多体問題の計算科学

#10

2017/6/20

Computational Science for Many-Body Problems

Linear Algebra for Quantum Many-Body Problems

1. Quantum mechanics by linear algebra
2. Linear algebra by comupter
3. Quantum many-body problems by linear algebra
4. Eigenvalue problems of large & sparse matrices

Quantum Mechanics by Linear Algebra

Quantum Mechanics by Linear Algebra

Naïvely, linear partial differential equations are rewritten by Linear equations

Schrödinger equation represented by partial diff. eq.

$$i\hbar\frac{d}{dt}\psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right]\psi(\vec{r},t)$$

Stationary solution: $\psi(\vec{r},t) = \phi(\vec{r})e^{-iEt/\hbar}$

$$\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right]\phi(\vec{r}) = E\phi(\vec{r})$$

Quantum Mechanics by Linear Algebra

Schrödinger equation represented by linear eqs.

$$\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right]\phi(\vec{r}) = E\phi(\vec{r})$$

Expanded by orthonormal basis

$$\phi(\vec{r}) = \sum_m c_m u_m(\vec{r})$$

$$\int d^3r \; u_\ell^*(\vec{r}) u_m(\vec{r}) = \delta_{\ell,m}$$

$$\int d^3r \phi^*(\vec{r})\phi(\vec{r}) = \sum_m |c_m|^2$$

Matrix representation

$$H_{\ell m} = \int d^3r u_\ell^*(\vec{r}) \left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right] u_m(\vec{r})$$

$$\sum_m H_{\ell m} c_m = E c_\ell$$

Quantum Mechanics by Linear Algebra

$$\sum_m H_{\ell m} c_m = E c_\ell$$

Hermitian matrix $H_{\ell m} = H^*_{m\ell}$

-Diagonalizable by unitary matrices
-Real eigenvalues

$$\sum_m H_{\ell m} U_{m\alpha} = U_{\ell\alpha} E_\alpha$$

$$\sum_m (U^\dagger)_{\beta m} U_{m\alpha} = \sum_m (U_{m\beta})^* U_{m\alpha} = \delta_{\beta,\alpha}$$

Quantum Mechanics by Linear Algebra

$$\sum_m H_{\ell m} c_m = E c_\ell$$

Vector representation of expectation value

$$\frac{\int d^3 r \phi^*(\vec{r}) \hat{O} \phi(\vec{r})}{\int d^3 r \phi^*(\vec{r}) \phi(\vec{r})} = \frac{\sum_{\ell,m} c_\ell^* c_m \int d^3 r u_\ell^*(\vec{r}) \hat{O} u_m(\vec{r})}{\sum_n |c_n|^2}$$

$$= \frac{\sum_{\ell,m} c_\ell^* O_{\ell m} c_m}{\sum_n |c_n|^2}$$

Linear Algebra by Computer

Linear Algebra by Computer

$$\sum_m H_{\ell m} U_{m\alpha} = U_{\ell\alpha} E_\alpha$$

Hermitian matrix $H_{\ell m} = H^*_{m\ell}$

LAPACK (Linear Algebra PACKage)

http://www.netlib.org/lapack/explore-html/index.html

zheev
z: double complex
he: hermitian
ev: eigenvalue & eigenvector

```
subroutine zheev ( character                          JOBZ,
                   character                          UPLO,
                   integer                            N,
                   complex*16, dimension( lda, * )    A,
                   integer                            LDA,
                   double precision, dimension( * )   W,
                   complex*16, dimension( * )         WORK,
                   integer                            LWORK,
                   double precision, dimension( * )   RWORK,
                   integer                            INFO
                 )
```

Linear Algebra by Computer

LAPACK (Linear Algebra PACKage)

http://www.netlib.org/lapack/explore-html/index.html

-Language: Fortran
C & C++ can call LAPACK

-License:
Modified BSD license

-Parallelized version:
ScaLAPACK

cf.) intel MKL
(commercial library)

-Transformation
-Eigenvalue
-Singular value

Quantum Many-Body Problems by Linear Algebra

Quantum Many-Body Problem by Linear Algebra

Hamiltonian in 2nd quantization form

Many-body electrons confined in one-body potential

(No spin-orbit coupling)

$$
\begin{aligned}
\hat{H} &= \sum_{\sigma}\int d^3r\hat{\phi}^{\dagger}_{\sigma}(\vec{r})\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2+V(\vec{r})\right]\hat{\phi}_{\sigma}(\vec{r}) \\
&+\frac{1}{2}\sum_{\sigma,\sigma'}\int d^3r\int d^3r'\hat{\phi}^{\dagger}_{\sigma}(\vec{r})\hat{\phi}_{\sigma}(\vec{r})v(|\vec{r}-\vec{r}'|)\hat{\phi}^{\dagger}_{\sigma'}(\vec{r}')\hat{\phi}_{\sigma'}(\vec{r}')
\end{aligned}
$$

Quantum Many-Body Problem by Linear Algebra

Field operator

$$\hat{\phi}_\sigma(\vec{r}) = \sum_\ell u_\ell(\vec{r})\hat{a}_{\ell\sigma}$$

$$\int d^3r\ u_\ell^*(\vec{r})u_m(\vec{r}) = \delta_{\ell,m}$$

Fermions

$$\{\hat{a}_{\ell\sigma}, \hat{a}^\dagger_{m\tau}\} = \hat{a}_{\ell\sigma}\hat{a}^\dagger_{m\tau} + \hat{a}^\dagger_{m\tau}\hat{a}_{\ell\sigma} = \delta_{\ell,m}\delta_{\sigma,\tau}$$

$$\{\hat{a}_{\ell\sigma}, \hat{a}_{m\tau}\} = \{\hat{a}^\dagger_{\ell\sigma}, \hat{a}^\dagger_{m\tau}\} = 0$$

Bosons

$$[\hat{a}_{\ell\sigma}, \hat{a}^\dagger_{m\tau}] = \hat{a}_{\ell\sigma}\hat{a}^\dagger_{m\tau} - \hat{a}^\dagger_{m\tau}\hat{a}_{\ell\sigma} = \delta_{\ell,m}\delta_{\sigma,\tau}$$

$$[\hat{a}_{\ell\sigma}, \hat{a}_{m\tau}] = [\hat{a}^\dagger_{\ell\sigma}, \hat{a}^\dagger_{m\tau}] = 0$$

Quantum Many-Body Problem by Linear Algebra

$$
\begin{aligned}
\hat{H} &= \sum_{\sigma} \int d^3r \hat{\phi}^{\dagger}_{\sigma}(\vec{r}) \left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] \hat{\phi}_{\sigma}(\vec{r}) \\
&+ \frac{1}{2} \sum_{\sigma,\sigma'} \int d^3r \int d^3r' \hat{\phi}^{\dagger}_{\sigma}(\vec{r}) \hat{\phi}_{\sigma}(\vec{r}) v(|\vec{r} - \vec{r}'|) \hat{\phi}^{\dagger}_{\sigma'}(\vec{r}') \hat{\phi}_{\sigma'}(\vec{r}')
\end{aligned}
$$

$\rightarrow$ General Hamiltonian with two-body interactions

$$
\hat{H} = \sum_{\ell,m,\sigma} K_{\ell m} \hat{a}^{\dagger}_{\ell\sigma} \hat{a}_{m\sigma} + \sum_{\ell_1,\ell_2,m_1,m_2} \sum_{\sigma,\sigma'} I_{\ell_1\ell_2 m_1 m_2} \hat{a}^{\dagger}_{\ell_1\sigma} \hat{a}_{\ell_2\sigma} \hat{a}^{\dagger}_{m_1\sigma'} \hat{a}_{m_2\sigma'}
$$

$$
K_{\ell m} = \int d^3r u^{*}_{\ell}(\vec{r}) \left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] u_m(\vec{r})
$$

$$
I_{\ell_1\ell_2 m_1 m_2} = \frac{1}{2} \int d^3r \int d^3r' u^{*}_{\ell_1}(\vec{r}) u_{\ell_2}(\vec{r}) v(|\vec{r} - \vec{r}'|) u^{*}_{m_1}(\vec{r}') u_{m_2}(\vec{r}')
$$

Quantum Many-Body Problem by Linear Algebra

Fock space of *N*-particle fermions expanded by

$$|\Phi\rangle = \sum_{\ell_1,\ell_2,\ldots,\ell_N} \sum_{\sigma_1,\sigma_2,\ldots,\sigma_N} C_{\ell_1\ell_2\cdots\ell_N} \hat{a}^\dagger_{\ell_1\sigma_1} \hat{a}^\dagger_{\ell_2\sigma_2} \cdots \hat{a}^\dagger_{\ell_N\sigma_N} |\mathrm{vac}\rangle$$

Orthonormalized many-body basis

$$\{\ell_j, \sigma_j\} = \{\ell_1, \sigma_1, \ell_2, \sigma_2, \ldots, \ell_N, \sigma_N\}$$

$$|\{\ell_j, \sigma_j\}\rangle = \hat{a}^\dagger_{\ell_1\sigma_1} \hat{a}^\dagger_{\ell_2\sigma_2} \cdots \hat{a}^\dagger_{\ell_N\sigma_N} |\mathrm{vac}\rangle$$

$$|\{m_j, \tau_j\}\rangle = \hat{a}^\dagger_{m_1\tau_1} \hat{a}^\dagger_{m_2\tau_2} \cdots \hat{a}^\dagger_{m_N\tau_N} |\mathrm{vac}\rangle$$

$$\langle\{m_j, \tau_j\}|\{\ell_j, \sigma_j\}\rangle = \begin{cases} 0 & (\{m_j, \tau_j\} \cup \{\ell_j, \sigma_j\} \neq \{\ell_j, \sigma_j\}) \\ 1 & (\{m_j, \tau_j\} \cup \{\ell_j, \sigma_j\} = \{\ell_j, \sigma_j\}) \end{cases}$$

Quantum Many-Body Problem by Linear Algebra

Common important formula
between Hilbert and Fock spaces

Closure by orthonormalized basis

$$1 = \sum_{\mu} |\mu\rangle\langle\mu|$$

$$\langle\mu|\nu\rangle = \delta_{\mu,\nu}$$

$$\begin{aligned}
\left(\sum_{\mu} |\mu\rangle\langle\mu|\right) \times |\Phi\rangle &= \left(\sum_{\mu} |\mu\rangle\langle\mu|\right) \times \sum_{\nu} d_{\nu}|\nu\rangle \\
&= \sum_{\nu} d_{\nu}|\nu\rangle \\
&= |\Phi\rangle
\end{aligned}$$

Quantum Many-Body Problem by Linear Algebra

Schrödinger equation $\hat{H}|\Phi\rangle = E|\Phi\rangle$

Hermitian $\hat{H}^\dagger = \hat{H} \quad H_{\mu\nu} = H^*_{\nu\mu}$

Many-body orthonormalized basis $\langle\mu|\nu\rangle = \delta_{\mu,\nu}$

Closure $1 = \sum_\mu |\mu\rangle\langle\mu|$

$$\langle\mu| \times \hat{H}|\Phi\rangle = \langle\mu| \times E|\Phi\rangle$$

$$\Leftrightarrow \quad \sum_\nu \langle\mu|\hat{H}|\nu\rangle\langle\nu|\Phi\rangle = E\langle\mu|\Phi\rangle$$

Rewritten Schrödinger equation

$$\sum_\nu H_{\mu\nu} d_\nu = E d_\mu$$

$$H_{\mu\nu} = \langle\mu|\hat{H}|\nu\rangle$$

$$|\Phi\rangle = \sum_\mu d_\mu |\mu\rangle$$

Eigenvalue Problems of Large and Sparse Matrices

Sparse Matrix

■ Particle or orbital number: N

■ Fock space dimension: exp[N x const.]

■ # of terms in Hamiltonian: Polynomial of N

→ # of matrix elements of Hamiltonian matrix:
(Polynomial of N) x exp[N x const.]

For sufficiently large N,
(Polynomial of N) x exp[N x const.]
<< (exp[N x const.])^2

Then, the Hamiltonian matrix is sparse

Larger TFIM Revisit

$$\hat{H} = J\sum_{i=0}^{L-1}\hat{S}_i^z\hat{S}_{i+1}^z - \Gamma\sum_{i=0}^{L-1}\hat{S}_i^x$$

-Non-commutative

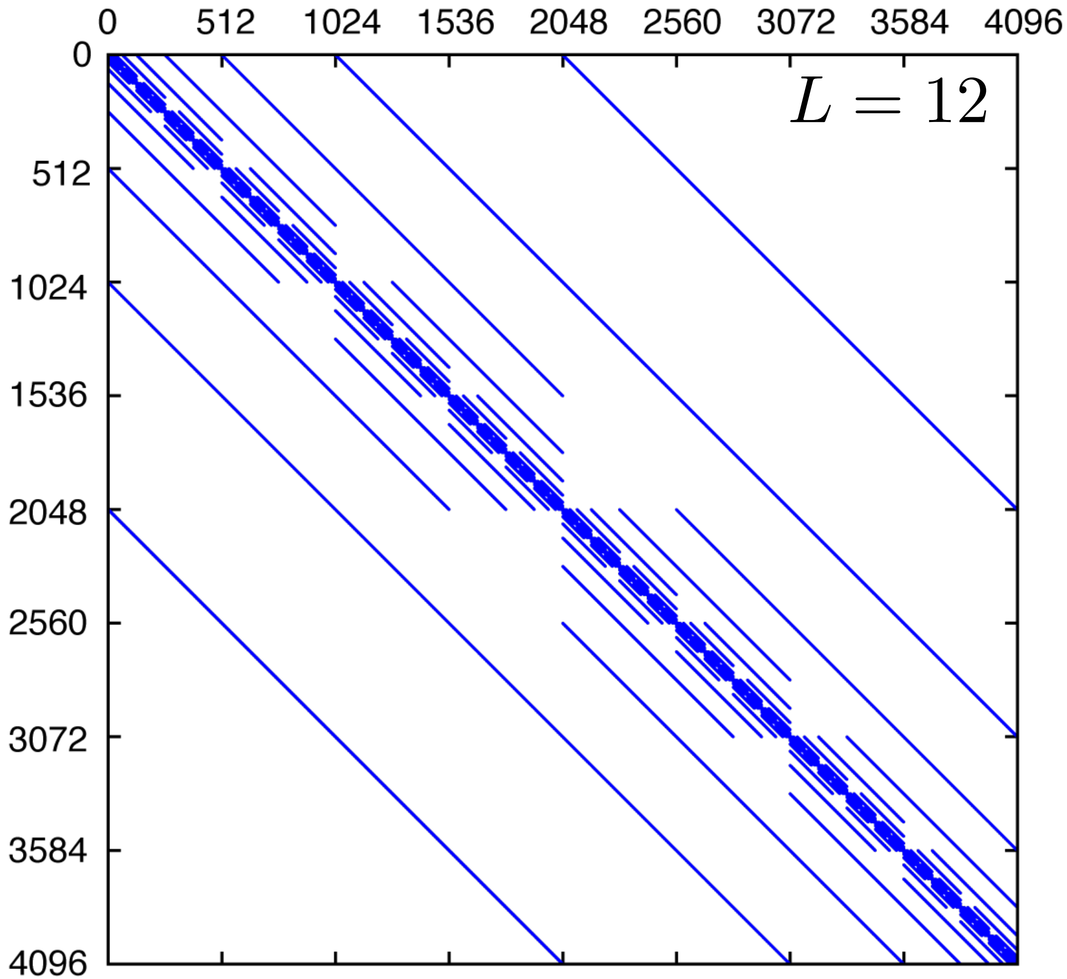
$$\left[\sum_{i=0}^{L-1}\hat{S}_i^z\hat{S}_{i+1}^z, \sum_{i=0}^{L-1}\hat{S}_i^x\right] \neq 0$$

→Quantum fluctuations
or Zero point motion

-Sparse
\# of elements ∝ $O(2^L)$

-Solvable

-Hierarchical matrix?



Computational and Memory Costs

Matrix-vector product of dense matrix

$$v_i = \sum_{j=0}^{N_{\mathrm{H}}-1} A_{ij} u_j$$

Computational: O((Fock space dimension)^2)
Memory: O((Fock space dimension)^2)

Matrix-vector product of large and sparse matrix

Computational: O(Fock space dimension)
Memory: O(Fock space dimension)
Hamiltonian is not stored in memory

Algorithm for Eigenvalue Problems of Large & Sparse Matrix: Power Method

Min. Eigenvalue of hermitian

$$\hat{H}|n\rangle = E_n|n\rangle$$

$$\langle n'|n\rangle = \delta_{n',n}$$

$$E_0 \leq E_1 \leq \cdots$$

Initial vector: $|v_1\rangle = \sum_{n=0} c_n|n\rangle$

Prameter: $\max_n\{E_n\} \leq \Lambda$

$$\lim_{m\to+\infty} \frac{(\Lambda - \hat{H})^m|v_1\rangle}{\sqrt{\langle v_1|(\Lambda - \hat{H})^{2m}|v_1\rangle}} = |0\rangle$$

$$(\Lambda - \hat{H})^m|v_1\rangle = \sum_n (\Lambda - E_n)^m c_n|n\rangle$$

$$\lim_{m\to+\infty} \frac{\sum_{n>0}(\Lambda - E_n)^{2m}|c_n|^2}{(\Lambda - E_0)^{2m}|c_0|^2} = 0$$

Advanced Algorithm: Krylov Subspace Method

Krylov subspace

$$\mathcal{K}_m(\hat{H}, |v_1\rangle) = \mathrm{span}\{|v_1\rangle, \hat{H}|v_1\rangle, \ldots, \hat{H}^{m-1}|v_1\rangle\}$$

Shift invariance:

$$\mathcal{K}_m(\hat{H}, |v_1\rangle) = \mathcal{K}_m(\hat{H} + z\mathbf{1}, |v_1\rangle)$$

Krylov subspace method:
-Lanczos method (symmetric/hermitian),
 Arnoldi method (general matrix)
-Conjugate gradient method (CG method)
 (many variation)

Lanczos Method

$$\textbf{Initial}: \beta_1 = 0,\ |v_0\rangle = 0$$

$$\textbf{for } j = 1, 2, \ldots, m \textbf{ do}$$

$$|w_j\rangle = \hat{H}|v_j\rangle - \beta_j|v_{j-1}\rangle$$

$$\alpha_j = \langle w_j|v_j\rangle$$

$$|w_j\rangle \leftarrow |w_j\rangle - \alpha_j|v_j\rangle$$

$$\beta_{j+1} = \sqrt{\langle w_j|w_j\rangle}$$

$$|v_{j+1}\rangle = |w_j\rangle/\beta_{j+1}$$

Lanczos Method

$$\alpha_j = \langle v_j|\hat{H}|v_j\rangle$$

$$\beta_j = \langle v_{j-1}|\hat{H}|v_j\rangle = \langle v_j|\hat{H}|v_{j-1}\rangle$$ ← Confirm

Orthogonalization

$$|v_j\rangle = \frac{\hat{H}|v_{j-1}\rangle - \sum_{\ell=1}^{j-1}|v_\ell\rangle\langle v_\ell|\hat{H}|v_{j-1}\rangle}{\langle v_j|\hat{H}|v_{j-1}\rangle}$$

$$\langle v_\ell|\hat{H}|v_{j-1}\rangle = \begin{cases} 0 & (\ell \leq j-3) \\ \beta_{j-1} & (\ell = j-2) \\ \alpha_{j-1} & (\ell = j-1) \end{cases}$$ ← Confirm

Lanczos Method

$$\textbf{Initial} : \beta_1 = 0,\ |v_0\rangle = 0$$

$$\textbf{for } j = 1, 2, \ldots, m \textbf{ do}$$

$$\boxed{|w_j\rangle = \hat{H}|v_j\rangle - \beta_j|v_{j-1}\rangle}$$

$$\alpha_j = \langle w_j|v_j\rangle$$

$$|w_j\rangle \leftarrow |w_j\rangle - \alpha_j|v_j\rangle$$

$$\beta_{j+1} = \sqrt{\langle w_j|w_j\rangle}$$

$$|v_{j+1}\rangle = |w_j\rangle/\beta_{j+1}$$

Lanczos Method

$$\alpha_j = \langle v_j | \hat{H} | v_j \rangle$$
$$\langle v_j | v_k \rangle = \delta_{j,k}$$
$$\beta_j = \langle v_{j-1} | \hat{H} | v_j \rangle = \langle v_j | \hat{H} | v_{j-1} \rangle$$

Hamiltonian projected onto *m* D Krylov subsace

$$H_m = \begin{pmatrix} \alpha_1 & \beta_2 & & & & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \beta_m & \alpha_m \end{pmatrix}$$

Eigenvalues of projected Hamiltonian
→ Approximate eigenvalues of original Hamiltonian

Lanczos Method: # of Vectors Required

$$\textbf{Initial}: \beta_1 = 0,\ |v_0\rangle = 0$$

$$\textbf{for } j = 1, 2, \ldots, m \textbf{ do}$$

$\color{blue}{\lvert w_j\rangle} \leftarrow \hat{H}\lvert v_j\rangle - \beta_j \color{blue}{\lvert v_{j-1}\rangle}$	$\lvert v_{j-1}\rangle \rightarrow \lvert w_j\rangle,\ \lvert v_j\rangle$
$\alpha_j = \langle w_j \vert v_j\rangle$	$\lvert w_j\rangle,\ \lvert v_j\rangle$
$\lvert w_j\rangle \leftarrow \lvert w_j\rangle - \alpha_j \lvert v_j\rangle$	$\lvert w_j\rangle,\ \lvert v_j\rangle$
$\beta_{j+1} = \sqrt{\langle w_j \vert w_j\rangle}$	$\lvert w_j\rangle,\ \lvert v_j\rangle$
$\lvert v_{j+1}\rangle = \lvert w_j\rangle / \beta_{j+1}$	$\lvert w_j\rangle \rightarrow \lvert v_{j+1}\rangle,\ \lvert v_j\rangle$

Convergence of Lanczos Method

Yousef Saad,
Numerical Methods for Large Eigenvalue Problems (2nd ed)
The Society for Industrial and Applied Mathematics 2011

Assumption: $\lambda_1 > \lambda_2 > \cdots > \lambda_n$

Convergence theorem for the largest eigenvalue

$$0 \leq \lambda_1 - \lambda_1^{(m)} \leq (\lambda_1 - \lambda_n) \left[\frac{\tan\theta(|v_1\rangle, |0\rangle)}{C_{m-1}(1 + 2\gamma_1)} \right]^2$$

$$\sim 4(\lambda_1 - \lambda_n) \left[\tan\theta(|v_1\rangle, |0\rangle)\right]^2 e^{-4\sqrt{\gamma_1}m}$$

$$\gamma_1 = \frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_n}$$

$$C_k(t) = \frac{1}{2}\left[\left(t + \sqrt{t^2 - 1}\right)^k + \left(t + \sqrt{t^2 - 1}\right)^{-k}\right]$$

Example of Distribution of Eigenvalues: Random Symmetric Matrices

Eugene P. Wigner, Annals of Mathematics, 2nd Series, 67, 325 (1958)

Wigner's random matrix $(A)_{ij} = a_{ij}$

$$a_{ij} = a_{ji}$$

(Not necessarily sparse)

$$\int p_{ij}(a)da = 1$$

$$p_{ij}(+a) = p_{ij}(-a)$$

$$\langle a_{ij}^n \rangle = \int p_{ij}(a)a^n da \leq B_n$$

$$\langle a_{ij}^2 \rangle = \int p_{ij}(a)a^2 da = 1$$

Example of Distribution of Eigenvalues: Random Symmetric Matrices

Eugene P. Wigner, Annals of Mathematics, 2nd Series, 67, 325 (1958)

Density of states of N_H x N_H symmetric random matirx

$$A\vec{v} = E\vec{v}$$

$$\sigma(E) = \begin{cases} \dfrac{\sqrt{4N_\mathrm{H} - E^2}}{2\pi N_\mathrm{H}} & (E^2 < 4N_\mathrm{H}) \\ 0 & (E^2 > 4N_\mathrm{H}) \end{cases}$$

Comment:
Sparse matrices in quantum many-body problems show smaller density of states than random matrices
→ Sparse around maximum/minimum eigenvalues
→ Lanczos method may work well

Report Problem

2nd report: Problem 1-1. (compulsory)

Derive the following relation in detail.
If it is too difficult, please assume *M*=4.

$$
\begin{aligned}
\mathrm{Tr} e^{-\beta \hat{H}[\hat{c}^\dagger, \hat{c}]} &= \mathrm{Tr}\left(e^{-\frac{\beta}{M}\hat{H}[\hat{c}^\dagger,\hat{c}]}\right)^M \\
&\simeq \int \langle -\overline{\psi}(1)| e^{-\frac{\beta}{M}\hat{H}[-\overline{\psi}(1),\psi(M)]} |\psi(M)\rangle e^{-\overline{\psi}(M)\psi(M)} \\
&\quad \times \langle \overline{\psi}(M)| e^{-\frac{\beta}{M}\hat{H}[\overline{\psi}(M),\psi(M-1)]} |\psi(M-1)\rangle e^{-\overline{\psi}(M-1)\psi(M-1)} \\
&\quad \times \cdots \\
&\quad \times \langle \overline{\psi}(2)| e^{-\frac{\beta}{M}\hat{H}[\overline{\psi}(2),\psi(1)]} |\psi(1)\rangle e^{-\overline{\psi}(1)\psi(1)} \prod_{\ell=1}^{M} d\overline{\psi}(\ell) d\psi(\ell)
\end{aligned}
$$

Report Problem

2nd report: Problem 1-2. (compulsory)

Evaluate the right-hand side of the following equation for arbitrary L.
If it is too difficult, please assume M=4.

$$\langle \hat{c}_{i\sigma}(L)\hat{c}^{\dagger}_{j\tau}(L)\rangle = \frac{\int \psi_{i\sigma}(L)\overline{\psi}_{j\tau}(L)e^{-S[\overline{\psi},\psi]}\left[d\overline{\psi}d\psi\right]}{\int e^{-S[\overline{\psi},\psi]}\left[d\overline{\psi}d\psi\right]}$$

$$S[\overline{\psi},\psi] = \sum_{L=1}^{M}\overline{\psi}(L)I\psi(L) + \overline{\psi}(1)B_1\psi(M) - \sum_{L=2}^{M}\overline{\psi}(L)B_L\psi(L-1)$$

$$\hat{c}_{i\sigma}(L) = e^{+L\frac{\beta}{M}\hat{H}}\hat{c}_{i\sigma}e^{-L\frac{\beta}{M}\hat{H}}$$

$$\int e^{-S[\overline{\psi},\psi]}\left[d\overline{\psi}d\psi\right] = \det\left[I + B_M\cdots B_1\right]$$

Report Problem

2nd report: Problem 2-1. (compulsory)

In the Lanczos algorithm, there are many implicit relationship between identities.
Please prove the following relation:

$$\beta_{j+1} = \sqrt{\langle w_j | w_j \rangle} = \langle v_{j-1} | \hat{H} | v_j \rangle$$

2nd report: Problem 2-2. (optional)

In the Lanczos algorithm, hermitian property of the Hamiltonian matrix is crucial to obtain the tridiagonalized matrix.
Please discuss what will happened if your target matrix is not hermitian, especially by paying attention to memory cost.

-Deadline: 7/31
-Submission by email or ITC-LMS