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Exact Diagonalization

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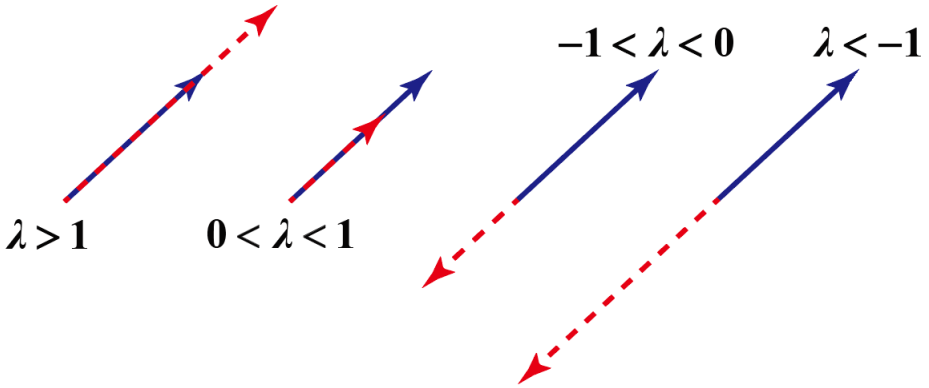
Outline

- Eigen problem
- Full Exact Diagonalization
- Lanczos Exact Diagonalization
- Summary

Eigen problem

lengthen, shorten and reverse directions



- Mathematic

$$Ax = \lambda x \Leftrightarrow (A - \lambda I)x = 0$$

$$\det\left(A - \lambda I\right) = 0$$

- Quantum Mechanic

$$\hat{H}\left|\Psi\right\rangle = E\left|\Psi\right\rangle \quad basis: \left|\Phi_1\right\rangle, \left|\Phi_2\right\rangle, \cdots, \left|\Phi_N\right\rangle \quad \hat{I} = \sum_{i=1}^{N}\left|\Phi_i\right\rangle\left\langle\Phi_i\right|$$

complete (and orthogonal) basis

$$\hat{I}\hat{H}\hat{I}\left|\Psi\right\rangle = E\hat{I}\left|\Psi\right\rangle$$

$$\sum_{i=1}^{N}\left|\Phi_i\right\rangle\left\langle\Phi_i\right|\hat{H}\sum_{j=1}^{N}\left|\Phi_j\right\rangle\left\langle\Phi_j\right|\left|\Psi\right\rangle = E\sum_{i=1}^{N}\left|\Phi_i\right\rangle\left\langle\Phi_i\right|\left|\Psi\right\rangle$$

$$\sum_{i=1}^{N}\left[\sum_{j=1}^{N}H_{ij}\Phi_j\right]\left|\Phi_i\right\rangle = \sum_{i=1}^{N}E\Phi_i\left|\Phi_i\right\rangle \Rightarrow \sum_{j=1}^{N}H_{ij}\Phi_j = E\Phi_i$$

Matrix mechanics

Eigen problem

Density matrix and partition function,

$$\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}} = \frac{1}{Z} \sum_i e^{-\beta E_i} \left| \Psi_i \right\rangle \left\langle \Psi_i \right|$$

$$Z = tr(e^{-\beta \hat{H}}) = \sum_i e^{-\beta E_i}$$

Many interesting physical variables,

$$\left\langle \hat{O} \right\rangle = tr(\hat{\rho}\hat{O}) = \frac{\sum_i e^{-\beta E_i} \left\langle \Psi_i \middle| \hat{O} \middle| \Psi_i \right\rangle}{\sum_i e^{-\beta E_i}} = \frac{\sum_i e^{-\beta (E_i - E_0)} \left\langle \Psi_i \middle| \hat{O} \middle| \Psi_i \right\rangle}{\sum_i e^{-\beta (E_i - E_0)}}$$

$$\underline{\underline{\beta \to \infty}} \frac{1}{m} \sum_{i=1}^{m} \left\langle \Psi_0^m \middle| \hat{O} \middle| \Psi_0^m \right\rangle$$

m is the number of degenerate ground states.

Finding roots of high-degree polynomials is a numerically tricky task

$$\det\left(A-\lambda I\right)=0$$

A better idea is to make use of the orthogonal or unitary transform

$$H'=U^{\dagger}HU, U^{\dagger}U=UU^{\dagger}=I, H'\Phi'=E\Phi'$$

$$\Rightarrow U^{\dagger}HU\Phi'=E\Phi' \Rightarrow H(U\Phi')=E(U\Phi')$$

Unitary transform does not change the eigenvalue of a matrix!

$$H\rightarrow U_1^{\dagger}HU_1\rightarrow U_2^{\dagger}U_1^{\dagger}HU_1U_2\rightarrow\cdots U_2^{\dagger}U_1^{\dagger}HU_1U_2\cdots\rightarrow\Lambda$$

$$\Lambda=U^{\dagger}HU,\ U=U_1U_2U_3\cdots$$ Jacobi iterative method, power method, …

Theorem: Suppose matrix A is real and symmetric, then

(1) All of the eigenvalues are real;

(2) Any two eigenvectors with different eigenvalues are orthogonal to each other;

(3) There exists a orthogonal matrix U that transforms A into a diagonal matrix.

For eigen problem of a hermitian matrix $C=A+iB$,

$$\left(A+iB\right)\cdot\left(u+iv\right)=\lambda\left(u+iv\right)$$

it can be mapped into the eigen problem of a real symmetric matrix

$$\begin{pmatrix} A & -B \\ B & A \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}=\lambda\begin{pmatrix} u \\ v \end{pmatrix}$$

$$C^{\dagger}=C\Rightarrow A^{T}=A, B^{T}=-B$$

Full Exact Diagonaliaztion

1. Jacobi method

$$H_0 = H, H_{k+1} = J_k^T H_k J_k, J_k^{-1} = J_k^T$$

$$J_k = \begin{pmatrix} 1 & & & & & & & & \\ & \ddots & & & & & & & \\ & & \cos\theta & & & & -\sin\theta & & \\ & & & 1 & & & & & \\ & & & & \ddots & & & & \\ & & & & & 1 & & & \\ & & \sin\theta & & & & \cos\theta & & \\ & & & & & & & \ddots & \\ & & & & & & & & 1 \end{pmatrix}$$

$$U = J_k J_{k-1} \cdots J_1 J_0$$

U is the product of all rotation matrices.

Example:

$$A_0 = \begin{pmatrix} 1 & 0 & 2 \\ 0 & 2 & 1 \\ 2 & 1 & 1 \end{pmatrix} \xrightarrow{J_0 = \begin{pmatrix} 0.707 & 0 & -0.707 \\ 0 & 1 & 0 \\ 0.707 & 0 & 0.707 \end{pmatrix}} A_1 = J_0^T A_0 J_0 = \begin{pmatrix} 3 & 0.707 & 0 \\ 0.707 & 2 & 0.707 \\ 0 & 0.707 & -1 \end{pmatrix}$$

$$\xrightarrow{J_1 = \begin{pmatrix} 0.888 & -0.460 & 0 \\ 0.460 & 0.888 & 0 \\ 0 & 0 & 1 \end{pmatrix}} A_2 = J_1^T A_1 J_1 = \begin{pmatrix} 3.366 & 0 & 0.325 \\ 0 & 1.634 & 0.628 \\ 0.325 & 0.628 & -1 \end{pmatrix}$$

$$\xrightarrow{J_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0.975 & -0.226 \\ 0 & 0.226 & 0.975 \end{pmatrix}} A_3 = J_2^T A_2 J_2 = \begin{pmatrix} 3.366 & 0.0735 & 0.317 \\ 0.0735 & 1.780 & 0 \\ 0.325 & 0 & -1.145 \end{pmatrix}$$

2. *QR* or *QU* factorization——widely used method

Decomposition of a matrix H into a product of an orthogonal matrix Q and an upper triangular matrix R,

$$H_0 = H \to H_k = Q_k R_k \to H_{k+1} = R_k Q_k \to H_{k+1} = Q_{k+1} R_{k+1} \to$$

It can be proved that H_{k+1} is similar to H_k,

$$H_{k+1} = R_k Q_k = Q_k^T Q_k R_k Q_k = Q_k^T H_k Q_k$$

$$= Q_k^T Q_{k-1}^T H_{k-1} Q_{k-1} Q_k = \cdots = Q_k^T Q_{k-1}^T \cdots Q_0^T H_0 Q_0 \cdots Q_{k-1} Q_k$$

$$\Rightarrow H = U \Lambda U^T, U = Q_1 Q_2 \cdots Q_\infty$$

Two strategies are used to improve covergence.

(1) shifted QR

$$A_k - \sigma_k I = Q_k R_k$$
$$A_{k+1} = R_k Q_k + \sigma_k I$$

(2) two steps

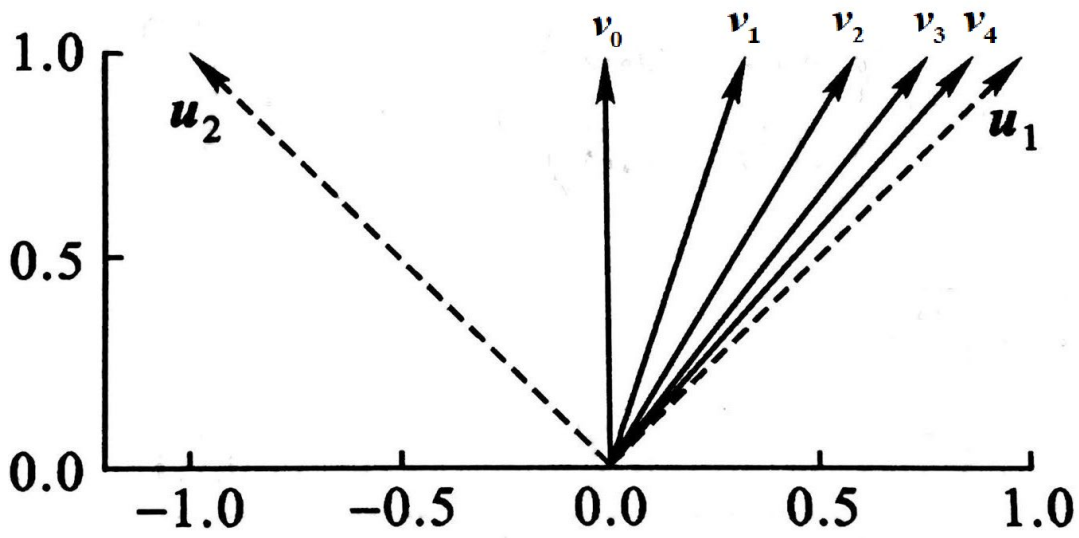
$$\boxed{\text{symmetric matrix}} \xrightarrow{\textbf{Householder transformation}} \boxed{\text{tridiagonal matrix}} \xrightarrow{\textbf{QR factorization}} \boxed{\text{diagonal matrix}}$$

Lanczos Exact Diagonalization

1. Power method

Eigenvalues: $|\lambda_1| > |\lambda_2| > |\lambda_3| > \ldots,$

Eigenvector: $u_1, u_2, u_3, \ldots.$



$$v_0 = \sum_{i=1}^{n} \alpha_i u_i, \alpha_1 \neq 0$$

$$v_k = Hv_{k-1} = H^2 v_{k-2} = \cdots = H^k v_0$$

$$= \sum_{i=1}^{n} \lambda_i^k \alpha_i u_i = \lambda_1^k \left[\alpha_1 u_1 + \sum_{i=2}^{n} \left(\lambda_i / \lambda_1 \right)^k \alpha_i u_i \right] \Rightarrow \begin{cases} \lambda_1 = \lim\limits_{k\to\infty} \dfrac{\|v_k\|_\infty}{\|v_{k-1}\|_\infty} \\ u_1 = \lim\limits_{k\to\infty} v_k \end{cases}$$

2. Krylov subspace

For $H \in C^{nxn}$ and $0 \neq v_0 \in C^{nxn}$,

$$\left\{ \boldsymbol{v}_0, \boldsymbol{H}\boldsymbol{v}_0, \boldsymbol{H}^2\boldsymbol{v}_0, \cdots, \boldsymbol{H}^{j-1}\boldsymbol{v}_0 \right\} : \textbf{Krylov sequence}$$

$$\mathcal{K}^m(\boldsymbol{H}; \boldsymbol{v}_0) = \textbf{span}\left\{ \boldsymbol{v}_0, \boldsymbol{H}\boldsymbol{v}_0, \boldsymbol{H}^2\boldsymbol{v}_0, \cdots, \boldsymbol{H}^{m-1}\boldsymbol{v}_0 \right\} : \textbf{Krylov subspace}$$

Ill-conditioned: $H^{m-1}v_0$ point more and more in the direction of the dominant eigenvector for increasing m, and hence the basis vectors become dependent in finite precision arithmetic. It is better to work with an orthonormal basis.

(1) symmetric matrices——Lanczos algorithm;

(2) unsymmetric matrices——Arnoldi algorithm.

3. (Modified) Lanczos algorithm

Lanczos method: construct a special orthogonal basis by numerically efficient recursion scheme where the Hamiltonian has a tridiagonal representation.

Since we use floating point arithemetic, when the basis size becomes large, round-off errors accumulation makes the orthogonality lost.

$$
\begin{cases}
v'_{n+1} = Hv_n - a_n v_n - b_{n-1} v_{n-1} \\
v_{n+1} = v'_{n+1} - \sum_{i=0}^{n} \frac{\left(v_i, v'_{n+1}\right)}{\left(v_i, v_i\right)} v_i \\
a_n = \frac{\left(v_n, Hv_n\right)}{\left(v_n, v_n\right)} \\
b_n = \sqrt{\frac{\left(v_n, v_n\right)}{\left(v_{n-1}, v_{n-1}\right)}}, b_0 = 0 \\
v_{-1} = 0, \text{choose } v_0 \text{ randomly}
\end{cases}
$$

Gram–Schmidt process

cost time and memory

Every iterative step generates one Krylov vector,

$$\left\{ \frac{v_0}{\sqrt{(v_0, v_0)}}, \frac{v_1}{\sqrt{(v_1, v_1)}}, \frac{v_2}{\sqrt{(v_2, v_2)}}, \cdots, \frac{v_{M-1}}{\sqrt{(v_{M-1}, v_{M-1})}} \right\}$$

These vectors form Krylov matrix V with orthonormal columns. This matrix can project the Hamiltonian matrix into a tridiagonal matrix in Krylov subspace.

$$T = V^{\dagger} H V = \begin{pmatrix} a_0 & b_1 & 0 & \cdots & 0 & 0 \\ b_1 & a_1 & b_2 & \cdots & 0 & 0 \\ 0 & b_2 & a_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & a_{M-2} & b_{M-1} \\ 0 & 0 & 0 & \cdots & b_{M-1} & a_{M-1} \end{pmatrix}$$

$M \sim 100$

Eigenvalues

$$\Lambda = U^{\dagger} T U$$

$$= U^{\dagger} V^{\dagger} H V U$$ **Eigenvectors**

How to get the orthogonal matrix U ?

QR(QL), MRRR, …

4. Sparse matrix storage format: Compressed Row Storage (CRS)

$$AX = \begin{bmatrix} 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 7 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 6 & 9 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 \\ \hline 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 7 & 6 & 0 & 0 & 0 \end{bmatrix} \begin{pmatrix} 3 \\ 4 \\ 1 \\ 9 \\ 3 \\ 6 \\ 1 \\ 2 \end{pmatrix}, \text{CRS format} \begin{cases} val = [2 \quad 4 \quad 7 \quad 6 \quad 9 \quad 5 \quad 3 \quad 1 \quad 7 \quad 6] \\ row\_prt = [1 \quad 2 \quad 2 \quad 4 \quad 4 \quad 6 \quad 7 \quad 8 \quad 11] \\ col\_ind = [3 \quad 2 \quad 6 \quad 5 \quad 6 \quad 8 \quad 2 \quad 3 \quad 4 \quad 5] \end{cases}$$

The row_ptr vector stores the locations in the val vector that start a row.

$$y = Ax, \quad y_i = \sum_j a_{i,j} x_j$$

```
for i=1, n
   y(i)=0
   for j = row_ptr(i), row_ptr(i+1)-1
      y(i)=y(i)+val(j)*x(col_ind(j))
   end
end
```

MPI .vs. OPENMP

5. Degenerate states and excited states

$$v_k = \lambda_1^k \left[\alpha_1 u_1 + \alpha_2 u_2 + \sum_{i=3}^{n} (\lambda_i / \lambda_1)^k \alpha_i u_i \right]$$

u_1, u_2 are degenate states.

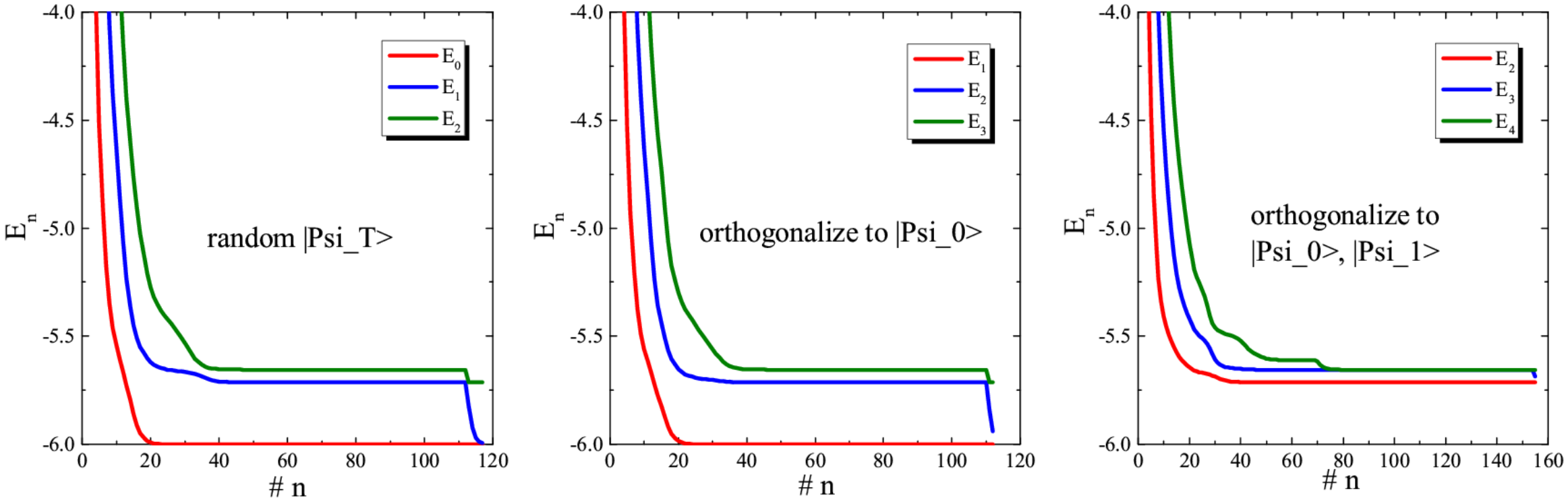
v_k is a superposition of u_1 and u_2。

(1) Gram–Schmidt process: each new Lanczos vector constructed is explicitly orthogonalized with respect to all previous basis vectors.

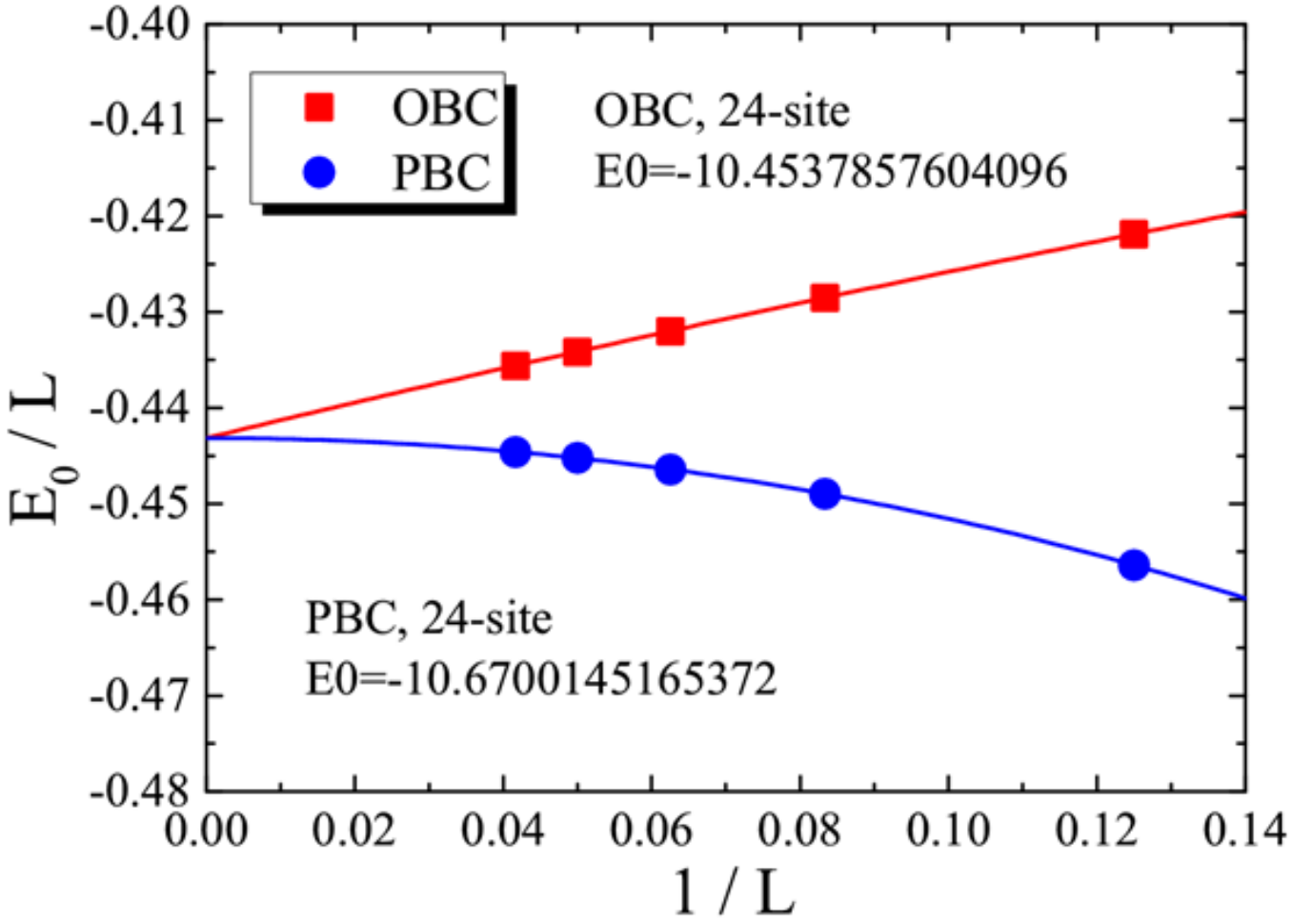
(2) Instead of converging several excited states in the same run, one can also target excited states one-by-one, starting each time from a vector which is orthogonal to all previous ones.

Anders W. Sandvik, AIP Conference Proceedings 1297, 135 (2010)

target excited states one-by-one



6. Download and run the source code



Finite-size gound state energies of 1D Heisenberg model.

Download the source code: https://github.com/hqwu/Lanczos-exact-diagonalization

Summary

1.Full exact diagonalization

(1)similarity transform to get the tridiagonal or diagonal matrix;

(2)QR or QL factorization to diagonal form.

2. Lanczos exact diagonalization

(1)Krylov subspace;

(2)degenerate states need to be careful ;

(3) excited states can be got by targeting one by one or using reorthogonalization.

Bibliography

(*1)Numerical Simulations of Frustrated Systems*, Andreas M. Läuchli, Springer Berlin Heidelberg, 2011.

(2)Anders W. Sandvik, AIP Conference Proceedings 1297, 135 (2010).

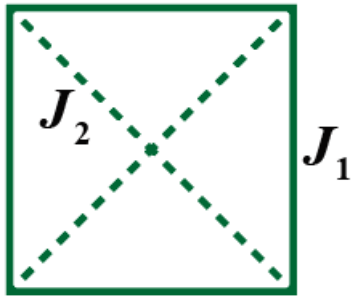
(*3)Numerical Recipes: The Art of Scientific Computing*, Third Edition (2007), 1256 pp. Cambridge University Press ISBN-10: 0521880688.

(4) *Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide*, Zhaojun Bai et al., Society for Industrial and Applied Mathematics, 2000

Appendix A

Four-site plaquette

$$\hat{H} = J_1\left(\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_3\right)\left(\hat{\mathbf{S}}_2 + \hat{\mathbf{S}}_4\right) + J_2\left(\hat{\mathbf{S}}_1\hat{\mathbf{S}}_3 + \hat{\mathbf{S}}_2\hat{\mathbf{S}}_4\right)$$



Basis of M_z=0 sector:

$$|\psi_1\rangle = |\uparrow_1\uparrow_2\downarrow_3\downarrow_4\rangle = |1_1 1_2 0_3 0_4\rangle = 3, \quad |\psi_2\rangle = |\uparrow_1\downarrow_2\uparrow_3\downarrow_4\rangle = |1_1 0_2 1_3 0_4\rangle = 5,$$

$$|\psi_3\rangle = |\downarrow_1\uparrow_2\uparrow_3\downarrow_4\rangle = |0_1 1_2 1_3 0_4\rangle = 6, \quad |\psi_4\rangle = |\uparrow_1\downarrow_2\downarrow_3\uparrow_4\rangle = |1_1 0_2 0_3 1_4\rangle = 9,$$

$$|\psi_5\rangle = |\downarrow_1\uparrow_2\downarrow_3\uparrow_4\rangle = |0_1 1_2 0_3 1_4\rangle = 10, \quad |\psi_6\rangle = |\downarrow_1\downarrow_2\uparrow_3\uparrow_4\rangle = |0_1 0_2 1_3 1_4\rangle = 12$$

$$\hat{H}\left|\psi_1\right\rangle = -\frac{J_2}{2}\left|\psi_1\right\rangle + \frac{J_1}{2}\left|\psi_2\right\rangle + \frac{J_2}{2}\left|\psi_3\right\rangle + \frac{J_2}{2}\left|\psi_4\right\rangle + \frac{J_1}{2}\left|\psi_5\right\rangle$$

$$\hat{H}\left|\psi_2\right\rangle = +\frac{J_1}{2}\left|\psi_1\right\rangle + \left(-J_1 + \frac{J_2}{2}\right)\left|\psi_2\right\rangle + \frac{J_1}{2}\left|\psi_3\right\rangle + \frac{J_1}{2}\left|\psi_4\right\rangle + \frac{J_1}{2}\left|\psi_6\right\rangle$$

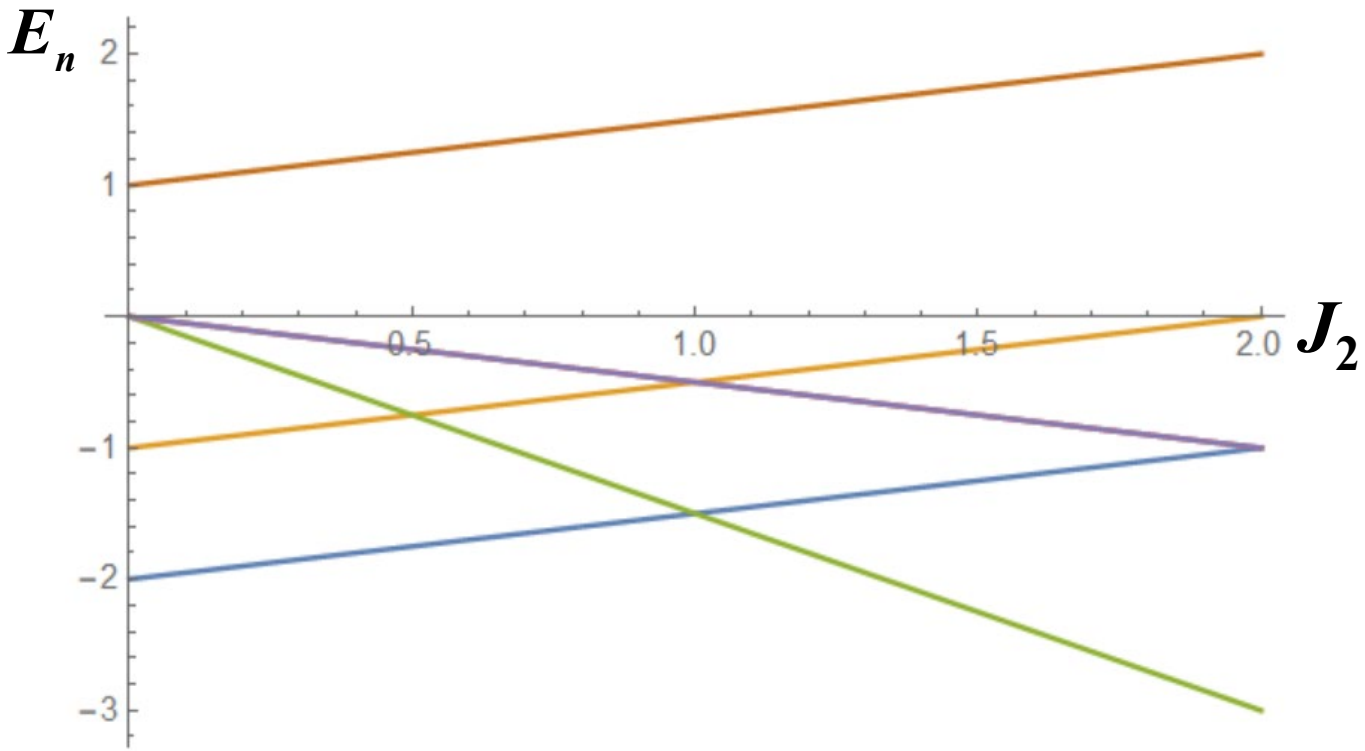
$$\hat{H}\left|\psi_3\right\rangle = +\frac{J_2}{2}\left|\psi_1\right\rangle + \frac{J_1}{2}\left|\psi_2\right\rangle - \frac{J_2}{2}\left|\psi_3\right\rangle + \frac{J_1}{2}\left|\psi_5\right\rangle + \frac{J_2}{2}\left|\psi_6\right\rangle$$

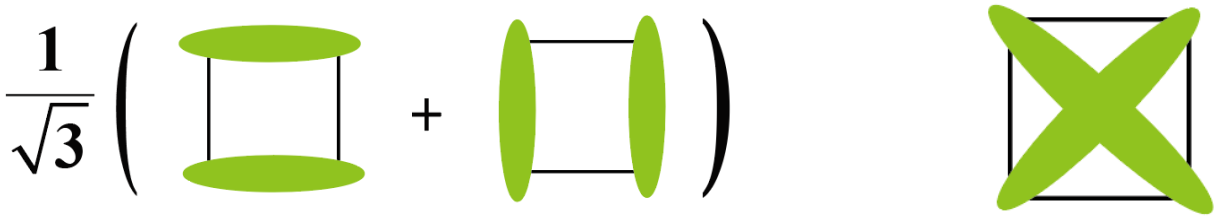
$$\hat{H}\left|\psi_4\right\rangle = +\frac{J_2}{2}\left|\psi_1\right\rangle + \frac{J_1}{2}\left|\psi_2\right\rangle - \frac{J_2}{2}\left|\psi_4\right\rangle + \frac{J_1}{2}\left|\psi_5\right\rangle + \frac{J_2}{2}\left|\psi_6\right\rangle$$

$$\hat{H}\left|\psi_5\right\rangle = +\frac{J_1}{2}\left|\psi_1\right\rangle + \frac{J_1}{2}\left|\psi_3\right\rangle + \frac{J_1}{2}\left|\psi_4\right\rangle + \left(-J_1 + \frac{J_2}{2}\right)\left|\psi_5\right\rangle + \frac{J_1}{2}\left|\psi_6\right\rangle$$

$$\hat{H}\left|\psi_6\right\rangle = +\frac{J_1}{2}\left|\psi_2\right\rangle + \frac{J_2}{2}\left|\psi_3\right\rangle + \frac{J_2}{2}\left|\psi_4\right\rangle + \frac{J_1}{2}\left|\psi_5\right\rangle - \frac{J_2}{2}\left|\psi_6\right\rangle$$

$$H = \begin{pmatrix} -\frac{J_2}{2} & \frac{J_1}{2} & \frac{J_2}{2} & \frac{J_2}{2} & \frac{J_1}{2} & 0 \\ \frac{J_1}{2} & \left(-J_1 + \frac{J_2}{2}\right) & \frac{J_1}{2} & \frac{J_1}{2} & 0 & \frac{J_1}{2} \\ \frac{J_2}{2} & \frac{J_1}{2} & -\frac{J_2}{2} & 0 & \frac{J_1}{2} & \frac{J_2}{2} \\ \frac{J_2}{2} & \frac{J_1}{2} & 0 & -\frac{J_2}{2} & \frac{J_1}{2} & \frac{J_2}{2} \\ \frac{J_1}{2} & 0 & \frac{J_1}{2} & \frac{J_1}{2} & \left(-J_1 + \frac{J_2}{2}\right) & \frac{J_1}{2} \\ 0 & \frac{J_1}{2} & \frac{J_2}{2} & \frac{J_2}{2} & \frac{J_1}{2} & -\frac{J_2}{2} \end{pmatrix}$$





$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Appendix B

$$C_V = \frac{\partial}{\partial T}\left(\frac{E}{N}\right) = \frac{\partial}{\partial T}\left(\frac{Tr\left(\hat{H}e^{-\beta\hat{H}}\right)}{NTr\left(e^{-\beta\hat{H}}\right)}\right) = \frac{1}{Nk_B T^2}\left(\left\langle \hat{H}^2 \right\rangle - \left\langle \hat{H} \right\rangle^2\right)$$

$$\left\langle \hat{H} \right\rangle = \frac{1}{Z}Tr\left(\hat{H}e^{-\beta\hat{H}}\right) = \frac{\sum_n \left\langle n \middle| \hat{H}e^{-\beta\hat{H}} \middle| n \right\rangle}{\sum_n \left\langle n \middle| e^{-\beta\hat{H}} \middle| n \right\rangle} = \frac{\sum_n E_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n}}$$

$$\left\langle \hat{H}^2 \right\rangle = \frac{1}{Z}Tr\left(\hat{H}^2 e^{-\beta\hat{H}}\right) = \frac{\sum_n \left\langle n \middle| \hat{H}^2 e^{-\beta\hat{H}} \middle| n \right\rangle}{\sum_n \left\langle n \middle| e^{-\beta\hat{H}} \middle| n \right\rangle} = \frac{\sum_n E_n^2 e^{-\beta E_n}}{\sum_n e^{-\beta E_n}}$$

$$\chi_u = \frac{\partial}{\partial H}\left(\frac{M_z}{N}\right) = \frac{1}{N}\frac{\partial}{\partial H}\left[\frac{Tr\left(e^{-\beta\hat{H}}\sum_i \hat{S}_i^z\right)}{Tr\left(e^{-\beta\hat{H}}\right)}\right] = \frac{\beta}{N}\left[\left\langle \hat{M}_z^2\right\rangle - \left\langle \hat{M}_z\right\rangle^2\right]$$

$$\left\langle \hat{M}_z^2\right\rangle = \frac{Tr\left[e^{-\beta\hat{H}}\left(\sum_i \hat{S}_i^z\right)^2\right]}{Tr\left(e^{-\beta\hat{H}}\right)} = \frac{\sum_n \left\langle n\right| e^{-\beta\hat{H}}\left(\sum_i \hat{S}_i^z\right)^2 \left|n\right\rangle}{\sum_n \left\langle n\right| e^{-\beta\hat{H}} \left|n\right\rangle} = \frac{\sum_n e^{-\beta E_n}\left(\sum_i S_i^z\right)^2}{\sum_n e^{-\beta E_n}}$$

$$\left\langle \hat{M}_z\right\rangle = \frac{Tr\left[e^{-\beta\hat{H}}\left(\sum_i \hat{S}_i^z\right)\right]}{Tr\left(e^{-\beta\hat{H}}\right)} = \frac{\sum_n \left\langle n\right| e^{-\beta\hat{H}}\left(\sum_i \hat{S}_i^z\right) \left|n\right\rangle}{\sum_n \left\langle n\right| e^{-\beta\hat{H}} \left|n\right\rangle} = \frac{\sum_n e^{-\beta E_n}\left(\sum_i S_i^z\right)}{\sum_n e^{-\beta E_n}}$$