多体問題の計算科学

#12

2017/7/4

Computational Science for Many-Body Problems

Numerical Methods for Quantum Many-Body Problems

1. Excitation spectrum
2. Conjugate gradient method 1
3. Typicality approach
4. Introduction to HΦ

Excitation Spectrum

An Example: Dynamical Spin Structure Factor

$$S(\vec{Q},\omega) = \sum_{\alpha=x,y,z}\sum_{m} |\langle m|\hat{S}^{\alpha}_{+\vec{Q}}|0\rangle|^2 \delta(\omega - E_m + E_0)$$

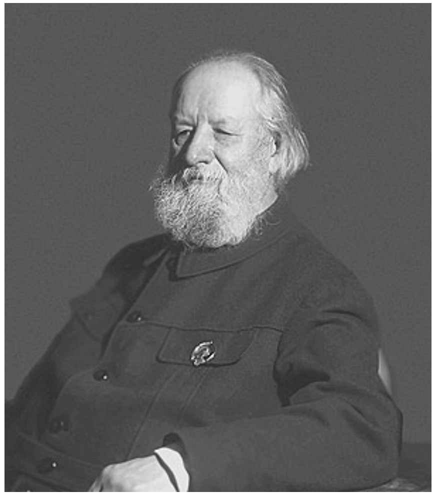
$$\hat{S}^{\alpha}_{\vec{Q}} = \frac{1}{N}\sum_{j=0}^{N-1} \hat{S}^{\alpha}_{j} e^{+i\vec{Q}\cdot\vec{r}_j}$$

Fermi's golden rule gives probability of transition (per unit time) from the ground state to excited states with energy $\omega = E_m - E_0$

Representation by using Green's function

$$\begin{aligned} S(\vec{Q},\omega) &= -\lim_{\delta\to 0+}\frac{1}{\pi}\mathrm{Im}\sum_{\alpha=x,y,z}\sum_{m}\frac{\langle 0|\hat{S}^{\alpha}_{-\vec{Q}}|m\rangle\langle m|\hat{S}^{\alpha}_{+\vec{Q}}|0\rangle}{\omega + i\delta - E_m + E_0} \\ &= -\lim_{\delta\to 0+}\frac{1}{\pi}\mathrm{Im}\sum_{\alpha=x,y,z}\sum_{m}\langle 0|\hat{S}^{\alpha}_{-\vec{Q}}\frac{1}{\omega + i\delta - \hat{H} + E_0}\hat{S}^{\alpha}_{+\vec{Q}}|0\rangle \end{aligned}$$

Krylov Subspace Method



Alexey Krylov
Aleksey Nikolaevich Krylov
1863-1945
Russian naval engineer and applied mathematician

Krylov subspace

$$\mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle) = \mathrm{span}\{|\rho\rangle, (\zeta - \hat{H})|\rho\rangle, \ldots, (\zeta - \hat{H})^{n-1}|\rho\rangle\}$$

Shift invariance

$$\mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle) = \mathcal{K}_n(\zeta' - \hat{H}, |\rho\rangle)$$

Green's Function by Solving Linear Equations

Green's function $G^{AB}(\zeta) = \langle 0|\hat{A}^\dagger(\zeta - \hat{H})^{-1}\hat{B}|0\rangle$

-Lanczos/Arnoldi methods

$$|\lambda\rangle = \hat{A}|0\rangle$$
$$|\rho\rangle = \hat{B}|0\rangle$$
$$|\chi(\zeta)\rangle = (\zeta - \hat{H})^{-1}|\rho\rangle$$

$$\rightarrow G^{AB}(\zeta) = \langle\lambda|\chi(\zeta)\rangle$$

→ Linear equations $(\zeta - \hat{H})|\chi(\zeta)\rangle = |\rho\rangle$

-CG-type methods, $\cdots$

Green's Function by Krylov Subspace Method

Searching solutions in Krylov subspaces

$$\mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle) = \mathrm{span}\{|\rho\rangle, (\zeta - \hat{H})|\rho\rangle, \ldots, (\zeta - \hat{H})^{n-1}|\rho\rangle\}$$

-Lanczos/Arnoldi methods, CG-type methods, $\cdots$

Initial: $|\chi_0(\zeta)\rangle = |\rho\rangle$

For n=1, 2, ..., m

$$\text{Find } |\chi_n(\zeta)\rangle \text{ in } \mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle)$$

$$|\rho_n(\zeta)\rangle = (\zeta - \hat{H})|\chi_n(\zeta)\rangle - |\rho\rangle$$

CG-type method

A. Frommer, Computing 70, 87 (2003).

Collinear residuals $|\rho_n(\zeta)\rangle \propto |\rho_n(\zeta')\rangle$

$$\mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle) = \mathcal{K}_n(\zeta' - \hat{H}, |\rho\rangle)$$

$\rightarrow$ Seed switch

S. Yamamoto, T. Sogabe, T. Hoshi, S.-L. Zhang, & T. Fujiwara, J. Phys. Soc. Jpn. 77, 114713 (2008).

Library Kω (released) by Dr. Kawamura (ISSP)

Conjugate Gradient Method

Linear Equations

Algorithm for linear equations
instead of eigenvalue problems

$$A\vec{x} = \vec{b}$$

A simple method: Gradient descent/steepest descent

Solving a linear equation is mapped onto
finding a minimum of a cost cuntion

For symmetric matrix A

$$f(\vec{x}) = \frac{1}{2}\vec{x}^T A\vec{x} - \vec{b}^T\vec{x}$$

$$\vec{\nabla}_x f(\vec{x}) = A\vec{x} - \vec{b}$$

$$\boxed{\vec{x}_{k+1} = \vec{x}_k - \alpha\vec{\nabla}_x f(\vec{x})|_{\vec{x}=\vec{x}_k}}$$

-Only local information is utilized,
and thus often captured by local minima

Conjugate Gradient Method

M. R. Hestenes & E. Stiefel, J. Res. Natl. Bur. Stand. 49, 409 (1952).

Find an approximate solution in a Krylov subspace

$$\vec{x}_k = \sum_{j=0}^{k-1} a_j \vec{p}_j$$

Conjugate basis set $\{\vec{p}_k\}$ $\quad \vec{p}_i^T A \vec{p}_j = 0 \ (i \neq j)$

Additional constraint: Find orthogonal residual vectors

$$\vec{r}_k = \vec{b} - A\vec{x}_k$$

Orthogonal basis set $\{\vec{r}_k\}$ $\quad \vec{r}_i^T \vec{r}_j = 0 \ (i \neq j)$

Conjugate Gradient Method: Algorithm

Linear equations $A\vec{x} = \vec{b}$

For symmetric matrix A

$$
\begin{aligned}
&\vec{p}_0 = \vec{r}_0 = \vec{b} - A\vec{x}_0 \\
&\text{For } k = 0, 1, \ldots, m \\
&\qquad \alpha_k = \frac{\vec{r}_k^T \vec{r}_k}{\vec{p}_k^T A \vec{p}_k} \\
&\qquad \vec{x}_{k+1} = \vec{x}_k + \alpha_k \vec{p}_k \\
&\qquad \vec{r}_{k+1} = \vec{r}_k - \alpha_k A \vec{p}_k \\
&\qquad \beta_k = \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k} \\
&\qquad \vec{p}_{k+1} = \vec{r}_{k+1} + \beta_k \vec{p}_k
\end{aligned}
$$

M. R. Hestenes & E. Stiefel,
J. Res. Natl. Bur. Stand. 49, 409 (1952).

The algorithm generates
-Conjugate basis set $\{\vec{p}_k\}$
-Orthogonal basis set $\{\vec{r}_k\}$

←A Krylov subspace

CG method finds an approximate solution
of the linear equation in a Krylov subspace

Sketch of Proof for CG Method 0.

Induction

Assume $\{\vec{r}_0, \vec{r}_1, \ldots, \vec{r}_k\}$ is orthogonal basis set

$$\vec{r}_i^T \vec{r}_j = 0 \quad (i \neq j, i \leq k, j \leq k)$$

Assume $\{\vec{p}_0, \vec{p}_1, \ldots, \vec{p}_k\}$ is conjugate basis set

$$\vec{p}_i^T A \vec{p}_j = 0 \quad (i \neq j, i \leq k, j \leq k)$$

Prove $\vec{r}_{k+1}$ satisfies $\quad \vec{r}_j^T \vec{r}_{k+1} = 0 \quad (j \leq k)$

Prove $\vec{p}_{k+1}$ satisfies $\quad \vec{p}_j^T A \vec{p}_{k+1} = 0 \quad (j \leq k)$

M. R. Hestenes & E. Stiefel, J. Res. Natl. Bur. Stand. 49, 409 (1952).

Sketch of Proof for CG Method 1.

Ansatz

$$\vec{x}_{k+1} = \vec{x}_k + \alpha_k \vec{p}_k$$

$$\begin{aligned} \to \vec{r}_{k+1} &= \vec{b} - A\vec{x}_{k+1} \\ &= \vec{r}_k - \alpha_k A\vec{p}_k \end{aligned}$$

Requirement

$$\vec{r}_k^T \vec{r}_{k+1} = 0$$

$$\to \vec{r}_k^T \vec{r}_{k+1} = \vec{r}_k^T \vec{r}_k - \vec{r}_k^T \alpha_k A\vec{x}_{k+1} = 0$$

$$\to \alpha_k = \frac{\vec{r}_k^T \vec{r}_k}{\vec{r}_k^T A\vec{p}_k}$$

$$\begin{cases} \vec{p}_k = \vec{r}_k + \beta_{k-1}\vec{p}_{k-1} \\ \vec{p}_{k-1}^T A\vec{p}_k = 0 \end{cases}$$ ←assumption

$$\to \alpha_k = \frac{\vec{r}_k^T \vec{r}_k}{\vec{r}_k^T A\vec{p}_k} = \frac{\vec{r}_k^T \vec{r}_k}{\vec{p}_k^T A\vec{p}_k}$$

$$\begin{aligned} \vec{r}_j^T \vec{r}_{k+1} &= \vec{r}_j^T \vec{r}_{k+1} - \alpha_k \vec{r}_j^T A\vec{p}_{k+1} \\ &= -\alpha_k \vec{p}_j^T A\vec{p}_{k+1} && (\vec{p}_j = \vec{r}_j + \beta_{j-1}\vec{p}_{j-1},\ \vec{r}_j^T \vec{r}_{k+1} = 0) \\ &= 0 && (j < k) \end{aligned}$$

Sketch of Proof for CG Method 2.

Ansatz & Requirement

$$\begin{cases} \vec{p}_{k+1} = \vec{r}_{k+1} + \beta_k \vec{p}_k \\ (\vec{p}_k^T A)\vec{p}_{k+1} = 0 \end{cases}$$

$$\rightarrow (\vec{p}_k^T A)\vec{p}_{k+1} = (\vec{p}_k^T A)\vec{r}_{k+1} + \beta_k (\vec{p}_k^T A)\vec{p}_k = 0$$

$$\rightarrow \beta_k = -\frac{\vec{p}_k^T A \vec{r}_{k+1}}{\vec{p}_k^T A \vec{p}_k}$$

$$\vec{r}_{k+1} = \vec{r}_k - \alpha_k A \vec{p}_k$$

$$\rightarrow A\vec{p}_k = \frac{\vec{r}_k - \vec{r}_{k+1}}{\alpha_k}$$

$$\beta_k = -\frac{\vec{p}_k^T A \vec{r}_{k+1}}{\vec{p}_k^T A \vec{p}_k} = -\frac{(\vec{r}_k - \vec{r}_{k+1})^T \vec{r}_{k+1}}{\alpha_k \vec{p}_k^T A \vec{p}_k}$$

$$= \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\frac{\vec{r}_k^T \vec{r}_k}{\vec{p}_k^T A \vec{p}_k} \vec{p}_k^T A \vec{p}_k} = \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k}$$

$$\boxed{\vec{p}_j^T A \vec{p}_{k+1} = 0 \quad (j < k)}$$

Variation of CG Method

Variation of CG method:
-A : symmetric → Conjugate Gradient
-A : hermitian → Conjugate Gradient (T → †)
-A+σ1: symmetric A and complex σ
→ Conjugate Orthogonal Conjugate Gradient (COCG)
-A+σ1: hermitian A and complex σ
→ Bi-Conjugate Gradient (BiCG)

An important application:
-Calculation of eigenvectors after the Lanczos method

Inverse iteration: $(\hat{H} - E_m)\vec{v}_{k+1} = \vec{v}_k$

$$\vec{v}_k \to |m\rangle$$

Preparation for Shifted Krylov Subspace Method

Collinear Residual

A. Frommer, Computing 70, 87 (2003).

$$A\vec{x} = \vec{b}$$
$$\vec{r}_0 = \vec{b} \text{ if } \vec{x}_0 = \vec{0}$$

$$(A + \sigma \mathbf{1})\vec{x}^\sigma = \vec{b}$$
$$\vec{r}_0^\sigma = \vec{b} \text{ if } \vec{x}_0^\sigma = \vec{0}$$

Shift invariance of Krylov subspace

$$\mathrm{span}\{\vec{r}_0, \vec{r}_1, \ldots, \vec{r}_k\} = \mathrm{span}\{\vec{r}_0^\sigma, \vec{r}_1^\sigma, \ldots, \vec{r}_k^\sigma\}$$

CG-type methods find a new residual vector

$$\vec{r}_{k+1} \perp \mathrm{span}\{\vec{r}_0, \vec{r}_1, \ldots, \vec{r}_k\} \qquad \vec{r}_{k+1}^\sigma \perp \mathrm{span}\{\vec{r}_0^\sigma, \vec{r}_1^\sigma, \ldots, \vec{r}_k^\sigma\}$$

Shift invariance of Krylov subspace

$$\mathrm{span}\{\vec{r}_0, \vec{r}_1, \ldots, \vec{r}_k, \vec{r}_{k+1}\} = \mathrm{span}\{\vec{r}_0^\sigma, \vec{r}_1^\sigma, \ldots, \vec{r}_k^\sigma, \vec{r}_{k+1}^\sigma\}$$

$$\vec{r}_{k+1} \propto \vec{r}_{k+1}^\sigma$$

Details of Collinear Residual 1.

Coefficient

A. Frommer, Computing 70, 87 (2003).

$$\vec{r}_k^\sigma = (1/\pi_k^\sigma)\vec{r}_k$$

$$\vec{x}_k = q_{k-1}(A)\vec{b}$$
$$\vec{r}_k = p_k(A)\vec{b} \ \left(= \vec{b} - Aq_{k-1}(A)\vec{b} = \vec{b} - A\vec{x}_k\right)$$

$$p_k(t) = 1 - tq_{k-1}(t)$$

$$q_{k-1}(t) = \sum_{m=0}^{k-1} d_m t^m$$

CG-type method

$$\vec{r}_k^\sigma = p_k^\sigma(A + \sigma\mathbf{1})\vec{b}$$
$$p_k^\sigma(A + \sigma\mathbf{1})\vec{b} = (1/\pi_k^\sigma)p_k(A)\vec{b}$$
$$\rightarrow p_k^\sigma(t + \sigma) = (1/\pi_k^\sigma)p_k(t)$$

$$\pi_k^\sigma = p_k(-\sigma) \quad (\text{since } p_k^\sigma(0) = 1)$$

Details of Collinear Residual 2.

A. Frommer, Computing 70, 87 (2003).

Recurrence formula for residual vectors

$$\vec{p}_{k-1} = \frac{1}{\beta_k}(\vec{r}_k - \vec{p}_k), \quad A\vec{p}_k = \frac{1}{\alpha_k}(\vec{r}_k - \vec{r}_{k+1})$$

$$\begin{aligned}
\to \vec{r}_k &= \vec{r}_{k-1} - \alpha_{k-1} A\vec{p}_{k-1} = \vec{r}_{k-1} - \frac{\alpha_{k-1}}{\beta_k} A(\vec{r}_k - \vec{p}_k) \\
&= \vec{r}_{k-1} - \frac{\alpha_{k-1}}{\beta_k} A\vec{r}_k + \frac{\alpha_{k-1}}{\alpha_k \beta_k}(\vec{r}_k - \vec{r}_{k+1})
\end{aligned}$$

$$\to \vec{r}_{k+1} = -\alpha_k A\vec{r}_k + \left(1 - \frac{\alpha_k \beta_k}{\alpha_{k-1}}\right)\vec{r}_k + \frac{\alpha_k \beta_k}{\alpha_{k-1}}\vec{r}_{k-1}$$

$$\to p_{k+1}(t) = -\alpha_k t \cdot p_k(t) + \left(1 - \frac{\alpha_k \beta_k}{\alpha_{k-1}}\right) p_k(t) + \frac{\alpha_k \beta_k}{\alpha_{k-1}} p_{k-1}(t)$$

$$\to \pi^\sigma_{k+1} = \left(1 + \alpha_k \sigma - \frac{\alpha_k \beta_k}{\alpha_{k-1}}\right)\pi^\sigma_k + \frac{\alpha_k \beta_k}{\alpha_{k-1}}\pi^\sigma_{k-1}$$

Typicality Approach

Typicality Approach: Numerical Background

Canonical ensemble average

$$\langle \hat{O} \rangle_{\beta}^{\mathrm{ens}} = \sum_n \frac{e^{-\beta E_n}}{Z(\beta)} \langle n | \hat{O} | n \rangle$$

Complexity	$\mathcal{O}(N_{\mathrm{H}}^3)$
Memory	$\mathcal{O}(N_{\mathrm{H}}^2)$

Is it necessary? Answer is No

M. Imada and M. Takahashi, J. Phys. Soc. Jpn. 55, 3354 (1986).
J. Skilling, Maximum entropy and bayesian methods: Cambridge, England, 1988,"
(Springer Science & Business Media, 2013) p. 455.
P. de Vries and H. De Raedt, Phys. Rev. B 47, 7929 (1993).
J. Jaklic and P. Prelovsek, Phys. Rev. B 49, 5065 (1994).
A. Hams and H. De Raedt, Phys. Rev. E 62, 4365 (2000).

Typicality Approach: Numerical Background

M. Imada and M. Takahashi, J. Phys. Soc. Jpn. 55, 3354 (1986).

Random wave function

$$|\phi_0\rangle = \sum_x c_x |x\rangle$$

$$\sum_x |c_x|^2 = 1$$

$$|x\rangle = |\sigma_0 \sigma_1 \cdots \sigma_{N-1}\rangle$$

Infinite-temperature result

$$\mathbb{E}[\langle\phi_0|\hat{O}|\phi_0\rangle] = N_{\mathrm{H}}^{-1} \sum_n \langle n|\hat{O}|n\rangle = \langle\hat{O}\rangle_{\beta=0}^{\mathrm{ens}}$$

$$\mathbb{E}[|c_x|^2] = N_{\mathrm{H}}^{-1}$$

$$|n\rangle = \sum_x U_{xn} |x\rangle$$

Complexity

Memory

$$\mathcal{O}(N_{\mathrm{H}})$$

Typicality Approach: Numerical Background

A. Hams and H. De Raedt, Phys. Rev. E 62, 4365 (2000).

$$\mathrm{Tr}\ \hat{O} = \sum_n \langle n|\hat{O}|n\rangle$$

Standard deviation

$$\mathbb{E}[\delta\hat{O}^\dagger\delta\hat{O}] = \frac{N_{\mathrm{H}}^{-1}\mathrm{Tr}[\hat{O}^\dagger\hat{O}] - N_{\mathrm{H}}^{-2}|\mathrm{Tr}\ \hat{O}|^2}{N_{\mathrm{H}}+1}$$

$$\delta\hat{O} = \langle\psi_0|\hat{O}|\psi_0\rangle - \langle\hat{O}\rangle^{\mathrm{ens}}_{\beta=0}$$

A. Sugita, Nonl. Phen. Compl. Sys. 10, 192 (2007).
P. Reimann, Phys. Rev. Lett. 99, 160404 (2007).

N. Ullah, Nucl. Phys. 58, 65 (1964).
-Uniform distribution on unit sphere in $\mathbb{R}^{2N_{\mathrm{H}}}$

$$\mathbb{E}[|c_x|^{2n}] = \frac{\Gamma(N_{\mathrm{H}})\Gamma(n+1)}{\Gamma(N_{\mathrm{H}}+n)}$$

Example 1: Energy at infinite temperature

$$N_{\mathrm{H}}^{-1}\mathrm{Tr}[\hat{H}^2] - N_{\mathrm{H}}^{-2}\mathrm{Tr}[\hat{H}]^2 \propto N$$

Example 2: Partition function

$$Z(\beta) = N_{\mathrm{H}}\mathbb{E}[\langle\phi_0|e^{-\beta\hat{H}}|\phi_0\rangle] \qquad \hat{O} = e^{-\beta\hat{H}}$$

$$\frac{\mathbb{E}\left[\left(N_{\mathrm{H}}\langle\phi_0|e^{-\beta\hat{H}}|\phi_0\rangle - Z(\beta)\right)^2\right]}{Z(\beta)^2} < e^{-S(\beta^*)}$$

$$\beta < \exists\beta^* < 2\beta,$$
$$e^{-S(\beta^*)} = e^{-2\beta[F(2\beta)-F(\beta)]}$$

Typicality Approach

Finite-temperature pure state

$$|\phi_\beta\rangle = e^{-\beta \hat{H}/2}|\phi_0\rangle$$

$$\langle \hat{O} \rangle_\beta^{\mathrm{ens}} = \frac{\mathbb{E}[\langle \phi_\beta | \hat{O} | \phi_\beta \rangle]}{\mathbb{E}[\langle \phi_\beta | \phi_\beta \rangle]}$$

M. Imada and M. Takahashi, J. Phys. Soc. Jpn. 55, 3354 (1986).
P. de Vries and H. De Raedt, Phys. Rev. B 47, 7929 (1993).
A. Hams and H. De Raedt, Phys. Rev. E 62, 4365 (2000).

S. Sugiura and A. Shimizu, Phys. Rev. Lett. 111, 010401 (2013).

$$\sigma_O^2 = \mathbb{E}\left[\left(\frac{\langle \phi_\beta |\, \hat{O} \,| \phi_\beta \rangle}{\langle \phi_\beta | \phi_\beta \rangle} - \langle \hat{O} \rangle_\beta^{\mathrm{ens}}\right)^2\right]$$

$$\sigma_O^2 \leq \frac{\langle (\Delta O)^2 \rangle_{2\beta}^{\mathrm{ens}} + (\langle O \rangle_{2\beta}^{\mathrm{ens}} - \langle O \rangle_\beta^{\mathrm{ens}})^2}{\exp[2\beta\{F(2\beta) - F(\beta)\}]}$$

Combination of Shifted Krylov Method and Typicality Approach

An Alternative to Spectral Projection

T. Kato, Progress of Theoretical Physics 4, 514 (1949).

$$\hat{P}_{\gamma,\rho} = \frac{1}{2\pi i}\oint_{C_{\gamma,\rho}} \frac{dz}{z - \hat{H}} \qquad z = \rho e^{i\theta} + \gamma$$

$$|\phi\rangle = \sum_n d_n |n\rangle$$

$$\hat{P}_{\gamma,\rho}|\phi\rangle = \sum_{E_n \in (\gamma-\rho,\gamma+\rho)} d_n |n\rangle$$

Discretized by Riemann sum

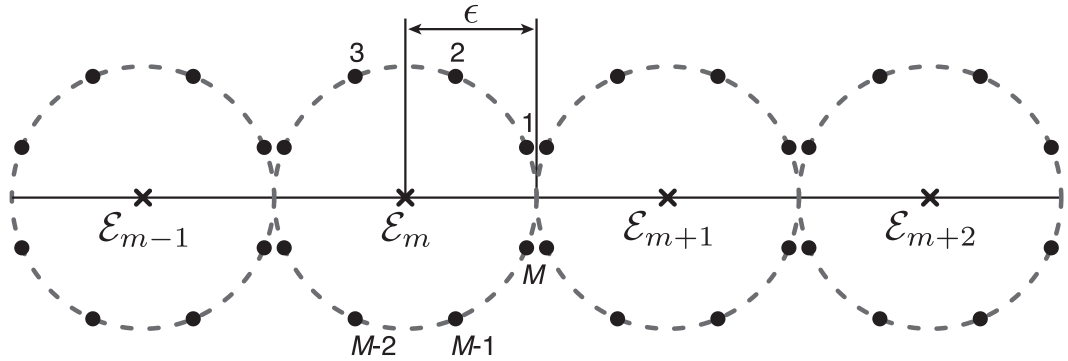
T. Sakurai and H. Sugiura,
J. Comput. Appl. Math. 159, 119 (2003).
T. Ikegami, T. Sakurai, and U. Nagashima,
J. Comput. Appl. Math. 233, 1927 (2010).

$$\hat{P}_{\gamma,\rho,M} = \frac{1}{M}\sum_{j=1}^{M} \frac{\rho e^{i\theta_j}}{\rho e^{i\theta_j} + \gamma - \hat{H}} \qquad \theta_j = 2\pi(j - 1/2)/M$$

Probability Distribution by Typical Pure States

$$|\phi^m_{\beta,\boldsymbol{\delta}}\rangle = \hat{P}_{\mathcal{E}_m,\epsilon,M}|\phi_\beta\rangle$$

$$\boldsymbol{\delta} = (E_0, \epsilon, M)$$



$$\mathcal{E}_m = E_0 + (2m-1)\epsilon$$

N. Shimizu, Y. Utsuno, Y. Futamura, T. Sakurai,T. Mizusaki, and T. Otsuka, Physics Letters B 753, 13 (2016).

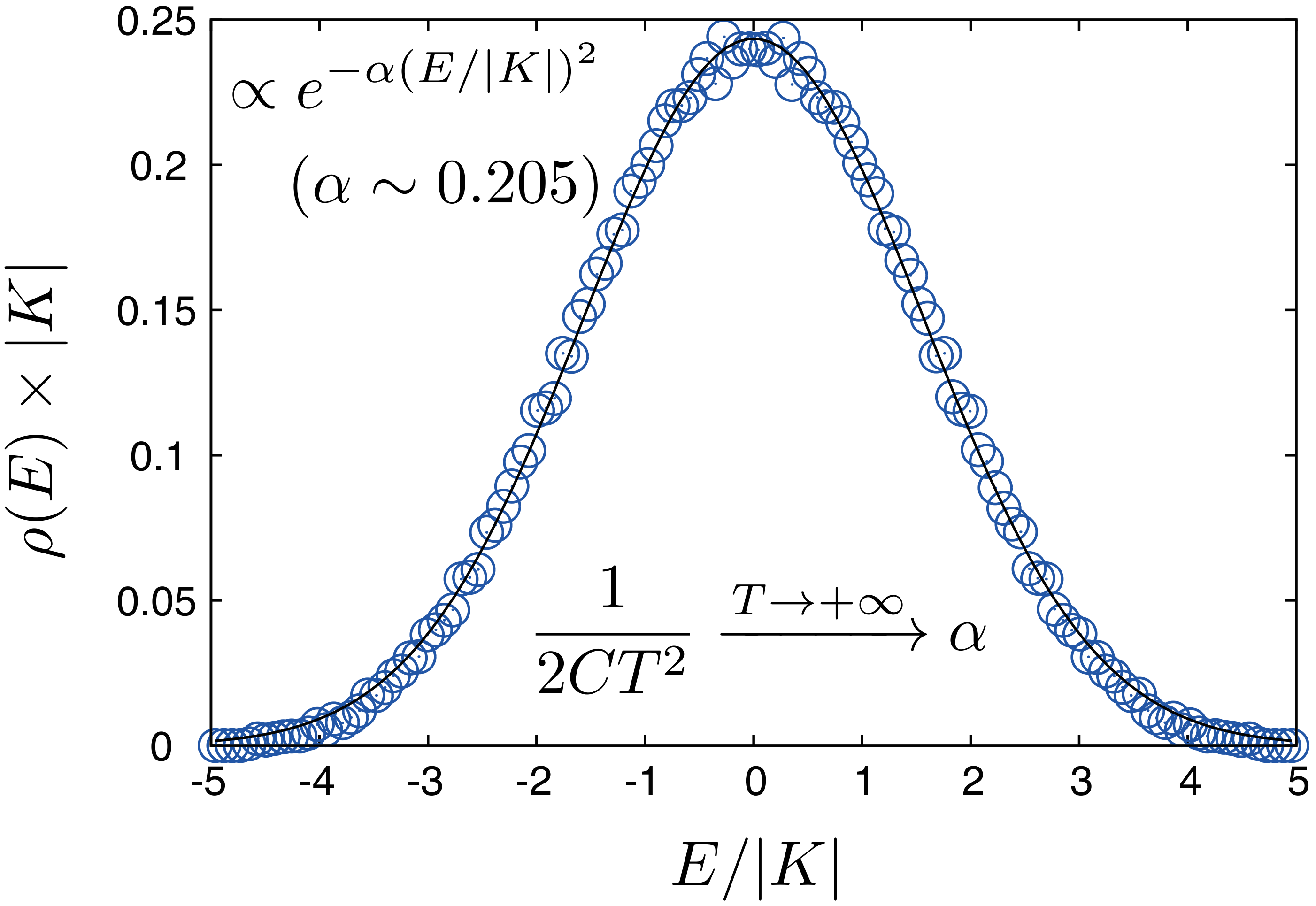
Probability distribution $\widetilde{P}_{\boldsymbol{\delta}}(\mathcal{E}_m) = \langle\phi^m_{\beta,\boldsymbol{\delta}}|\phi^m_{\beta,\boldsymbol{\delta}}\rangle$

An Example of Density of State

24 site cluster of Kitaev model
(frustrated S =1/2 spins)

A. Kitaev, Annals Phys. 321, 2 (2006).

2^{24} = 16,777,216



Introduction of HΦ

(Please visit MateriApps)

HΦ

For direct comparison between experiments and theory and promoting development of other numerical solvers

Numerical diagonalization package for lattice hamiltonian

-For wide range of quantum lattice hamiltonians

  Ab initio effective hamiltonians

-Lanczos method [1]:

  Ground state and low-lying excited states

  Excitation spectra of ground state

-Thermal pure quantum (TPQ) state [2]: Finite temperatures

-Parallelization with MPI and OpenMP

[1] E. Dagotto, Rev. Mod. Phys. 66, 763 (1994) .
[2] S. Sugiura, A. Shimizu, Phys. Rev. Lett. 108, 240401 (2012).

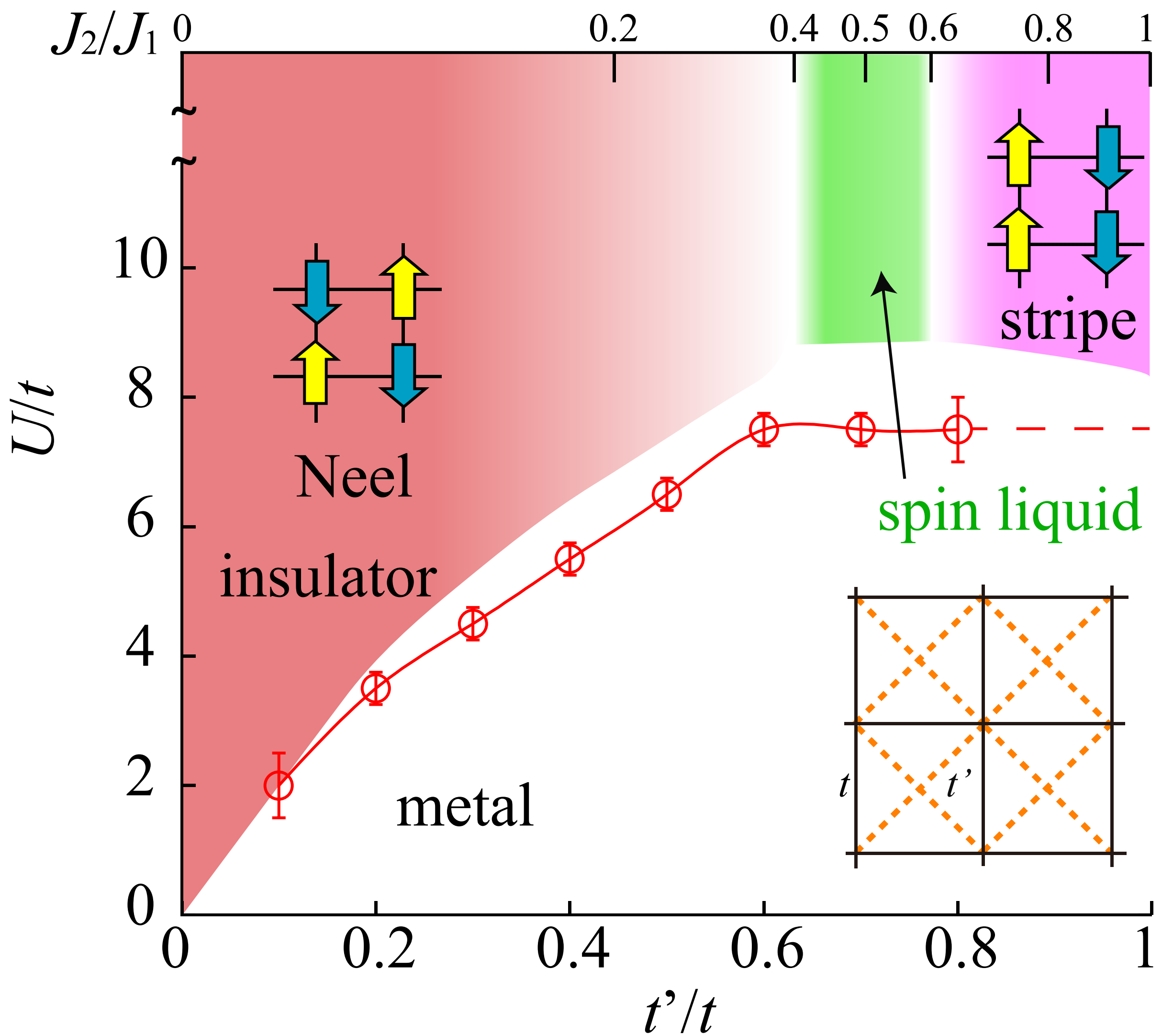
Open source program package (latest release: ver.2.0.0)

Licence: GNU GPL version3

Project for advancement of software usability in materials science" by ISSP

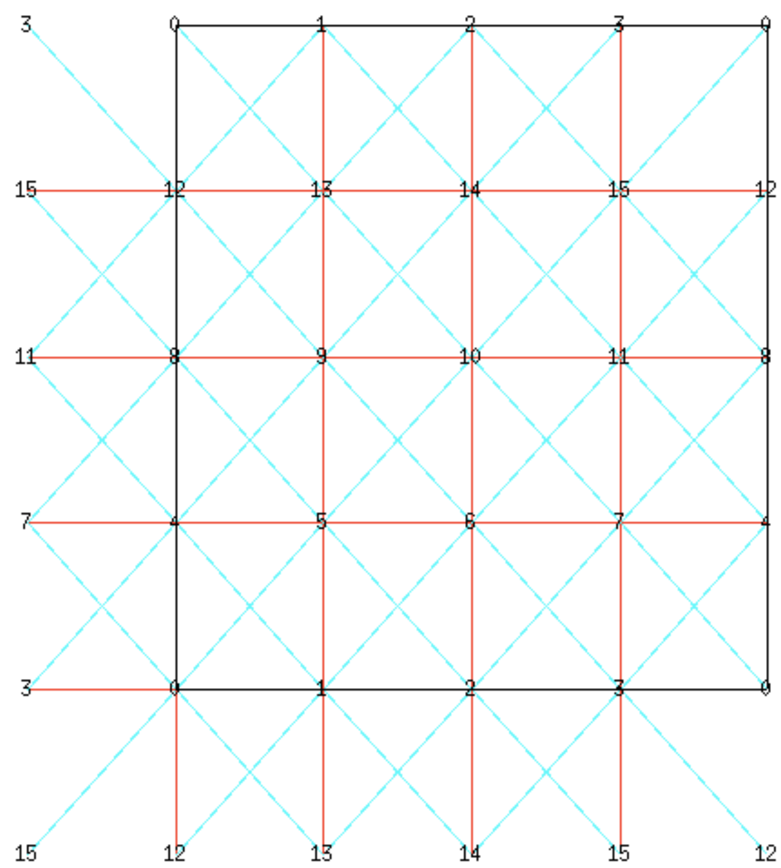
An Example: *t-t'* Hubbard

T. Misawa & Y. Yamaji, arXiv:1608.09006



“Standard” Input

```
W = 4
L = 4
model = "Hubbard"
//method = "Lanczos”
method = "TPQ"
//method = "FullDiag"
lattice = "Square"
t = 1.0
t' = 0.5
U = 8.0
nelec = 16
2Sz = 0
```



Output

Ground-state/finite-temperature
-Energy
-Square of energy
-One-body equal time Green's function
-Two-body equal time Green's/correlation function

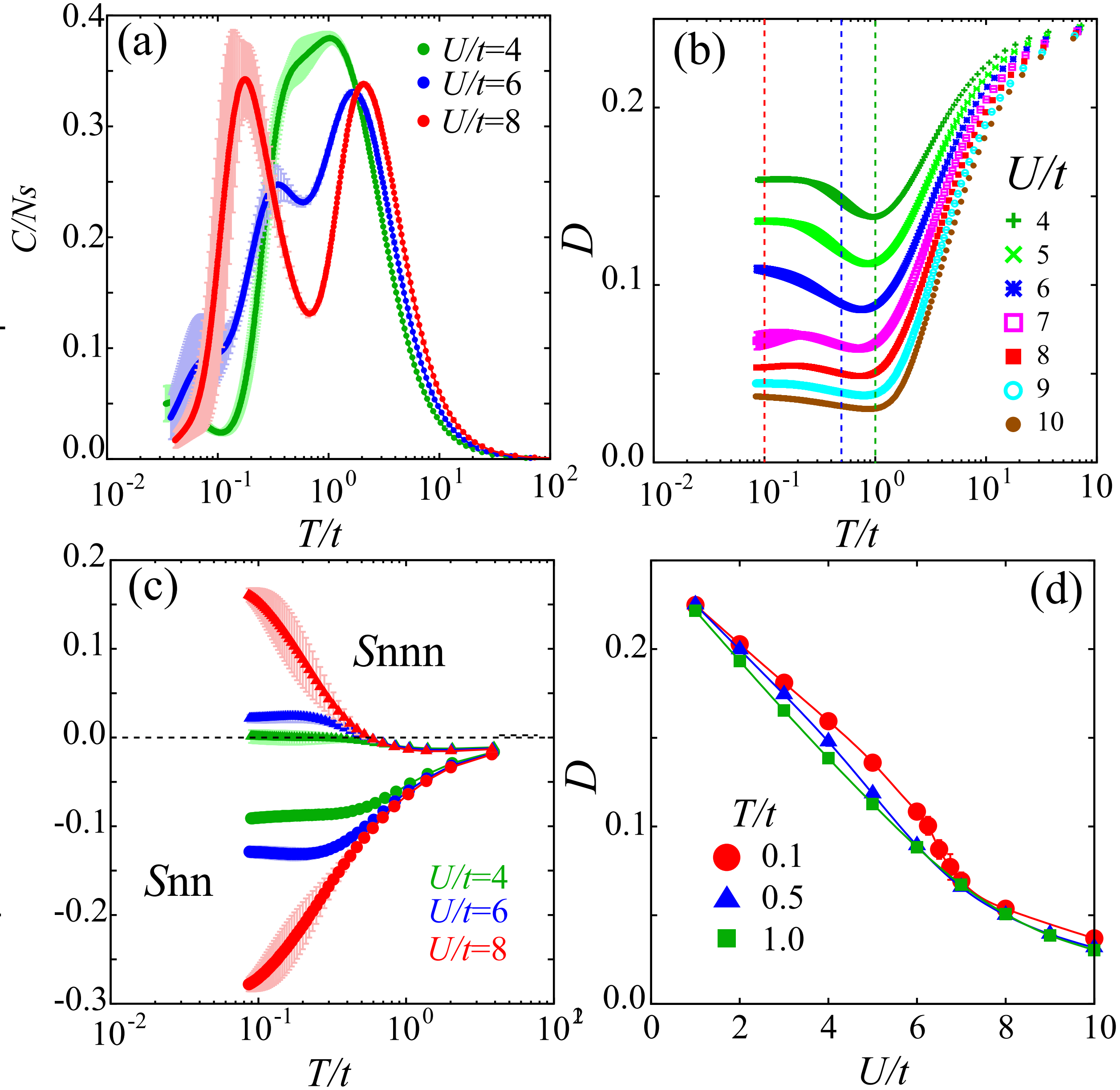
$$\langle H\rangle,\ \langle H^2\rangle,\ \langle c^\dagger_{i\sigma_1} c_{j\sigma_2}\rangle,\ \langle c^\dagger_{i\sigma_1} c_{j\sigma_2} c^\dagger_{k\sigma_3} c_{\ell\sigma_4}\rangle$$

$$t'/t = 0.5$$

$$C = \frac{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}{k_{\rm B} T^2}$$

$$\frac{\langle \phi | \vec{\hat{S}}_i \cdot \vec{\hat{S}}_j | \phi \rangle}{\langle \phi | \phi \rangle}$$

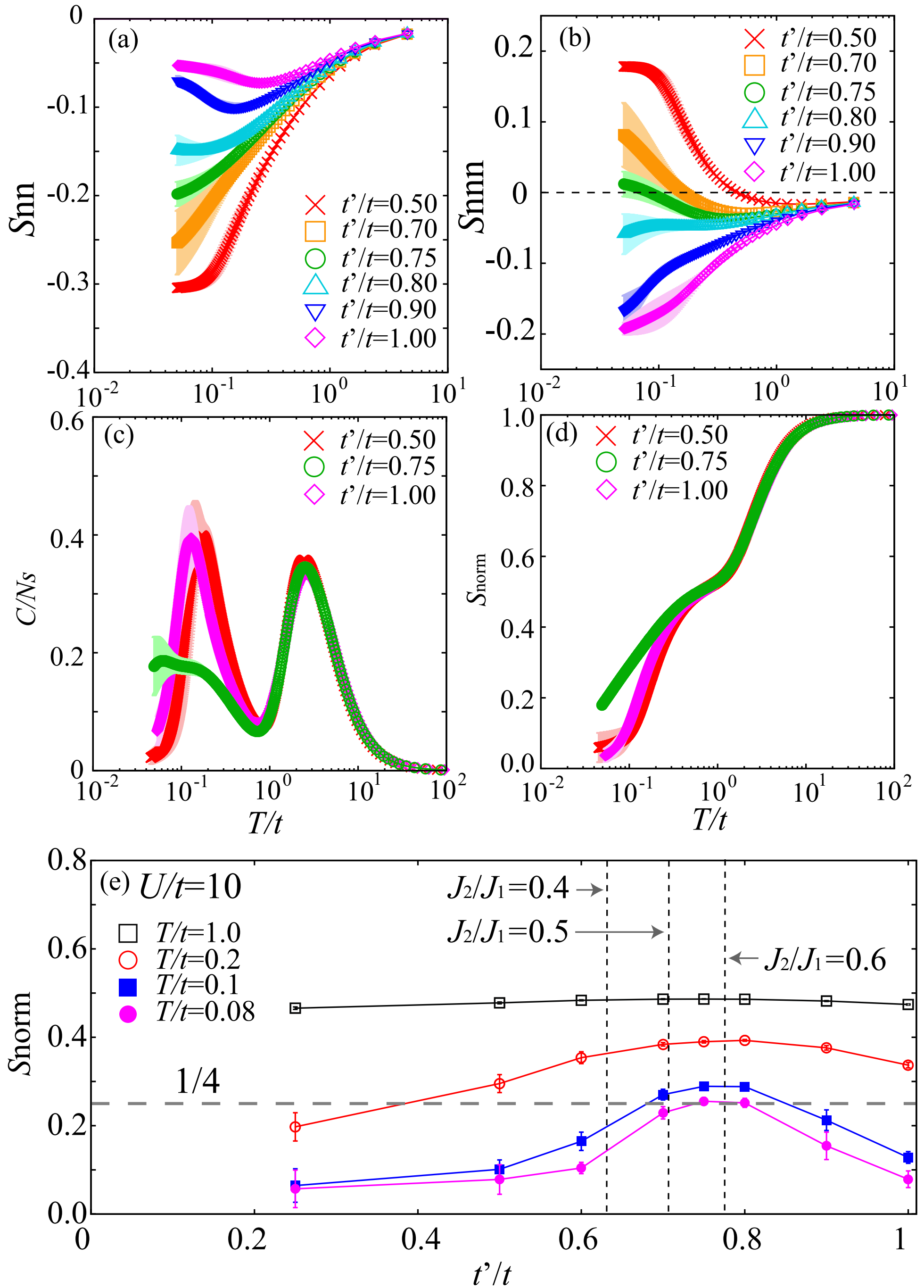
$$D = \frac{\langle \phi | \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} | \phi \rangle}{\langle \phi | \phi \rangle}$$



$U/t = 10$

$$\frac{\langle\phi|\vec{\hat{S}}_i\cdot\vec{\hat{S}}_j|\phi\rangle}{\langle\phi|\phi\rangle}$$

$$C = \frac{\langle\hat{H}^2\rangle - \langle\hat{H}\rangle^2}{k_\mathrm{B}T^2}$$



Standard input

```
W = 4
L = 4
model = "Hubbard"
//method = "Lanczos"
method = "TPQ"
//method = "FullDiag"
lattice = "Square"
t = 1.0
t' = 0.5
U = 8.0
nelec = 16
2Sz = 0
```

```
Standard interface
```

Making input files from scratch

Expert input

```
Def. files for Hamiltonian
Def. files for controlling simulation
```

```
Expert interface
```

```
Subroutines:
-Lanczos
-TPQ
-Full diag. (LAPACK)
```

Models

Standard input: Simplified input for typical lattice models

Hubbard

$$H = -\mu \sum_{i=1}^{N} \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^{\dagger} c_{i\sigma} - \sum_{i \neq j} \sum_{\sigma=\uparrow,\downarrow} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow} + \sum_{i \neq j} V_{ij} n_i n_j$$

Quantum spins

$$H = -h \sum_{i=1}^{N} S_i^z + \Gamma \sum_{i} S_i^x + D \sum_{i} S_i^z S_i^z + \sum_{i,j} \sum_{\alpha,\beta=x,y,z} J_{ij}^{\alpha\beta} S_i^{\alpha} S_j^{\beta}$$

Kondo lattice

$$H = -\mu \sum_{i=1}^{N} \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^{\dagger} c_{i\sigma} - t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{J}{2} \sum_{i=1}^{N} \left\{ S_i^{+} c_{i\downarrow}^{\dagger} c_{i\uparrow} + S_i^{-} c_{i\uparrow}^{\dagger} c_{i\downarrow} + S_i^{z} (n_{i\uparrow} - n_{i\downarrow}) \right\}$$

Expert input: Flexible input for any one- and two-body hamiltonian

$$H = \sum_{i,j} \sum_{\sigma_1,\sigma_2} t_{i\sigma_1 j\sigma_2} c_{i\sigma_1}^{\dagger} c_{j\sigma_2} + \sum_{i,j,k,\ell} \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} I_{i\sigma_1 j\sigma_2;k\sigma_3\ell\sigma_4} c_{i\sigma_1}^{\dagger} c_{j\sigma_2} c_{k\sigma_3}^{\dagger} c_{\ell\sigma_4}$$

Next Week

-Shifted Krylov subspace method 2
-Implementation of Lanczos method
-Parallelization
-Other numerical methods
-Report problems

The next week is the last since 7/18 is reserved
for supplementary classes in the faculty of engineering