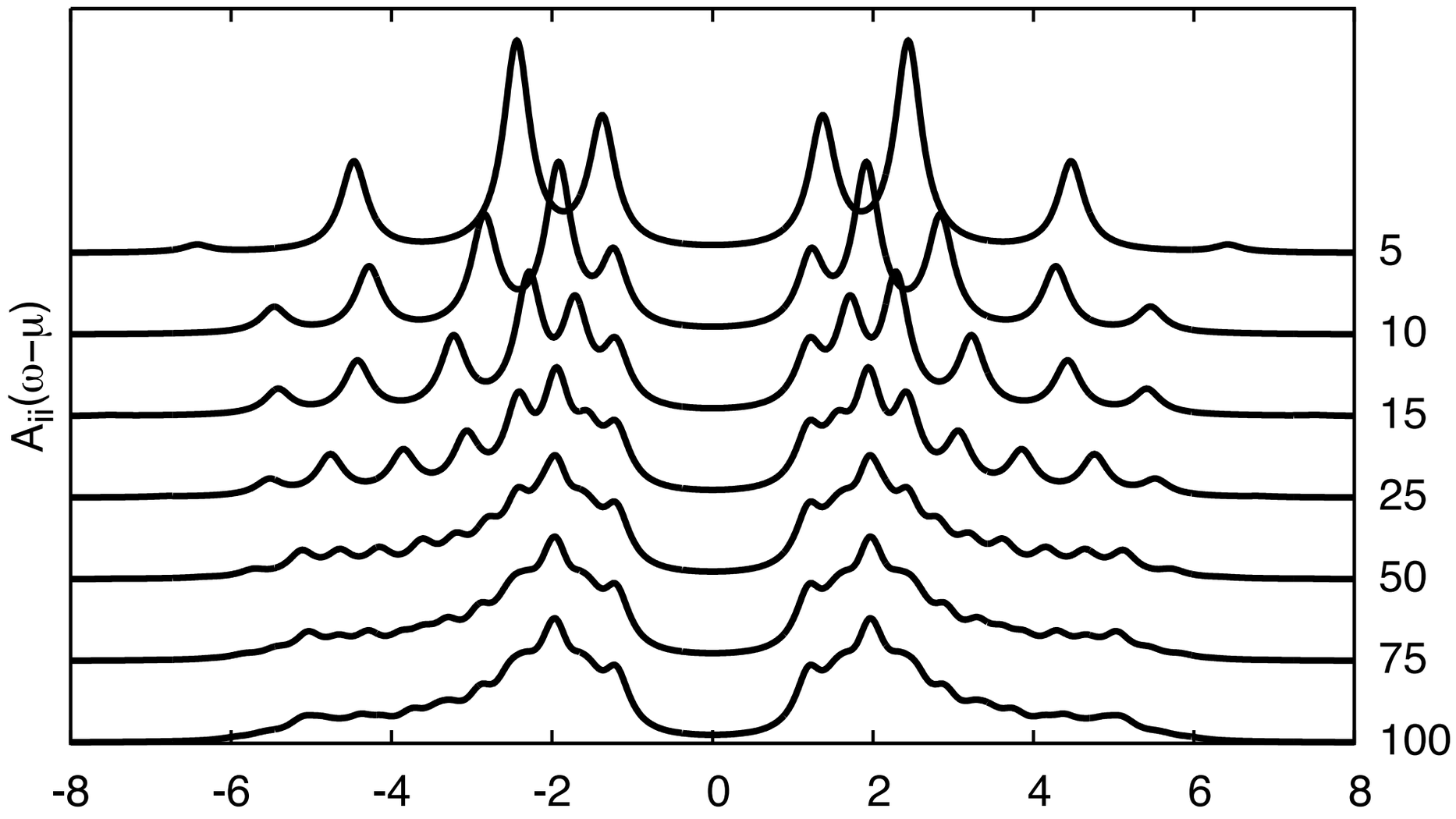
$$C\tilde{A} + D\tilde{C} = 0 \rightsquigarrow \tilde{C} = -D^{-1}C\tilde{A}$$

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

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

$$= \left\langle 0 \middle| \hat{\psi}(x_1) \cdots \hat{\psi}(x_N)\ c^\dagger_{\alpha_N} \cdots c^\dagger_{\alpha_1} \middle| 0 \right\rangle$$

$$\hat{\psi}(x)|0\rangle = 0 \qquad \{\hat{\psi}(x), \hat{\psi}(x')\} = 0 = \{\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x')\}$$

$$\langle 0|0\rangle = 1 \qquad \{\hat{\psi}(x), \hat{\psi}^\dagger(x')\} = \delta(x-x')$$

occupation number representation

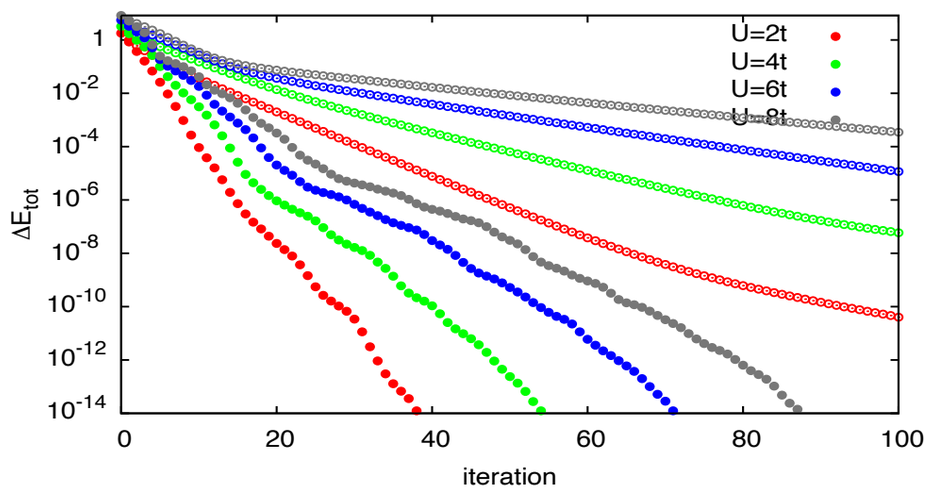
$$|n_{K-1}, \ldots, n_0\rangle := \prod \left(c^\dagger_k\right)^{n_k} |0\rangle$$

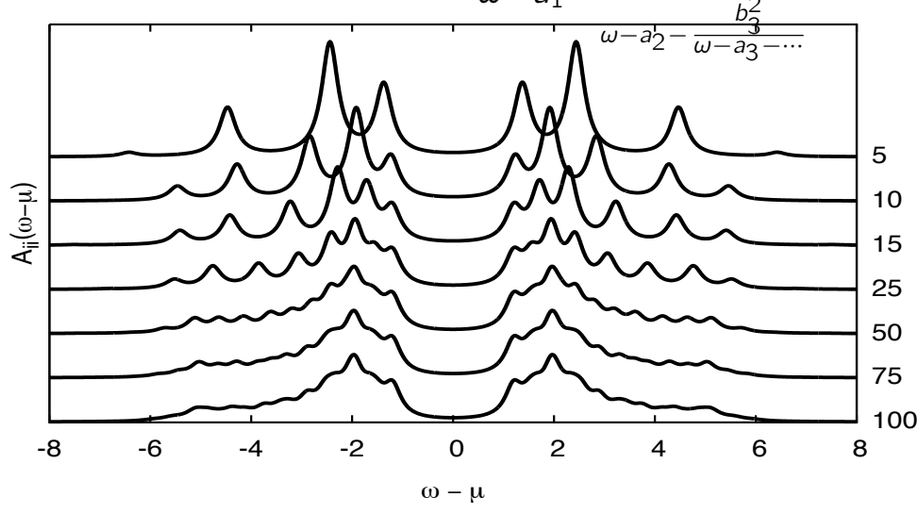
bit counting

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

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

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