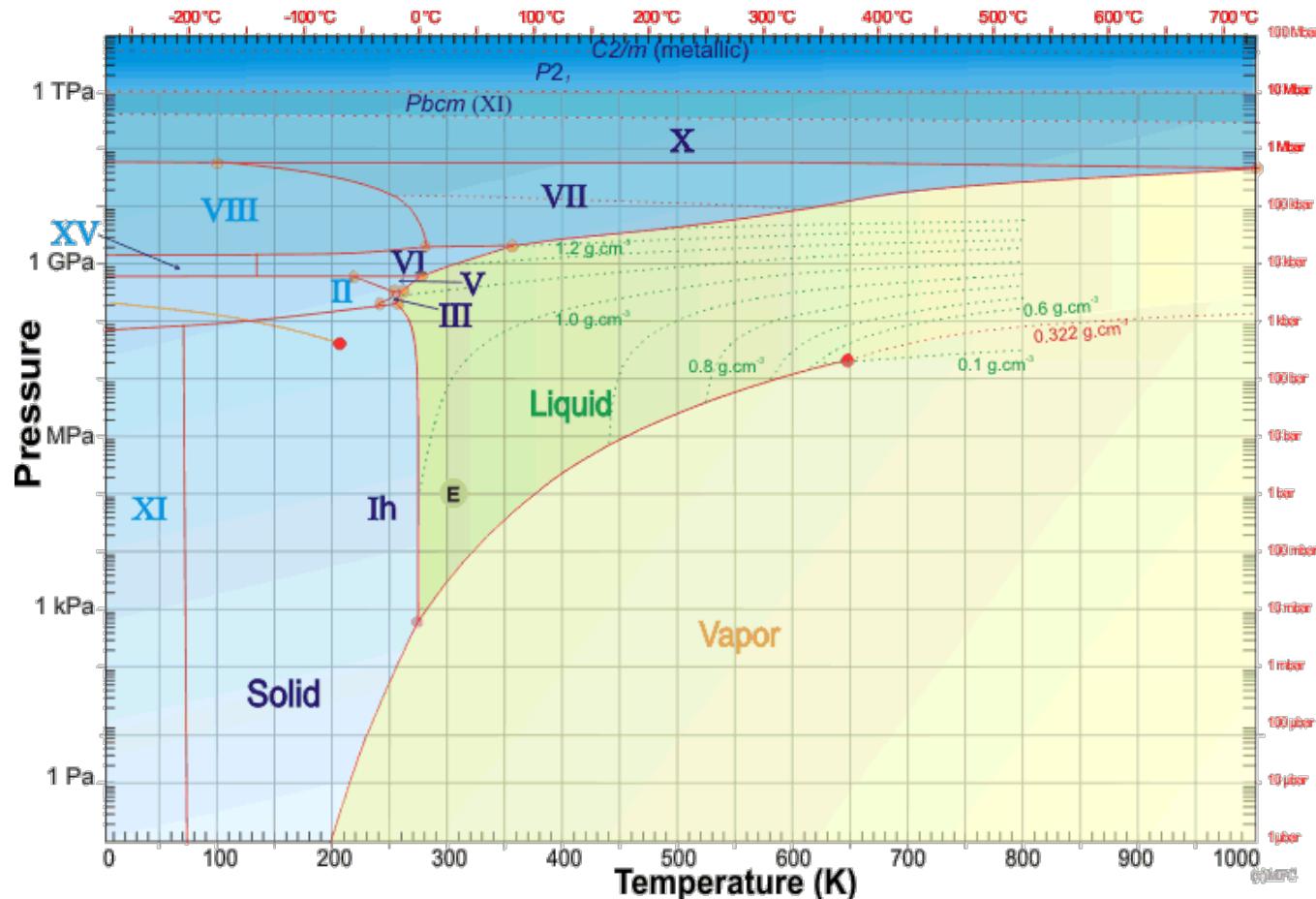


CSA Summer School Lecture 3

#1
2017/8/23

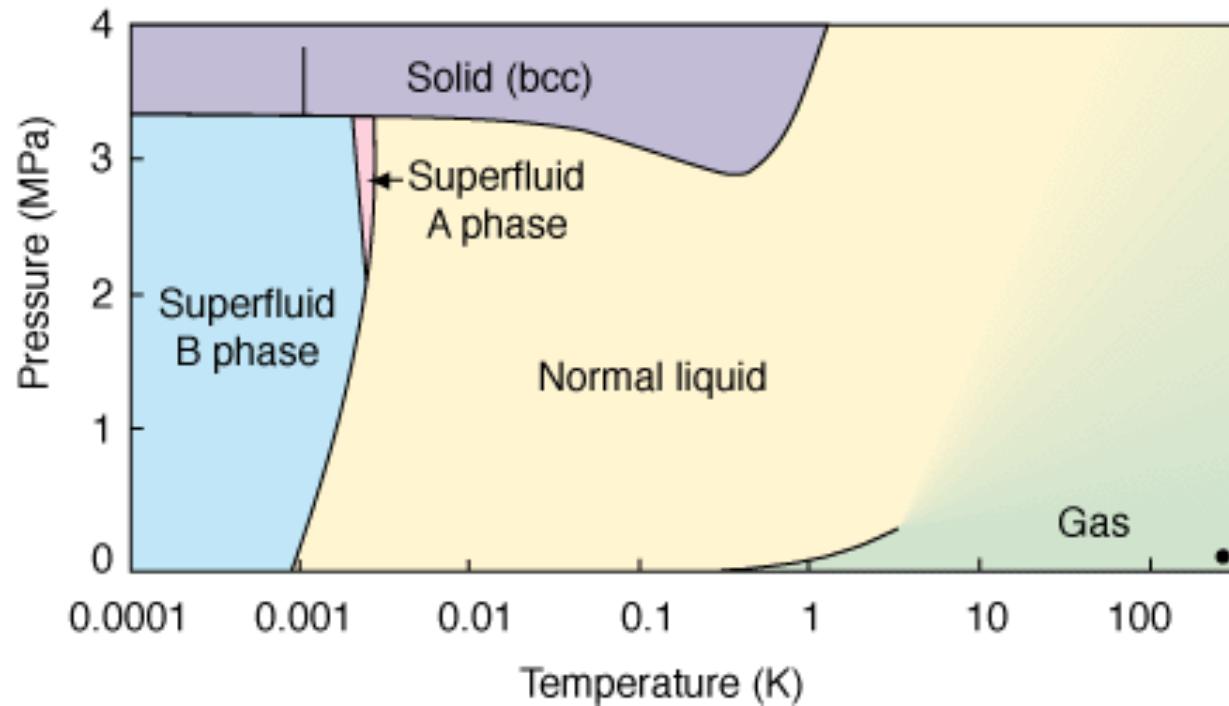
Quantum Many-Body Problems:
Numerical Exact Diagonalization
& Haldane Gap

Phase diagram of H₂O



Martin Chaplin
Water Structure and Science
<http://www1.lsbu.ac.uk/water/>

Phase diagram of ${}^3\text{He}$



D. D. Osheroff, R. C. Richardson, and D. M. Lee,
Phys. Rev. Lett. 28, 885 (1972).

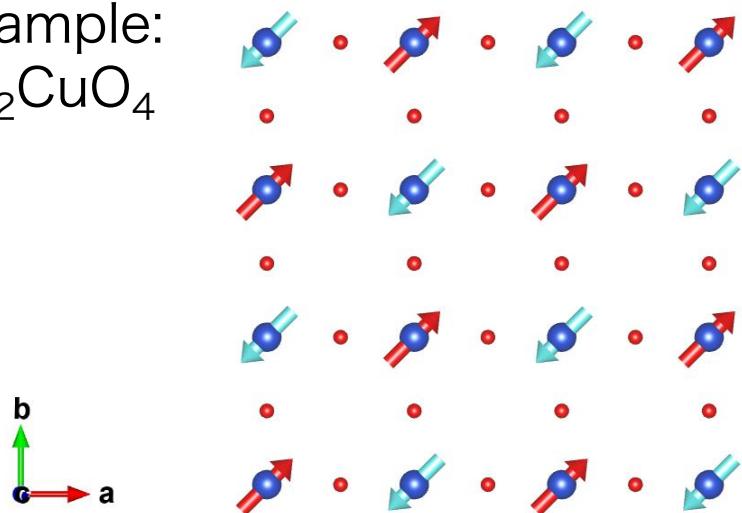
Why Quantum Many-Body Systems?

Quantum Phases: More is different

-Spontaneous symmetry breaking (SSB)

Superfluidity, superconductivity, magnetic order

Example:



$$J \left[\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \hat{S}_i^z \hat{S}_j^z \right]$$

-Topology

Classification of Crystalline Solids In One-Body Picture

- Metal
- Zero gap semiconductor
- Band insulator
- Mott insulator

Trivial insulator

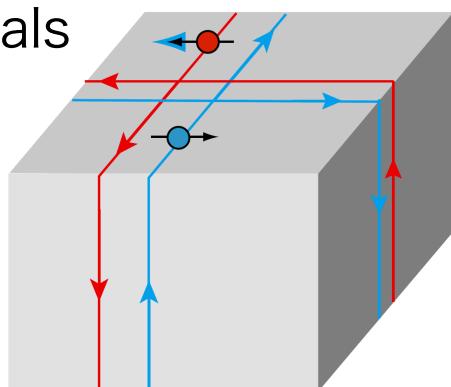
Si

Topological insulator

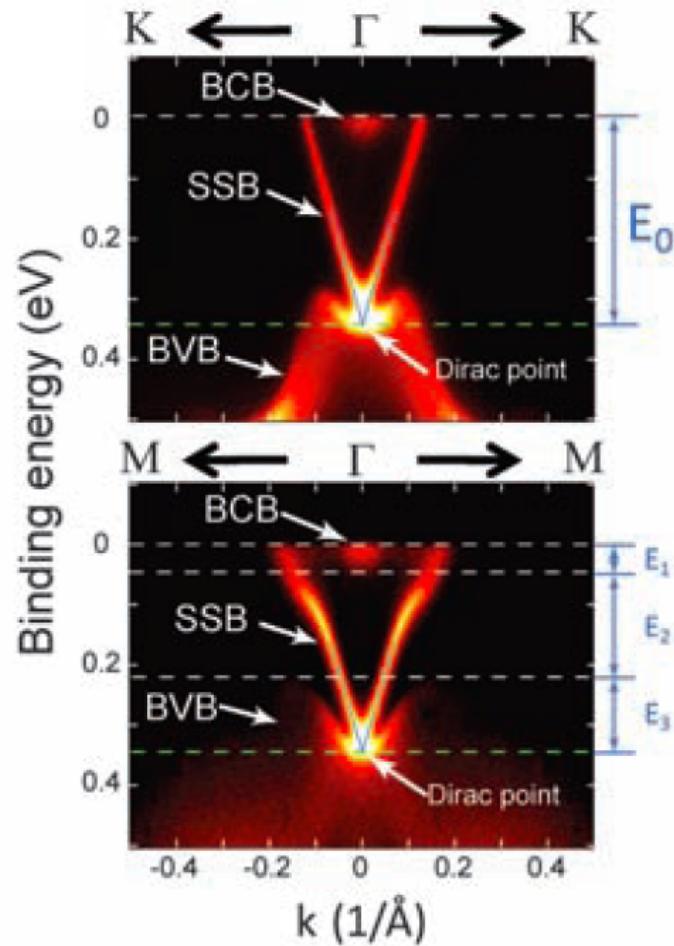
Bi_2Te_3

Thermoelectric

Surface metals



Y. L. Chen, *et al.*, Science 325, 178 (2009)



An example: Chern insulator

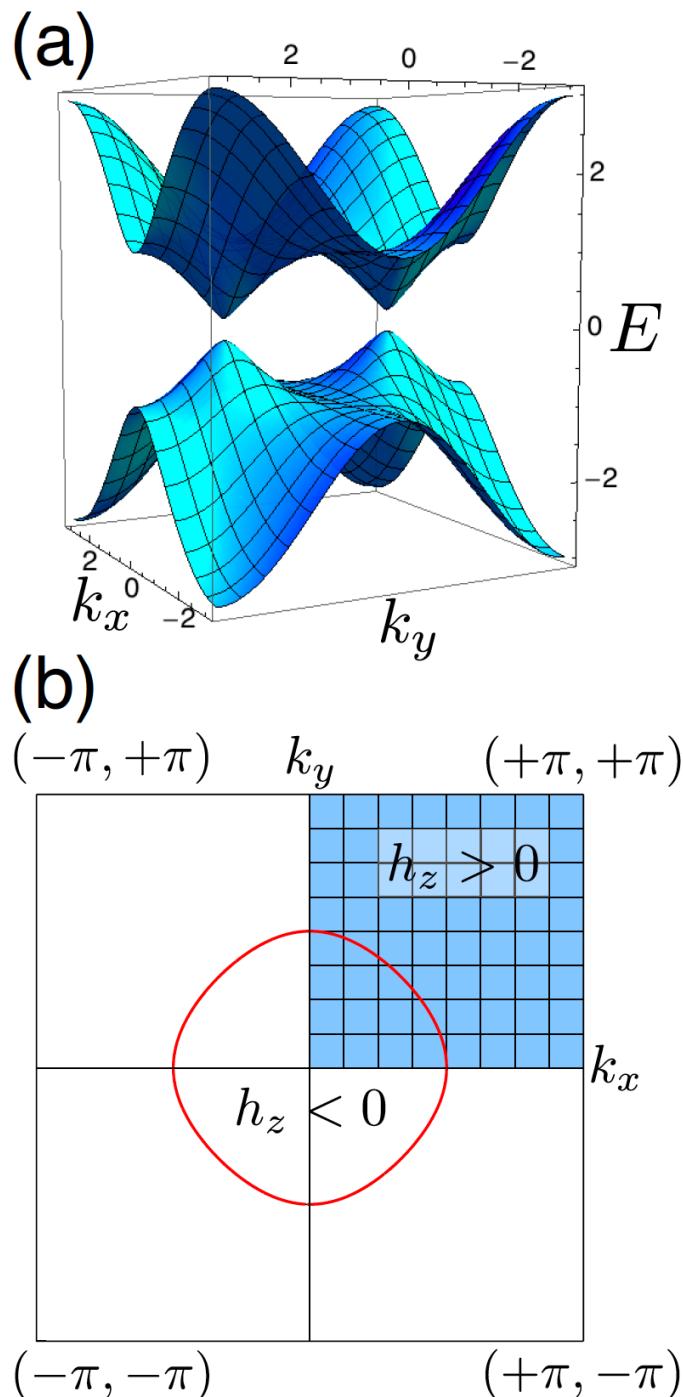
$$\hat{H}_{\text{2D}}(\vec{k}) = h_x(\vec{k})\hat{\sigma}_x + h_y(\vec{k})\hat{\sigma}_y + h_z(\vec{k})\hat{\sigma}_z,$$

$$h_\alpha(\vec{k}) = v_\alpha \sin k_\alpha \ (\alpha = x, y),$$

$$h_z(\vec{k}) = r \sum_{\alpha=x,y} [1 - \cos k_\alpha] - m.$$

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

$$E = E_{\pm}(\vec{k}) = \pm \sqrt{|h_x(\vec{k})|^2 + |h_y(\vec{k})|^2 + |h_z(\vec{k})|^2}$$



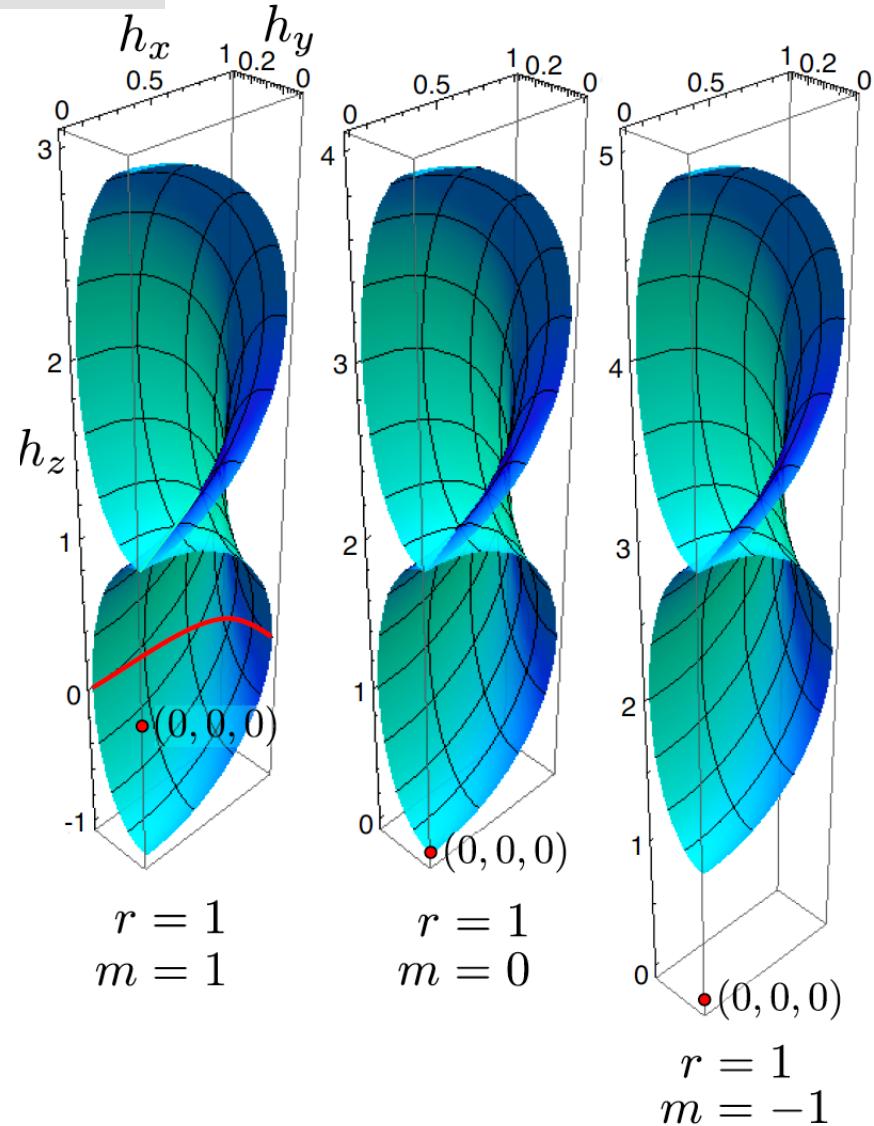
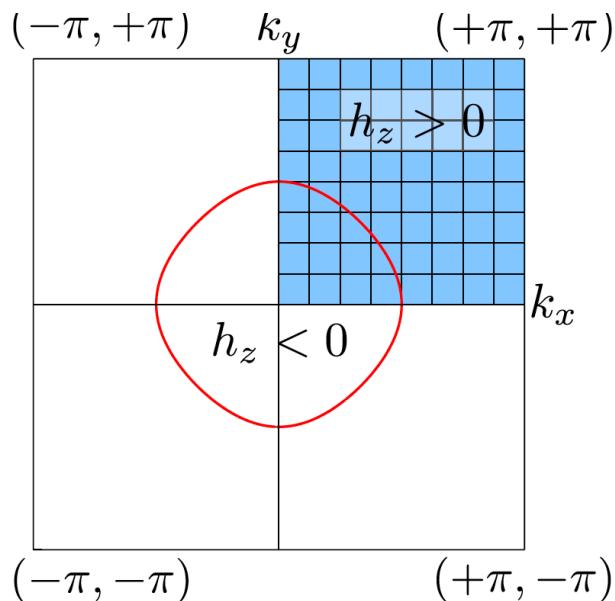
An example: Chern insulator

Mapping: T^2 to R^3

$$\hat{H}_{2D}(\vec{k}) = h_x(\vec{k})\hat{\sigma}_x + h_y(\vec{k})\hat{\sigma}_y + h_z(\vec{k})\hat{\sigma}_z,$$

$$h_\alpha(\vec{k}) = v_\alpha \sin k_\alpha \ (\alpha = x, y),$$

$$h_z(\vec{k}) = r \sum_{\alpha=x,y} [1 - \cos k_\alpha] - m.$$



If we keep a finite gap, we find infinite number (Z) of topologically distinct phases

Difficulties in Quantum Many-Body Systems

Exponential wall

Nobel lecture by Walter Kohn (1999)

B. Many Electrons – Encountering an Exponential Wall

In the same spirit as our last “guesstimates” for H_2 , let us now consider a general molecule consisting of N atoms with a total of N interacting electrons, where $N \gg 10$ say. We ignore symmetries and spin, which will not affect our general conclusions. Reasoning as before, we see that the number M of parameter required is

$$M = p^{3N}, \quad 3 \leq p \leq 10. \quad (2.12)$$

The energy needs to be minimized in the space of these M parameters. Call \bar{M} the maximum value feasible with the best available computer software and hardware; and \bar{N} the corresponding maximum number of electrons. Then, from Eq. (2.12) we find

$$\bar{N} = \frac{1}{3} \frac{\log \bar{M}}{\log p}. \quad (2.13)$$

Let us optimistically take $\bar{M} \approx 10^9$ and $p = 3$. This gives the shocking result

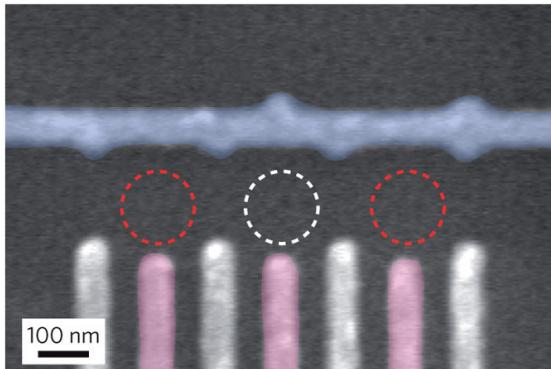
$$\bar{N} = \frac{1}{3} \frac{9}{0.48} = 6(!). \quad (2.14)$$

In practice, by being “clever”, one can do better than this, perhaps by one half order of magnitude, up to say $\bar{N} \approx 20$. But the exponential in Eq. (2.12) represents a “wall” severely limiting \bar{N} .

Quantum Many-Body Problems

An example: 3 Quantum dots

F. R. Braakman, et al., Nat. Nano. 8, 432 (2013)

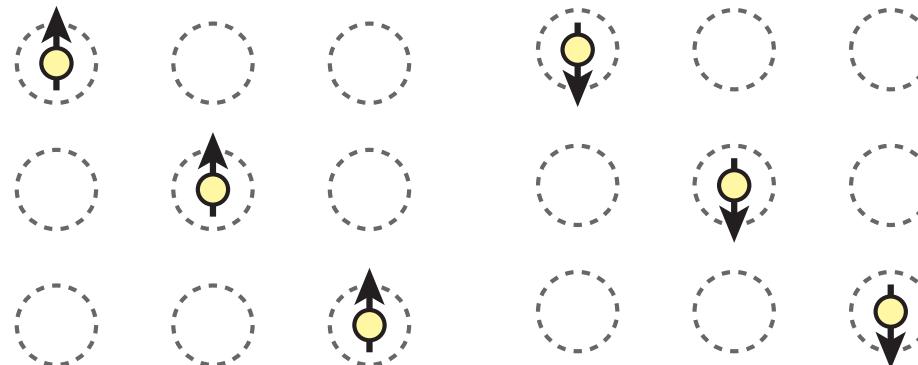


Quantum dot:

- A quantum box can confine a single electron
- Utilized for single electron transistor, quantum computers

One-body problem:

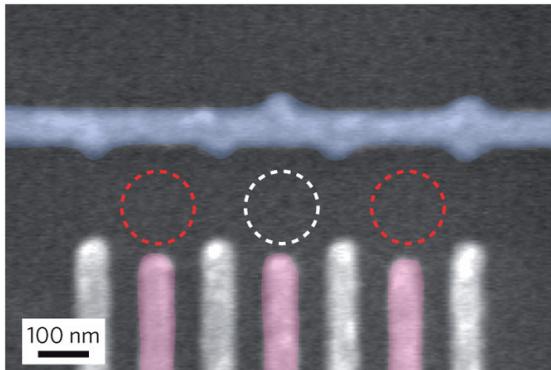
One electron confined in three quantum dot
→ Number of states = 2×3 (factor 2 from spin)



Quantum Many-Body Problems

An example: 3 Quantum dots

F. R. Braakman, et al., Nat. Nano. 8, 432 (2013)

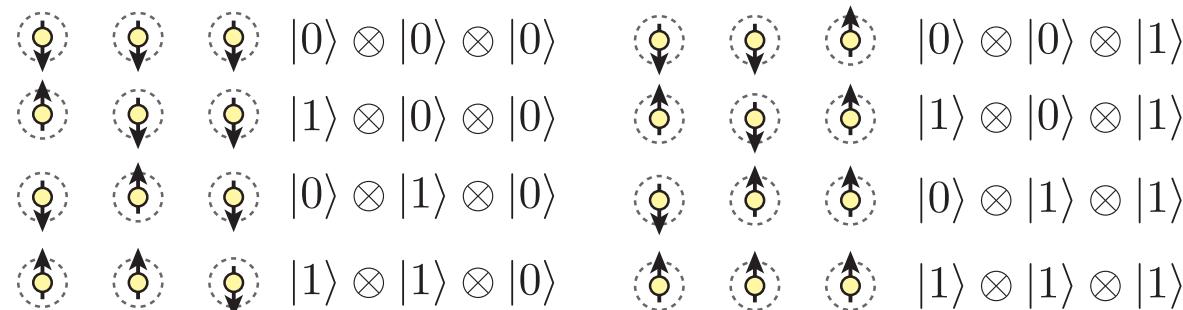


Quantum dot:

- A quantum box can confine a single electron
- Utilized for single electron transistor, quantum computers

Three-body problem:

→ Number of states = 2^3 (factor 2 from spin)



States represented by superposition

$$\mathcal{F} = \left\{ \sum_{n_0=0,1} \sum_{n_1=0,1} \sum_{n_2=0,1} C_{n_0 n_1 n_2} |n_0\rangle \otimes |n_1\rangle \otimes |n_2\rangle : C_{n_0 n_1 n_2} \in \mathbb{C} \right\}$$

Quantum Many-Body Problems

N Quantum dots

One-body problem:

$$\rightarrow \text{Number of states} = 2 \times N$$

N-body problem:

$$\rightarrow \text{Number of states} = 2^N$$

Further example: N=12



One-body problem \rightarrow Number of states = $2 \times N = 24$

N-body problem \rightarrow Number of states = $2^N = 4096$

Extreme example: N=36

One-body $\rightarrow 2 \times N = 72$
N-body $\rightarrow 2^N \sim 6.9 \times 10^{10}$

Quantum Many-Body Problems

Q. Is exponentially large degrees of freedom necessary to describe quantum phases?

A. Practically No!

By carefully choosing targets, we can find a relevant Fock subspace with much smaller dimension or an effective representation of many-body states

Today: A relevant subspace found by Lanczos/CG-type method (implemented in $\text{H}\Phi$)

Tomorrow: An effective representation by matrix product states (MPS)

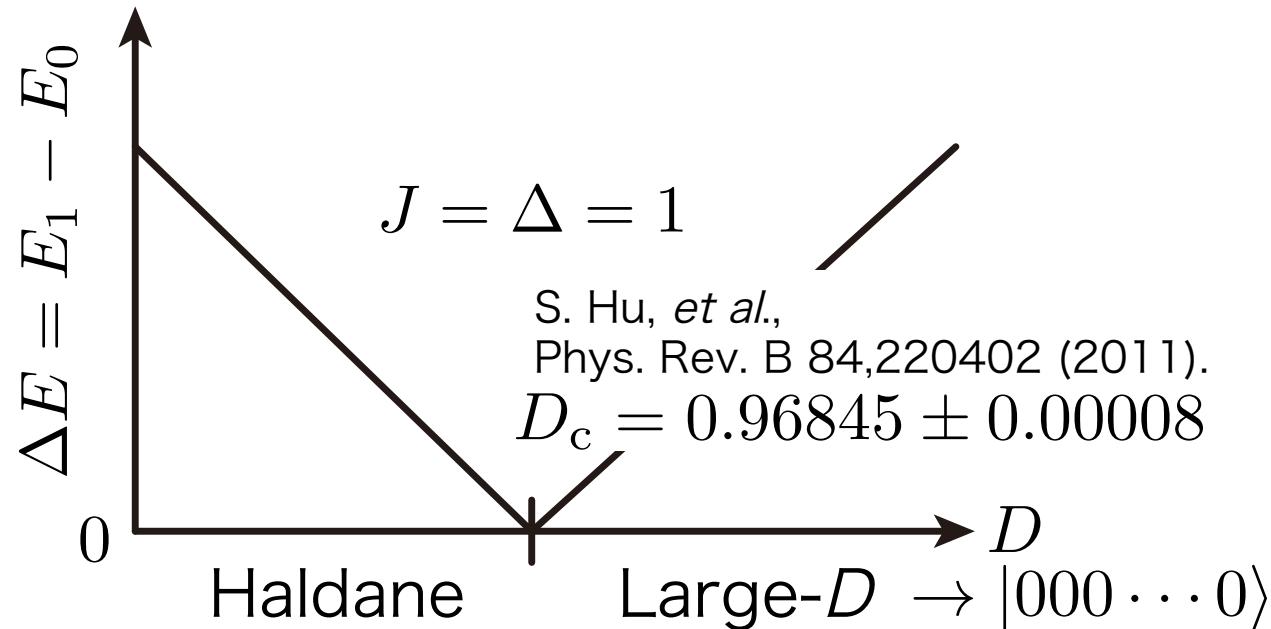
Target: Haldane Gap and Topology

Model: $S=1$ XXZ model
with single ion anisotropy

$$\hat{H} = J \sum_{\langle i,j \rangle} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \Delta \hat{S}_i^z \hat{S}_j^z \right) + D \sum_i (\hat{S}_i^z)^2$$

$\Delta = 1$: Heisenberg model

Topological phase transition (No SSB)



Background: $S=1$ Heisenberg Model

Haldane gap $\Delta = 1, D = 0$

F. D. M. Haldane, Phys. Rev. Lett. 50, 1153 (1983); Phys. Lett. 93A, 464 (1983).

-*Conjecture* about excitation gap

Gapless: $S = 1/2, 3/2, 5/2, \dots$

Gapful: $S = 1, 2, 3, \dots$

cf.) AKLT I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki,
Commun. Math. Phys. 115, 477 (1988).

$$\Delta(S) = \begin{cases} 0.41048(6) & \text{for } S = 1 \\ 0.08917(4) & \text{for } S = 2 \\ 0.01002(3) & \text{for } S = 3 \end{cases}$$

S. Todo and K. Kato, Phys. Rev. Lett. 87, 047203 (2001).

→ Symmetry Protected Topological (SPT) state

Spin Coupling

- 電子1つが持つスピンは $S=1/2$, スピン角運動量は $h/4\pi$
- 磁石の磁性の源は、複数の電子のスピン角運動量の合成による
(角運動量も合算される)
例: 希土類磁性体ガドリニウム Gd^{+3} $S=7/2$
- $S \rightarrow +\infty$ の極限が古典ハイゼンベルグ・スピンを再現

$S=1$ の場合

$$|m_z = +1; S = 1\rangle = |\uparrow\uparrow\rangle$$

$$|m_z = 0; S = 1\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$|m_z = -1; S = 1\rangle = |\downarrow\downarrow\rangle$$

Quantum Spin $S=1$ Operator

For $S=1$

$$\hat{S}^x \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & +1 & 0 \\ +1 & 0 & +1 \\ 0 & +1 & 0 \end{pmatrix}$$

$$\hat{S}^y \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & -i \\ 0 & +i & 0 \end{pmatrix}$$

$$\hat{S}^z \doteq \begin{pmatrix} +1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

\hat{S}^x	+1	0	-1
+1	0	$+1/\sqrt{2}$	0
0	$+1/\sqrt{2}$	0	$+1/\sqrt{2}$
-1	0	$+1/\sqrt{2}$	0

\hat{S}^y	+1	0	-1
+1	0	$-i/\sqrt{2}$	0
0	$+i/\sqrt{2}$	0	$-i/\sqrt{2}$
-1	0	$+i/\sqrt{2}$	0

\hat{S}^z	+1	0	-1
+1	+1	0	0
0	0	0	0
-1	0	0	-1

Simulation by HΦ

Model: $S=1$ XXZ model
with single ion anisotropy

$$\hat{H} = J \sum_{\langle i,j \rangle} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \Delta \hat{S}_i^z \hat{S}_j^z \right) + D \sum_i (\hat{S}_i^z)^2$$

How to install HΦ

For ECCS

1. Google “csa lecture github”
2. Visit repository:
[compsci-alliance/introduction-to-computational-science](https://github.com/compsci-alliance/introduction-to-computational-science)
3. Download CSA_SS_Lect3-1.zip
4. Unzip CSA_SS_Lect3-1.zip
5. \$ cd ./CSA_SS_Lect3-1/.
6. Unzip qlmpack-develop.zip
7. \$./build-hphi-dev.sh

For PC clusters/SC

1. Google “MateriApps HPhi”
2. Visit HΦ’ page

Importance of Numerically Exact Wave Functions

Fractional quantum Hall effect

D. C. Tsui, *et al.*, Phys. Rev. Lett. 48, 1559 (1982).

R. B. Laughlin, Phys. Rev. Lett. 50, 1395 (1983).

F. D. M. Haldane, Phys. Rev. Lett. 55, 2095 (1985).

-ED used for examining Laughlin's wave function

Thermalization of isolated quantum systems

M. Rigol, V. Dunjko, and M. Olshanii, Nature 452, 854 (2008).

-Simulating dynamics of isolated quantum systems

New emergent concepts have been examined by ED

ED Solvers for Quantum Many-Body Problems

TITPACK by Y. Taguchi & H. Nishimori (1985-)
Heisenberg & XXZ model

KOBEPACK by M. Kaburagi, T. Nishino, & T. Tonegawa (1992-)
-S=1 Heisenberg

SPINPACK by J. Schulenburg (1995-)
-MPI & PTHREAD
-XXZ, Hubbard, & t - J model
-Symmetries

ALPS IETL library by P. Dayal, M. Troyer, & R. Villiger

Mainly for fundamental lattice models



A Numerical Solver for
Quantum Many-Body Problems:
 $H\Phi$

$\mathcal{H}\Phi$

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 \(latest release: ver.2.0.3\)](#)

Licence: GNU GPL version3

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

$\text{H}\Phi$ Developers



Dr. Takahiro Misawa
The Institute for Solid State Physics,
The University of Tokyo



Dr. Mitsuaki Kawamura
The Institute for Solid State Physics,
The University of Tokyo



Dr. Yoshikazu Yoshimi
The Institute for Solid State Physics,
The University of Tokyo

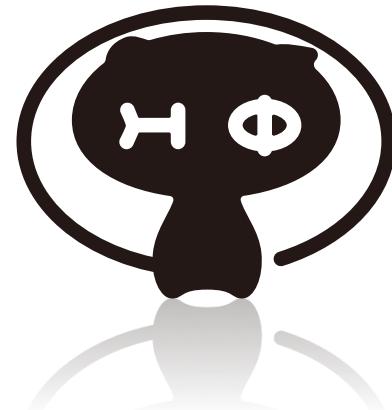


Prof. Synge Todo
Department of Physics,
The University of Tokyo



Prof. Naoki Kawashima
The Institute for Solid State Physics,
The University of Tokyo

Youhei Yamaji
Department of Applied Physics,
The University of Tokyo



Acknowledgement:

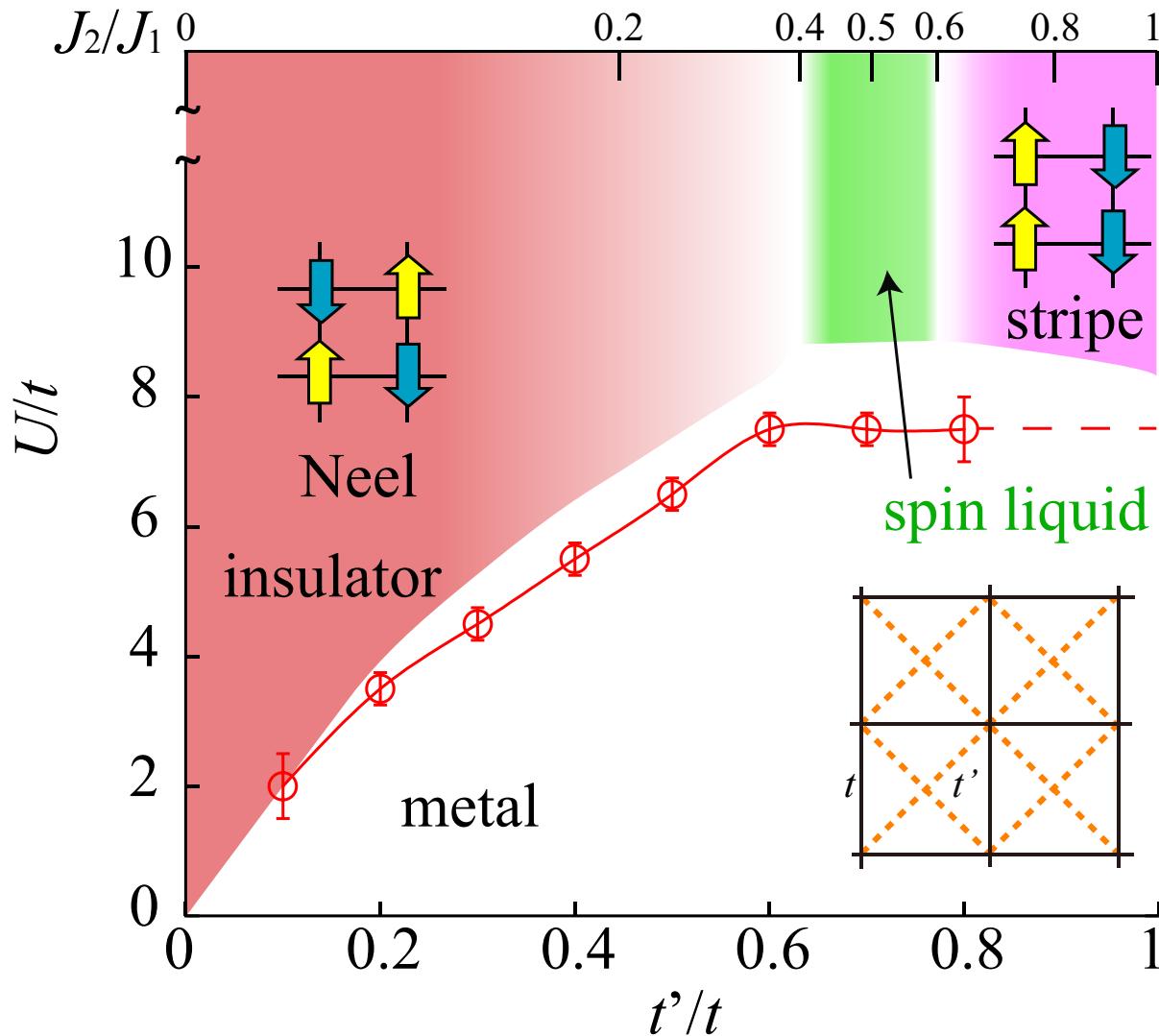
Prof. Takeo Hoshi (Tottori Univ.)

Prof. Tomohiro Sogabe (Nagoya Univ.)

“Project for advancement of software usability in materials science” by ISSP

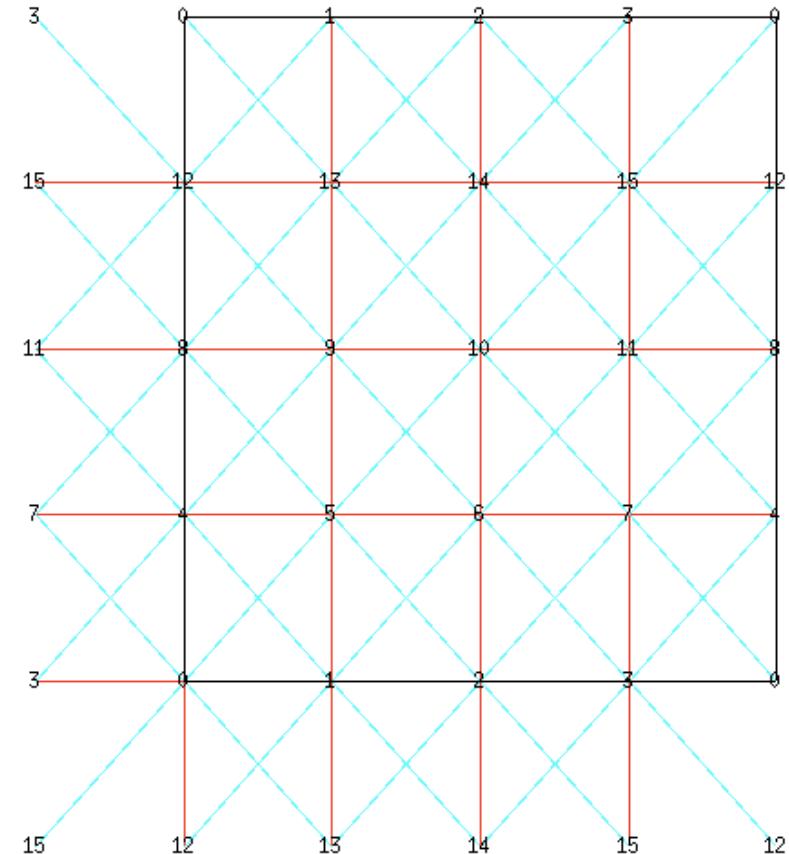
An Example: t - t' Hubbard

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

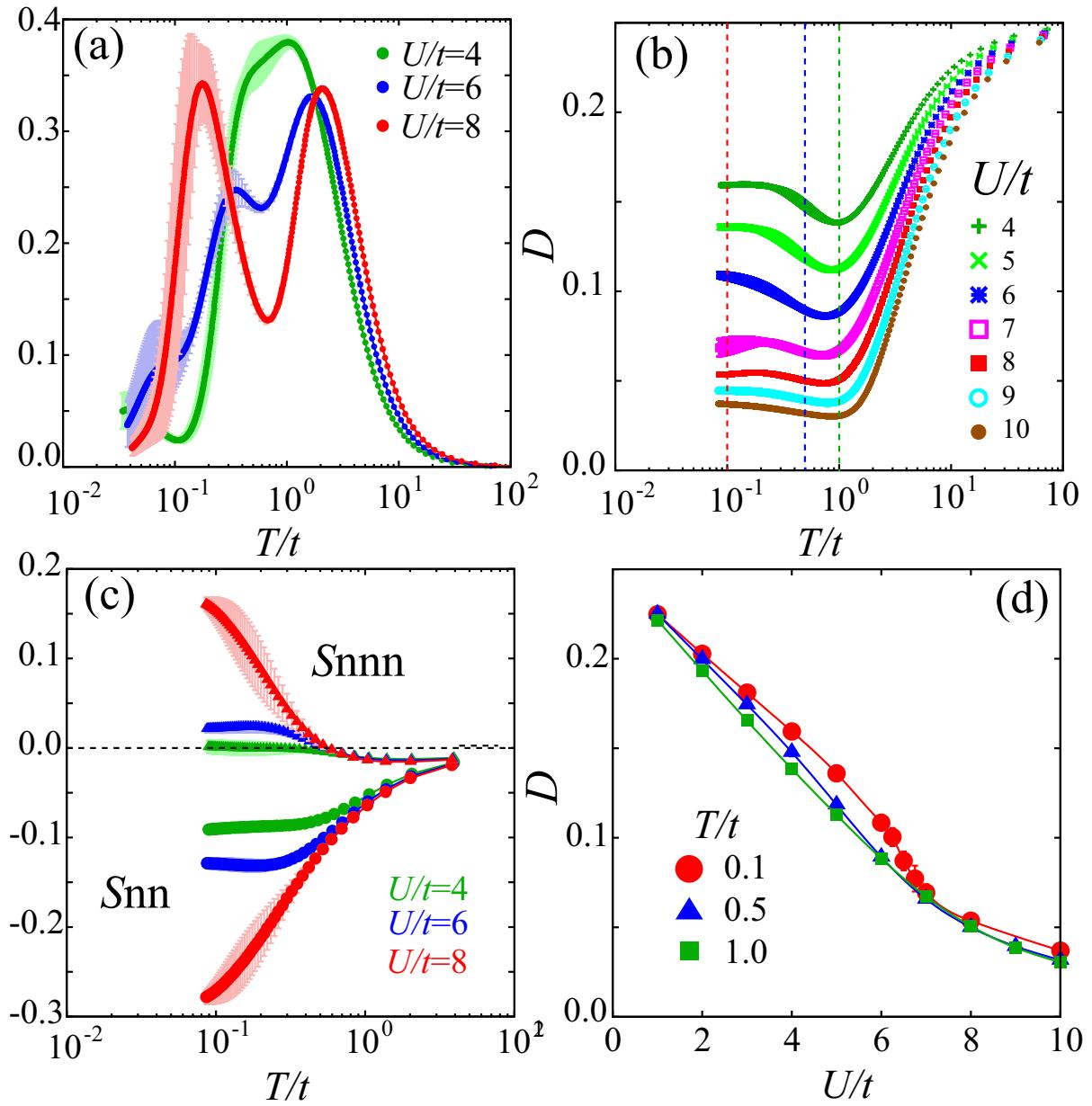
$$\langle H \rangle, \langle H^2 \rangle, \langle c_{i\sigma_1}^\dagger c_{j\sigma_2} \rangle, \langle c_{i\sigma_1}^\dagger c_{j\sigma_2} c_{k\sigma_3}^\dagger c_{\ell\sigma_4} \rangle$$

$$t'/t = 0.5$$

$$C = \frac{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}{k_B T^2}$$

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

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



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

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

Exercise: Use Standard Mode

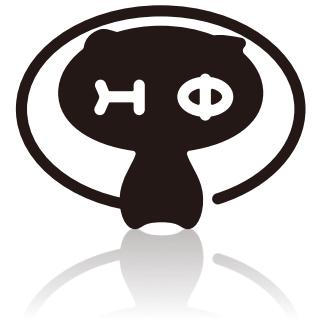
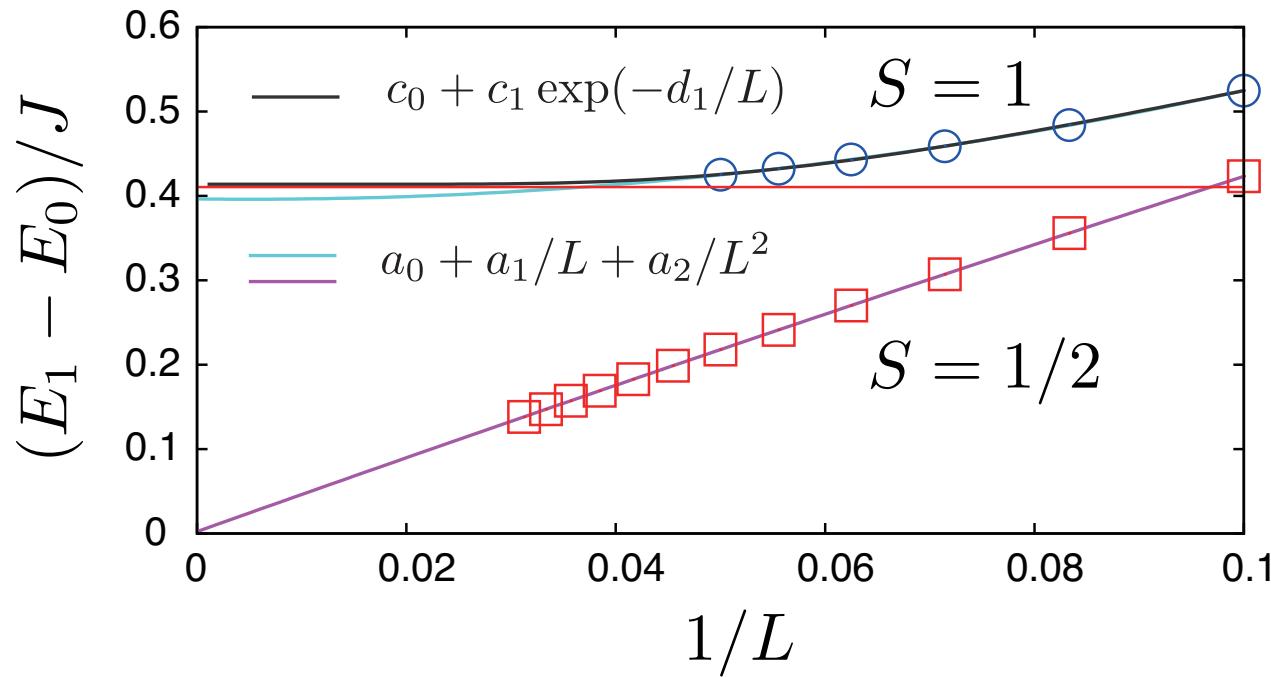
$$\hat{H} = J \sum_{\langle i,j \rangle} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \Delta \hat{S}_i^z \hat{S}_j^z \right) + D \sum_i (\hat{S}_i^z)^2$$

Standard input file for a 12 site $S=1$ Heisenberg model

```
L = 12           ←Number of sites * “//” means a comment line
model = "SpinGC" ←Any total Sz
//model = "Spin" ←Fixed total Sz
lattice = "Chain" ←Periodic 1D chain
method = "Lanczos"
//method = "CG"
//method = "TPQ"
//method = "FullDiag"
2S=2           ←Spin quantum number S
//2Sz=0        ←Total Sz
D=1.0          ←Sorry, we have a bug for D in the current release
                (will be fixed in the next release)
Jx=1.0
Jy=1.0
Jz=1.0        ←You can control Δ
```

$S=1$ Heisenberg Model

Haldane gap



ED: $S=1$ up to 22 sites

O. Golinelli, Th. Jolicoeur, and R. Lacaze, Phys. Rev. B 50, 3037 (1994).

QMC: S. Todo and K. Kato, Phys. Rev. Lett. 87, 047203 (2001).

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)

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

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

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

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

Bosons

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

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

Quantum Many-Body Problem by Linear Algebra

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

→ General Hamiltonian with two-body interactions

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

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

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

Quantum Many-Body Problem by Linear Algebra

Fock space of N -particle fermions expanded by

$$|\Phi\rangle = \sum_{\ell_1, \ell_2, \dots, \ell_N} \sum_{\sigma_1, \sigma_2, \dots, \sigma_N} C_{\ell_1 \ell_2 \dots \ell_N} \hat{a}_{\ell_1 \sigma_1}^\dagger \hat{a}_{\ell_2 \sigma_2}^\dagger \cdots \hat{a}_{\ell_N \sigma_N}^\dagger |\text{vac}\rangle$$

Orthonormalized many-body basis

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

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

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

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

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

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

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

$$\begin{aligned} & \langle\mu| \times \hat{H}|\Phi\rangle = \langle\mu| \times E|\Phi\rangle \\ \Leftrightarrow & \sum_\nu \langle\mu|\hat{H}|\nu\rangle\langle\nu|\Phi\rangle = E\langle\mu|\Phi\rangle \end{aligned}$$

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: $\exp[N \times \text{const.}]$
- # of terms in Hamiltonian: Polynomial of N
 - # of matrix elements of Hamiltonian matrix:
(Polynomial of N) $\times \exp[N \times \text{const.}]$

For sufficiently large N ,
(Polynomial of N) $\times \exp[N \times \text{const.}]$
 $\ll (\exp[N \times \text{const.}])^2$

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

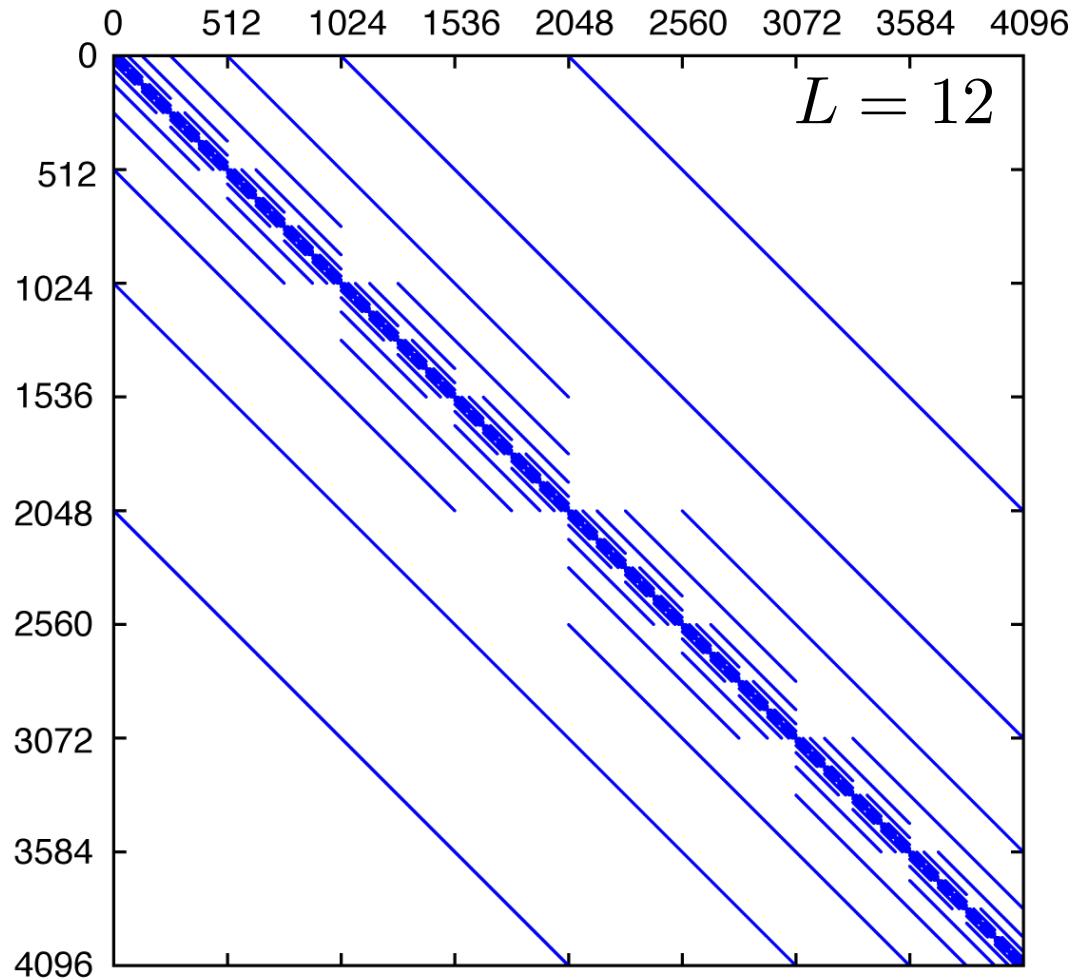
$$\left[\sum_{i=0}^{L-1} \hat{S}_i^z \hat{S}_{i+1}^z, \sum_{i=0}^{L-1} \hat{S}_i^x \right] \neq 0$$

→ Quantum fluctuations
or Zero point motion

-Sparse
of elements $\propto O(2^L)$

-Solvable

-Hierarchical matrix?



Computational and Memory Costs

Matrix-vector product of dense matrix

$$v_i = \sum_{j=0}^{N_H-1} A_{ij} u_j$$

Computational: $O((\text{Fock space dimension})^2)$

Memory: $O((\text{Fock space dimension})^2)$

Matrix-vector product of
large and sparse matrix

Computational: $O(\text{Fock space dimension})$

Memory: $O(\text{Fock space dimension})$

Hamiltonian is not stored in memory

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

Min. Eigenvalue of hermitian

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

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

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

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

$$E_0 \leq E_1 \leq \dots$$

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

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

$$\sum_n (\Lambda - E_n)^{2m} |c_n|^2$$

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

Advanced Algorithm: Krylov Subspace Method

Krylov subspace

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

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

Initial : $\beta_1 = 0, |v_0\rangle = 0$

for $j = 1, 2, \dots, m$ **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

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

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

Orthogonalization

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

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

Lanczos Method

Initial : $\beta_1 = 0, |v_0\rangle = 0$

for $j = 1, 2, \dots, m$ **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

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

$$\langle v_j | v_k \rangle = \delta_{j,k}$$

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

Hamiltonian projected onto m D Krylov subspace

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

Eigenvalues of projected Hamiltonian

→ Approximate eigenvalues of original Hamiltonian

Lanczos Method: # of Vectors Required

Initial : $\beta_1 = 0, |v_0\rangle = 0$

for $j = 1, 2, \dots, m$ **do**

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

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

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

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

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

$$|v_{j-1}\rangle \rightarrow |w_j\rangle, |v_j\rangle$$

$$|w_j\rangle, |v_j\rangle$$

$$|w_j\rangle, |v_j\rangle$$

$$|w_j\rangle, |v_j\rangle$$

$$|w_j\rangle \rightarrow |v_{j+1}\rangle, |v_j\rangle$$

Convergence of Lanczos Method

Yousef Saad,

Numerical Methods for Large Eigenvalue Problems (2nd ed)

The Society for Industrial and Applied Mathematics 2011

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

Convergence theorem for the largest eigenvalue

$$0 \leq \lambda_1 - \lambda_1^{(m)} \leq (\lambda_1 - \lambda_n) \left[\frac{\tan \theta(|v_1\rangle, |0\rangle)}{C_{m-1}(1 + 2\gamma_1)} \right]^2$$
$$\sim 4(\lambda_1 - \lambda_n) [\tan \theta(|v_1\rangle, |0\rangle)]^2 e^{-4\sqrt{\gamma_1}m}$$

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

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

Representation of S=1 Spin

$$\hat{H} = J \sum_{\langle i,j \rangle} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \Delta \hat{S}_i^z \hat{S}_j^z \right) + D \sum_i (\hat{S}_i^z)^2$$

Two body interaction can be defined by `interall.def`

$$\hat{H}_I = \sum_{i,j,k,\ell} \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} I_{ijkl}^{\sigma_1\sigma_2\sigma_3\sigma_4} \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{k\sigma_3}^\dagger \hat{c}_{\ell\sigma_4}$$

Bogoliubov representation for S=1

$$\hat{S}_i^z = \sum_{\sigma=-1,0,+1} \sigma \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$$

$$(\hat{S}_i^z)^2 = \left(\hat{c}_{i,+1}^\dagger \hat{c}_{i,+1} - \hat{c}_{i,-1}^\dagger \hat{c}_{i,-1} \right)^2$$

σ	ternary
-1	0
0	1
+1	2

Lines define the single ion anisotropy of 0th site in `interall.def`

$(\hat{S}_0^z)^2$	0	0	0	0	0	0	0	1.00	0.00
	0	0	0	0	2	0	2	-2.00	0.00
	0	2	0	2	0	2	2	1.00	0.00

Exercise: Use Expert Mode

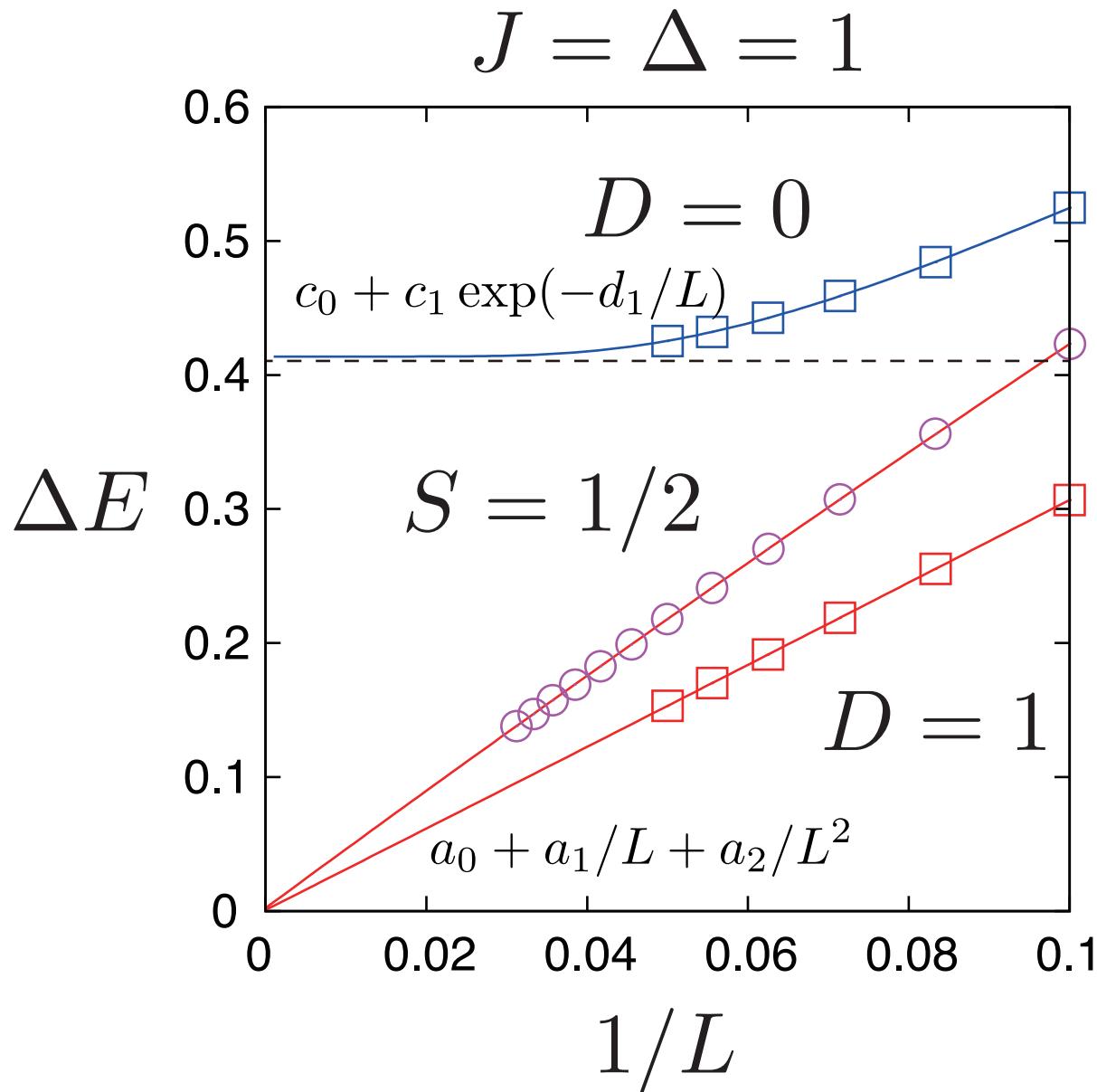
Perform conjugate gradient (CG) with changing L and D
to obtain excited states accurately

LOB(P)CG by A. V. Knyazev, SIAM j. Sci. Compt. 23, 517 (2001).
CG method is selected by CalcType in calcmod.def

modpara.def

```
-----
Model_Parameters    0
-----
HPhi_Cal_Parameters
-----
CDataFileHead      zvo
CParaFileHead     zqp
-----
Nsite              12
Lanczos_max        2000
initial_iv         -1
exct               1   ← How many states you will obtain
LanczosEps          14   from the lowest eigenstate
LanczosTarget       2
LargeValue          1.20000000000000e+01
NumAve              5
```

A Goal: Gap Estimate

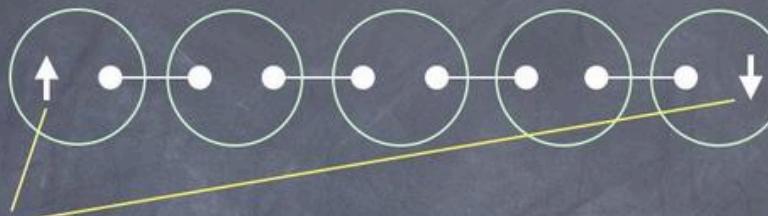


Beyond: Open Boundary with Edge States

M. Oshikawa
From seminar @KITP

Edge states

Consider a chain with open boundary condition



"free" $S=1/2$ appears at each end, interacting with each other. Effective coupling: $J_{\text{eff}} \sim e^{-L/\xi}$

$2 \times 2 = 4$ groundstates below the Haldane gap (nearly degenerate)

Kennedy (1990)

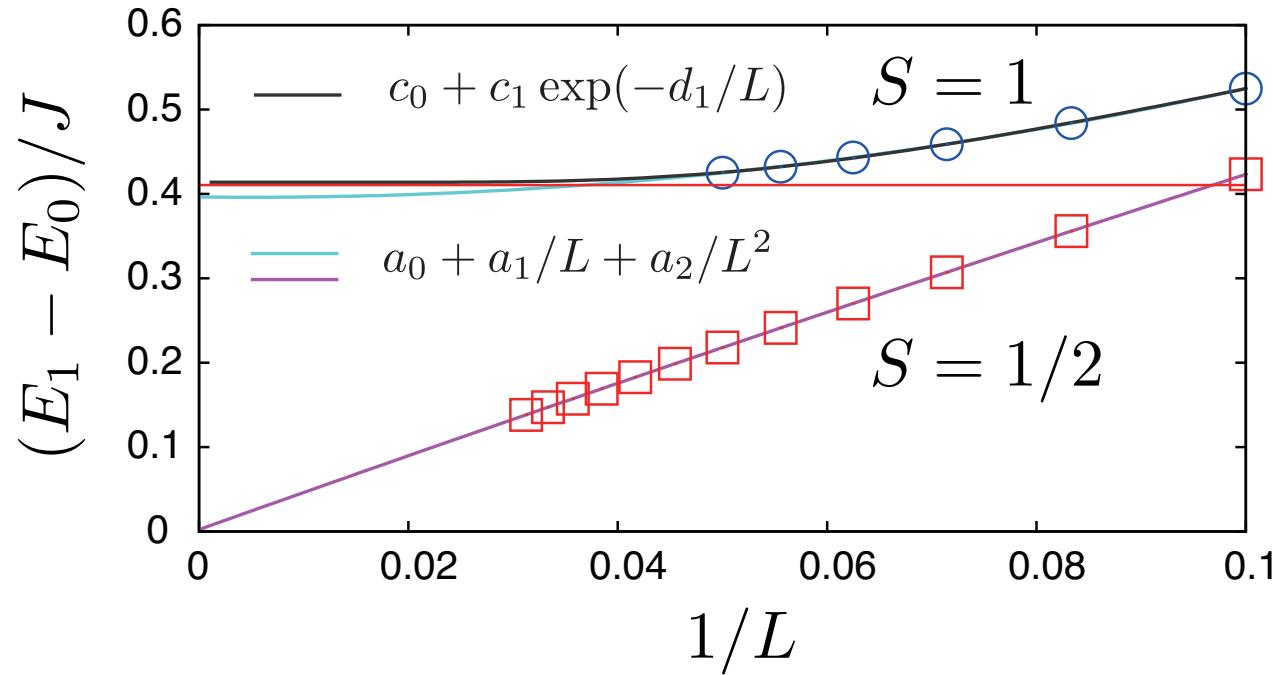
7

Existence of edge modes is **not** the necessary condition

F. Pollmann, A. M. Turner, E. Berg, and M. Oshikawa,
Phys. Rev. B 81, 064439 (2010).

$S=1$ Heisenberg Model

Haldane gap



ED: $S=1$ up to 22 sites

O. Golinelli, Th. Jolicoeur, and R. Lacaze, Phys. Rev. B 50, 3037 (1994).

QMC: S. Todo and K. Kato, Phys. Rev. Lett. 87, 047203 (2001).

Exercise: Use Standard Mode 2

$$\hat{H} = J \sum_{\langle i,j \rangle} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \Delta \hat{S}_i^z \hat{S}_j^z \right) + D \sum_i (\hat{S}_i^z)^2$$

Two body interaction can be defined by `interall.def`

$$\hat{H}_I = \sum_{i,j,k,\ell} \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} I_{ijkl}^{\sigma_1\sigma_2\sigma_3\sigma_4} \hat{c}_{i\sigma_1}^\dagger \hat{c}_{j\sigma_2} \hat{c}_{k\sigma_3}^\dagger \hat{c}_{\ell\sigma_4}$$

Bogoliubov representation for $S=1$

$$\hat{S}_i^z = \sum_{\sigma=-1,0,+1} \sigma \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$$

$$(\hat{S}_i^z)^2 = \left(\hat{c}_{i,+1}^\dagger \hat{c}_{i,+1} - \hat{c}_{i,-1}^\dagger \hat{c}_{i,-1} \right)^2$$

σ	ternary
-1	0
0	1
+1	2

Lines define the single ion anisotropy of 0 th site

$(\hat{S}_0^z)^2$	0	0	0	0	0	0	0	1.00	0.00
	0	0	0	0	0	2	0	2	-1.00
	0	2	0	2	0	0	0	-1.00	0.00
	0	2	0	2	0	2	0	1.00	0.00

After adding lines in `interall.def`, please update `NInterAll`