

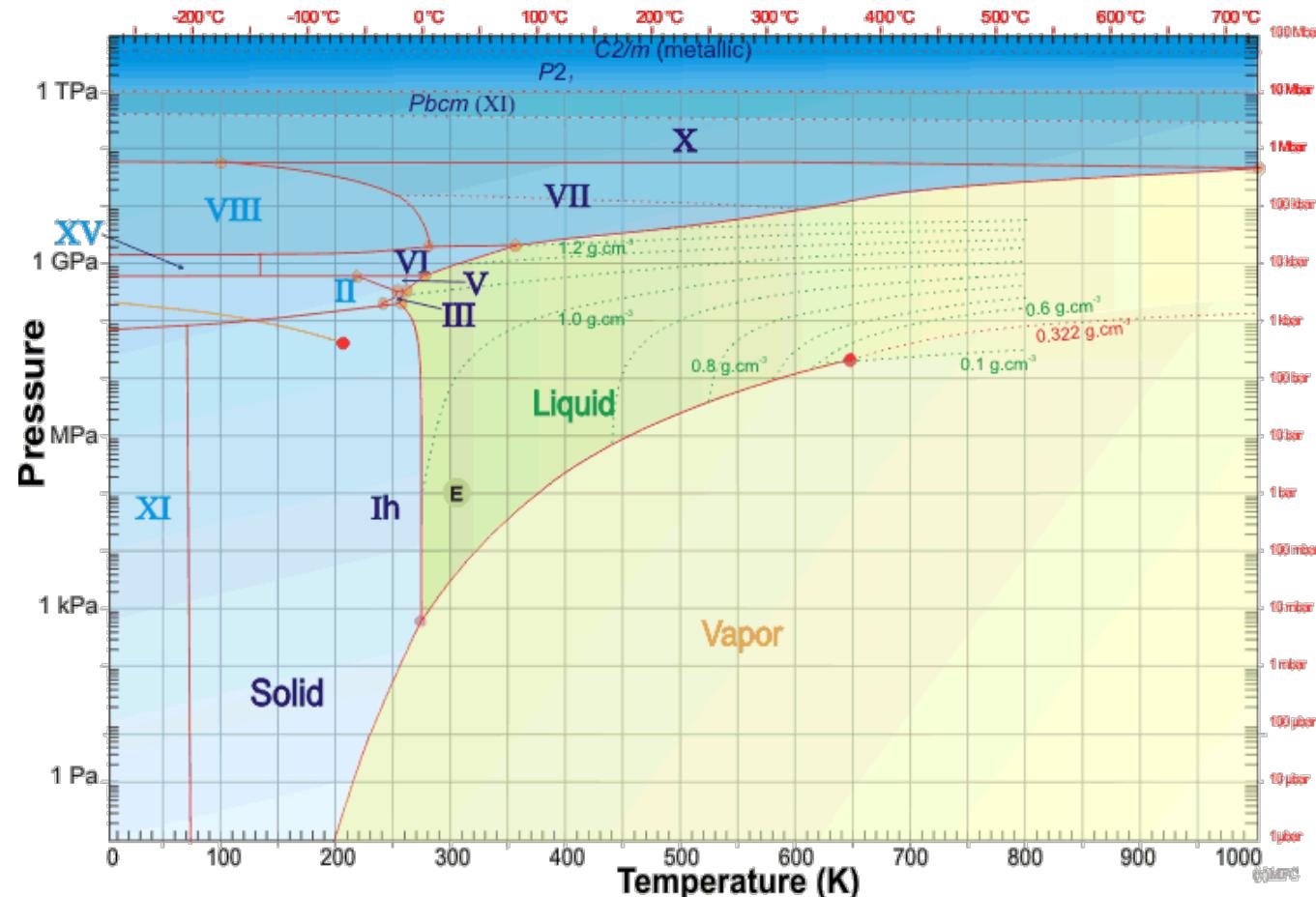
CSA Summer School Lecture 3

#1

2017/8/23

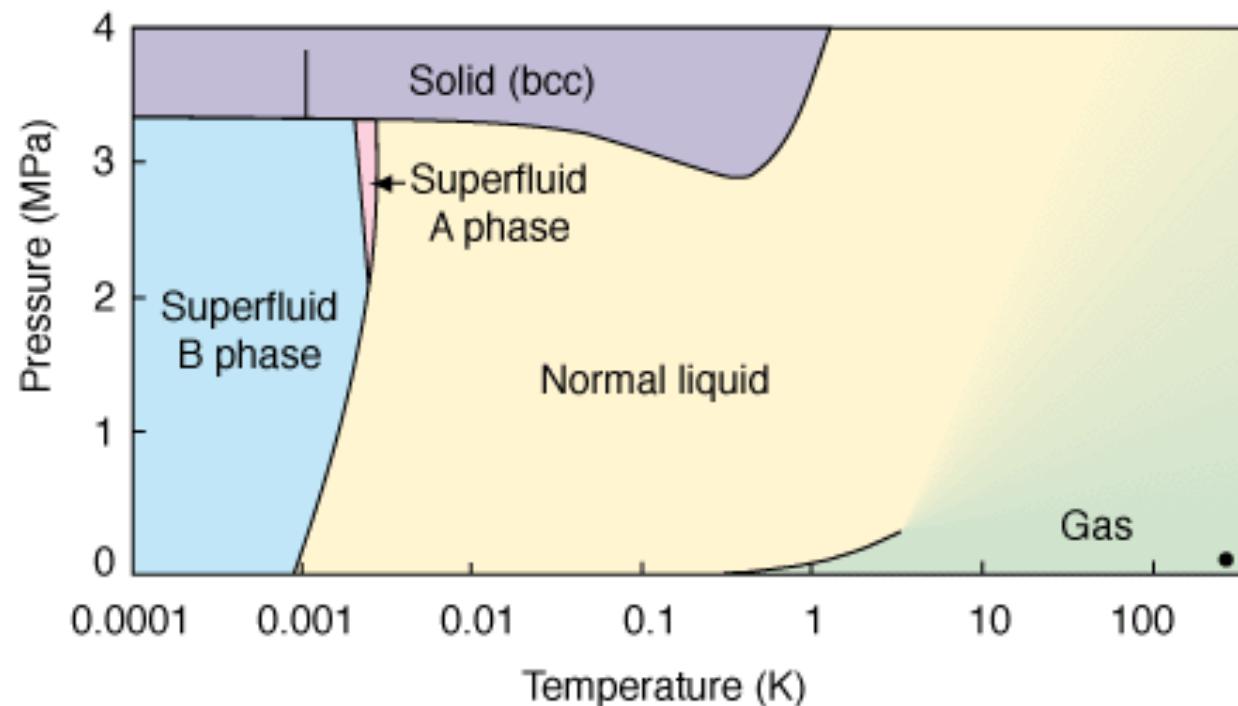
Quantum Many-Body Problems:
Numerical Exact Diagonalization
& Haldane Gap

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?

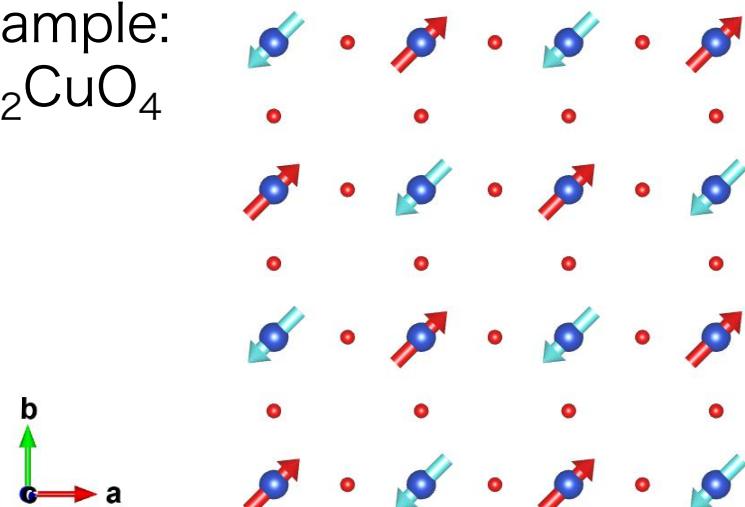
Quantum Phases: More is different

-Spontaneous symmetry breaking (SSB)

Superfluidity, superconductivity, magnetic order

Example:

La_2CuO_4



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

-Topology

Classification of Crystalline Solids In One-Body Picture

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

Trivial insulator

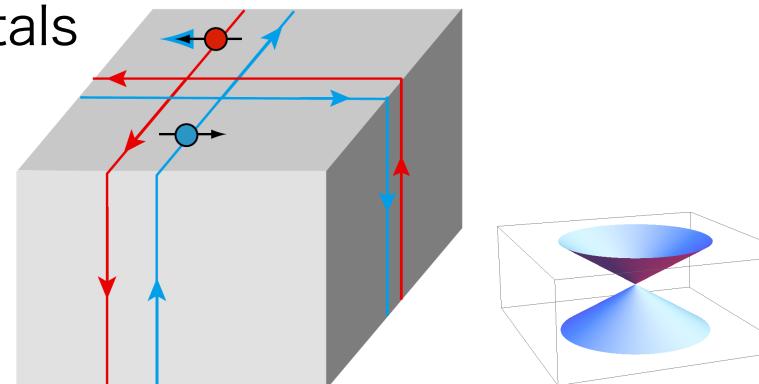
Si

Topological insulator

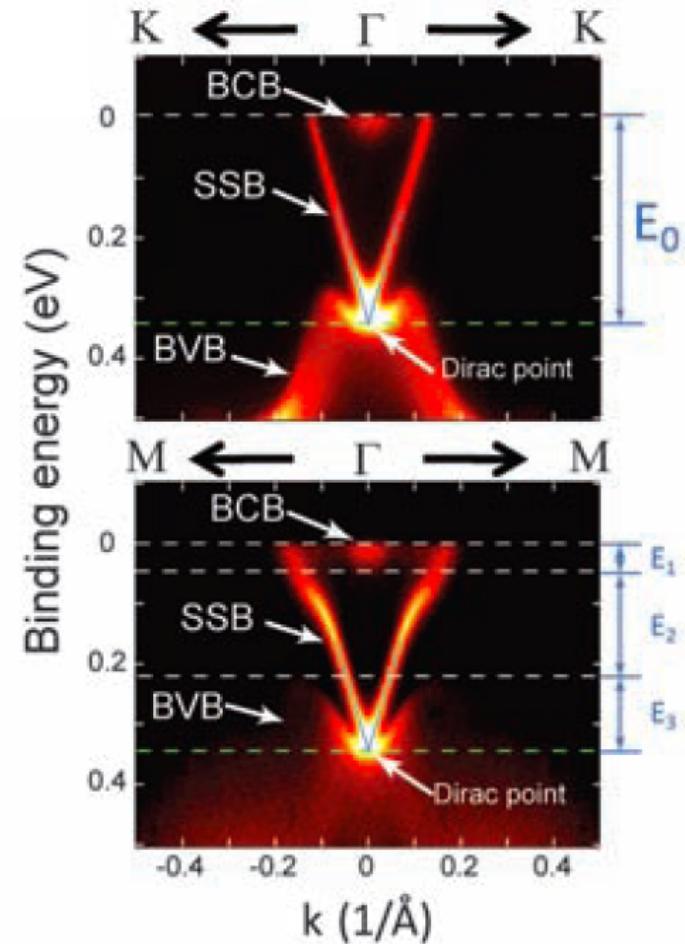
Bi_2Te_3

Thermoelectric

Surface metals



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



An example: Chern insulator

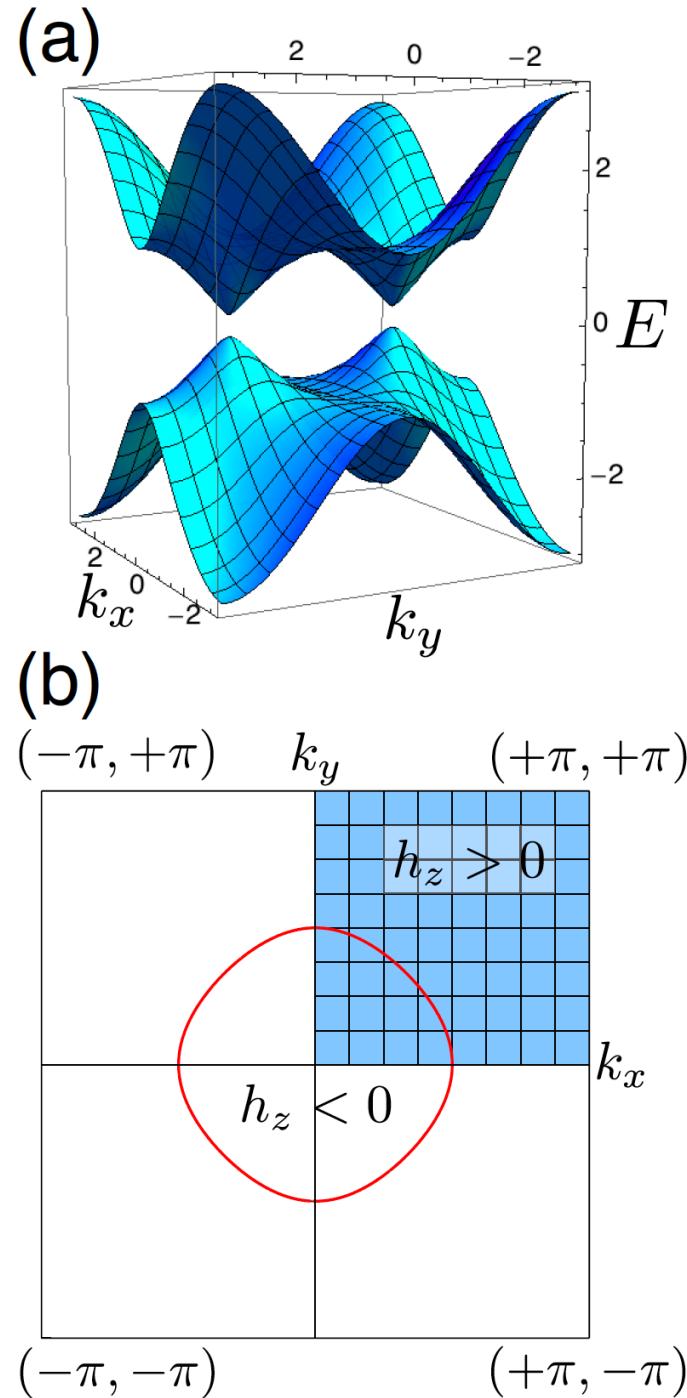
$$\hat{H}_{\text{2D}}(\vec{k}) = h_x(\vec{k})\hat{\sigma}_x + h_y(\vec{k})\hat{\sigma}_y + h_z(\vec{k})\hat{\sigma}_z,$$

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

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

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

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



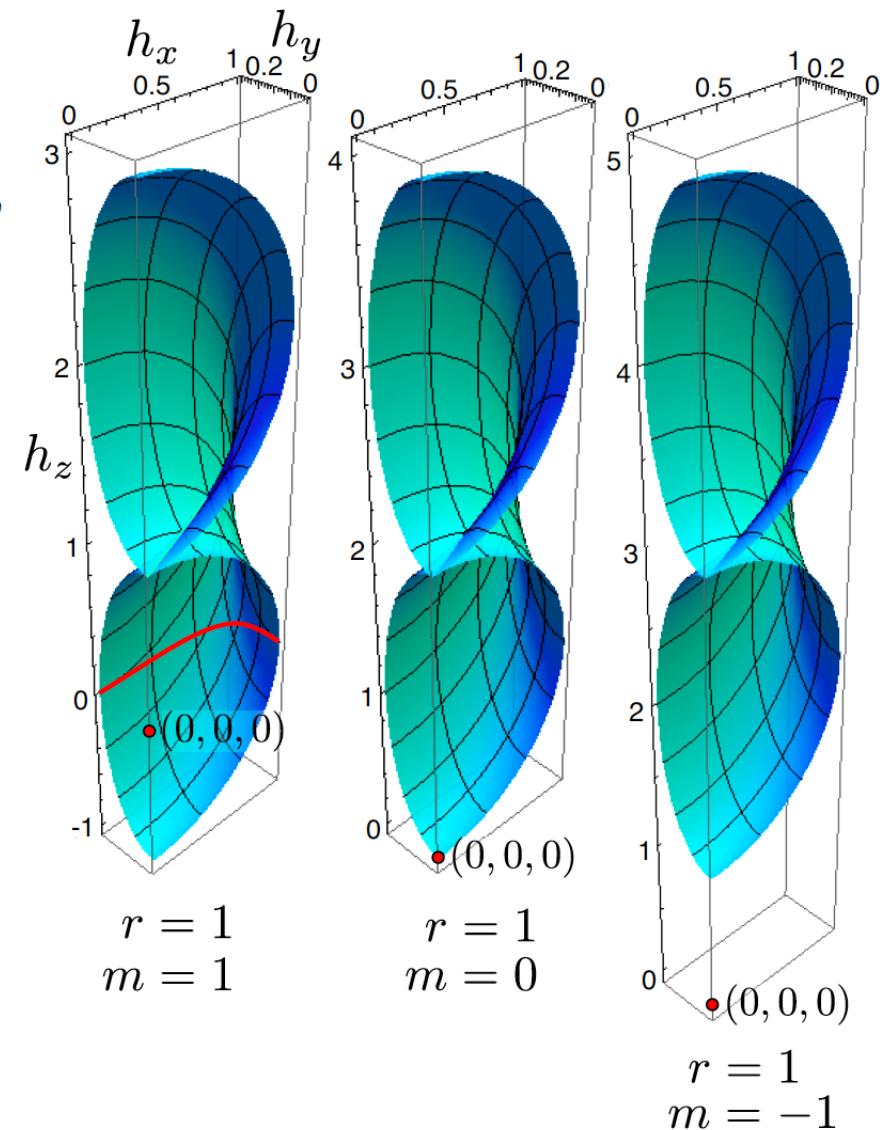
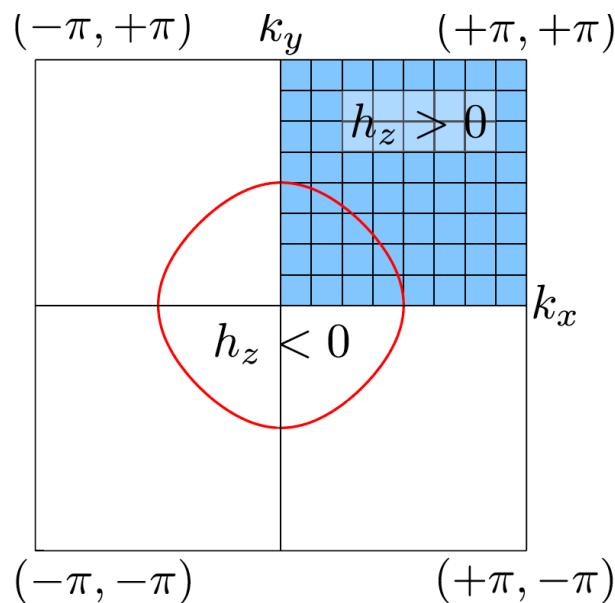
An example: Chern insulator

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 of 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

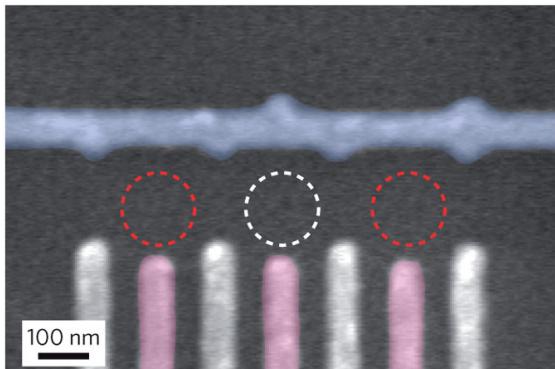
$$\bar{N} = \frac{1}{3} \frac{9}{0.48} = 6(!). \quad (2.14)$$

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)



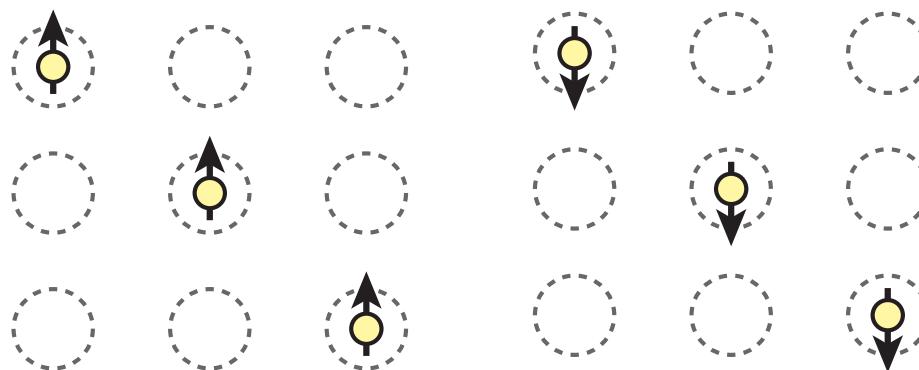
Quantum dot:

- 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

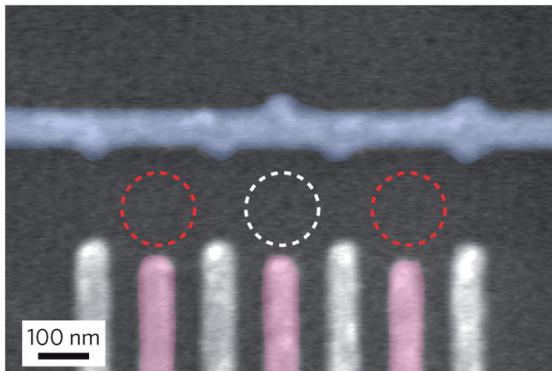
→ Number of states = 2×3 (factor 2 from spin)



Quantum Many-Body Problems

An example: 3 Quantum dots

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

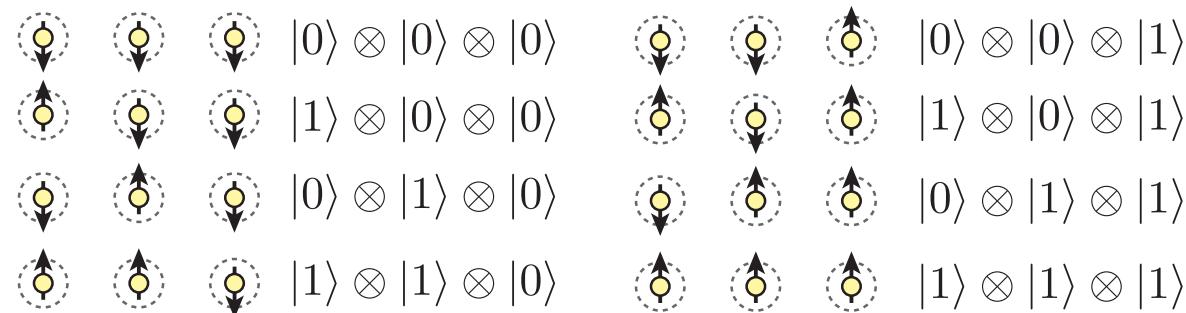


Quantum dot:

- 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)

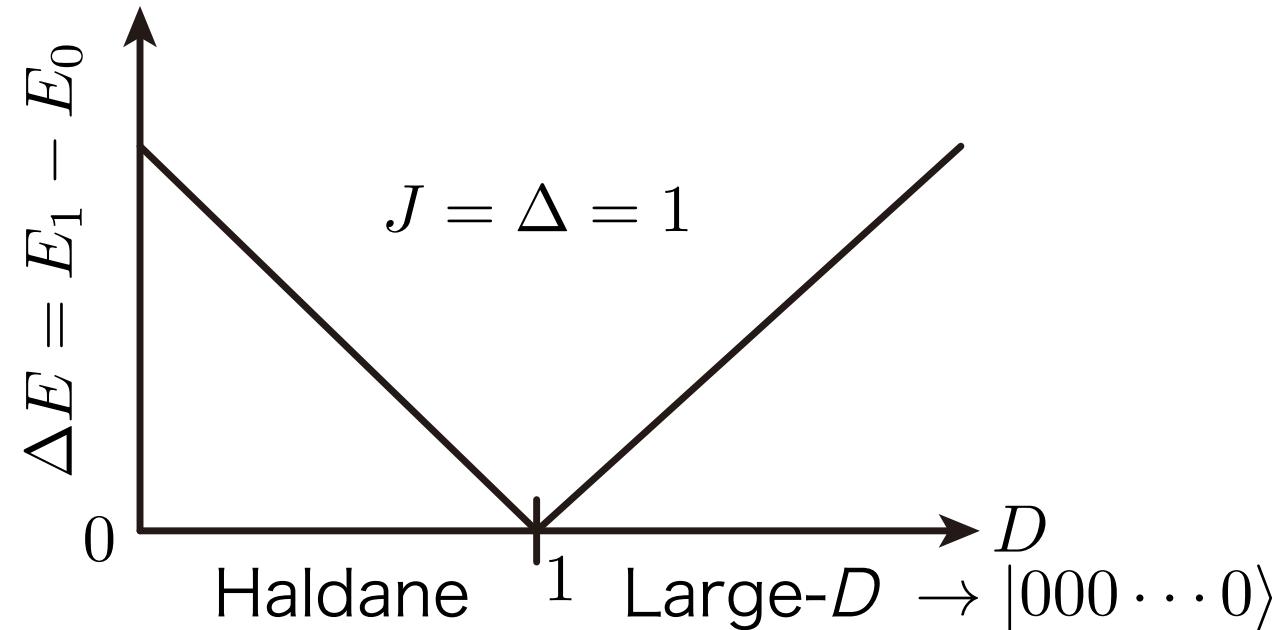
Target: Haldane Gap and Topology

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

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

\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

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

\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
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

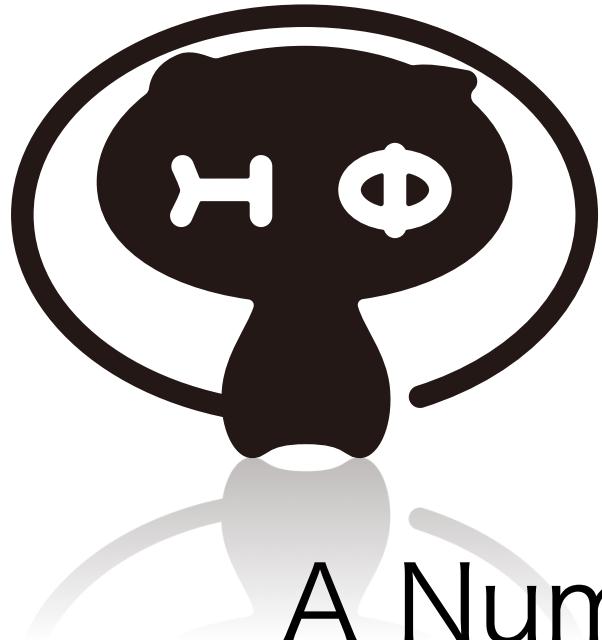
TITPACK by Y. Taguchi & H. Nishimori (1985-)
Heisenberg & XXZ model

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:
 $H\Phi$

$\text{H}\Phi$

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

HΦ Developers



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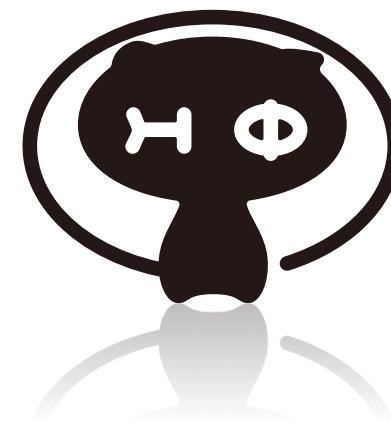
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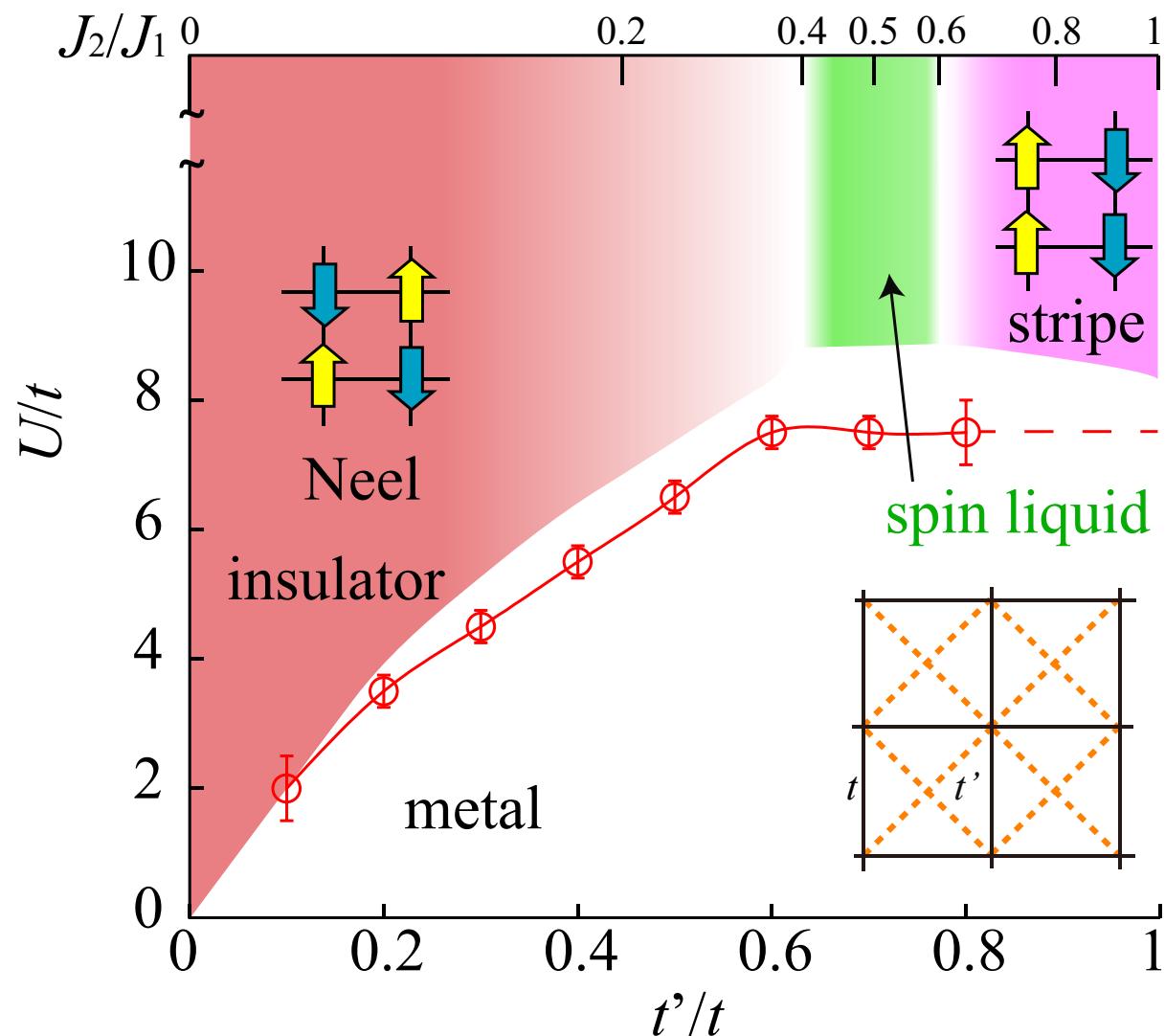
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Acknowledgement:
Prof. Takeo Hoshi (Tottori Univ.)
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“*Project for advancement of software usability in materials science*” by ISSP



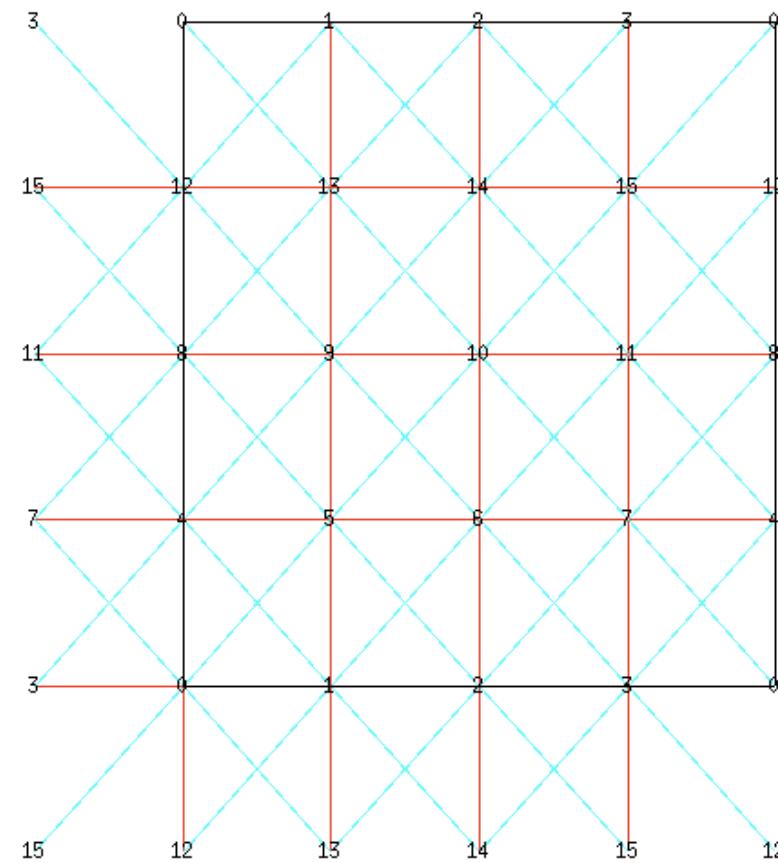
An Example: t - t' Hubbard

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

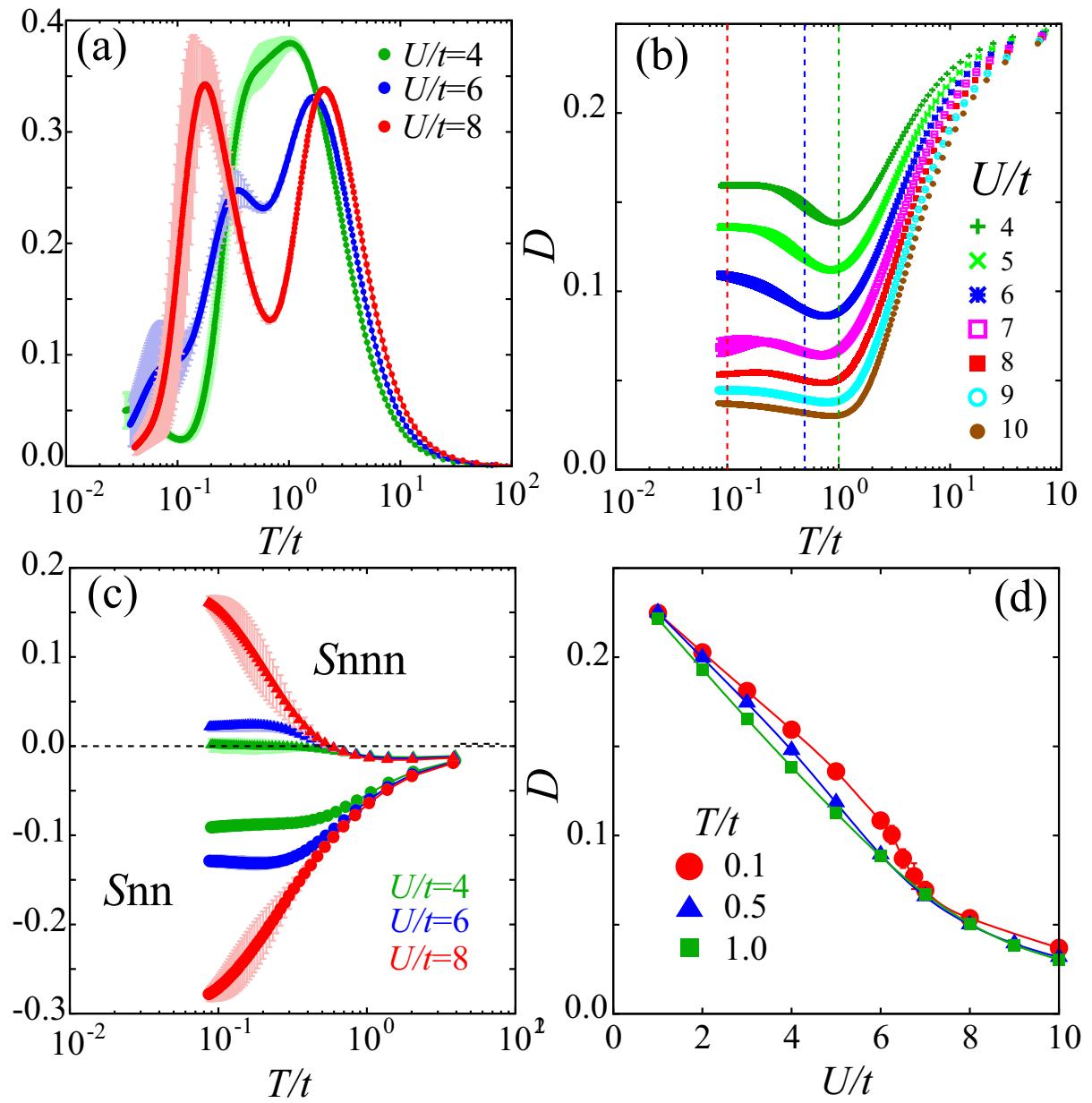
$$\langle H \rangle, \langle H^2 \rangle, \langle c_{i\sigma_1}^\dagger c_{j\sigma_2} \rangle, \langle c_{i\sigma_1}^\dagger c_{j\sigma_2} c_{k\sigma_3}^\dagger c_{l\sigma_4} \rangle$$

$$t'/t = 0.5$$

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

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

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



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

Expert input

Def. files for Hamiltonian
Def. files for controlling simulation

Making input files
from scratch

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

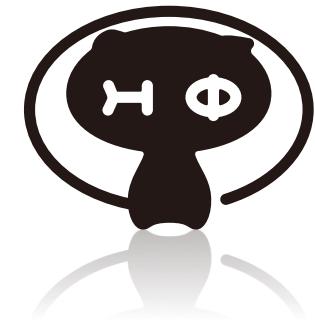
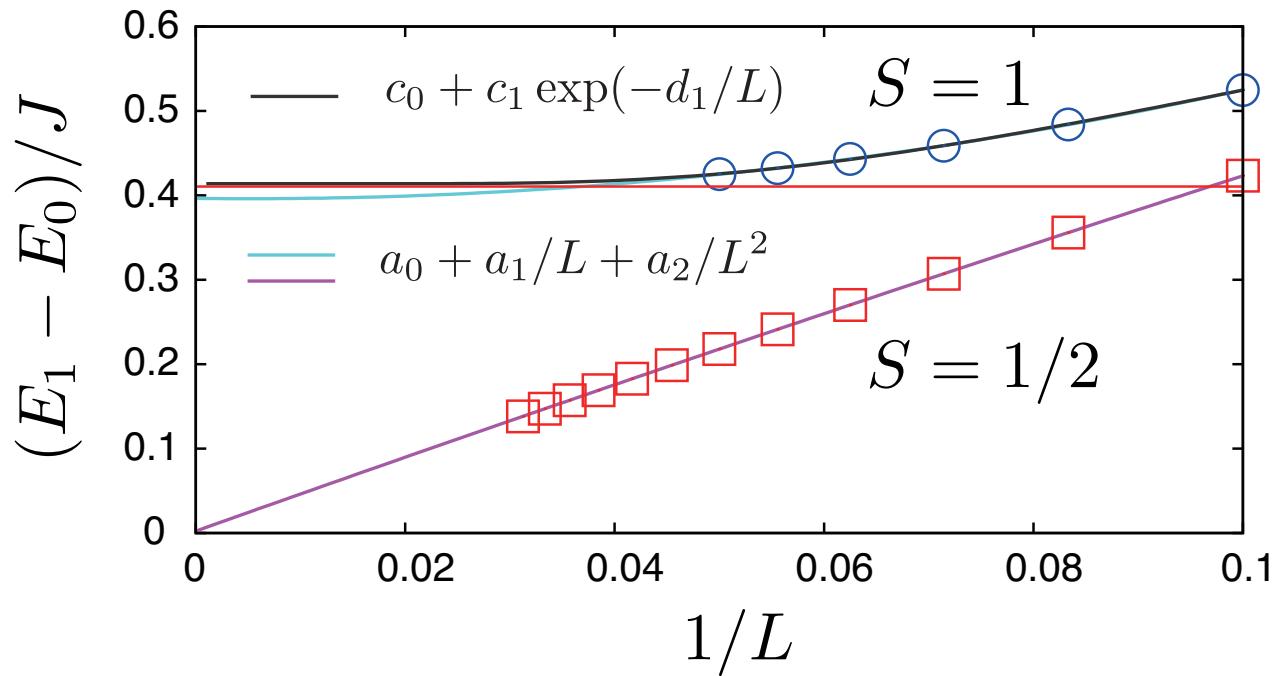
$$\hat{H} = J \sum_{\langle i,j \rangle} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \Delta \hat{S}_i^z \hat{S}_j^z \right) + D \sum_i (\hat{S}_i^z)^2$$

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

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

Orthonormalized many-body basis

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

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

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

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

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

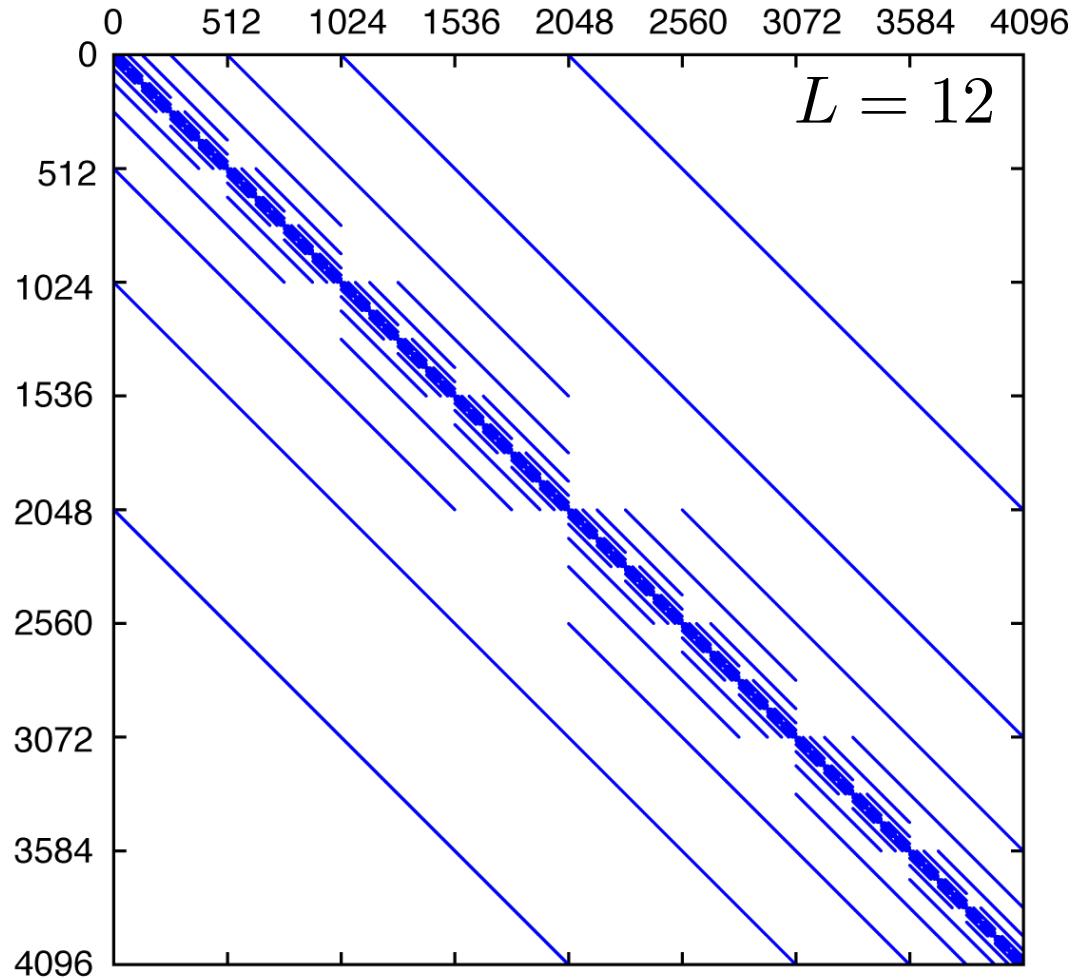
$$\left[\sum_{i=0}^{L-1} \hat{S}_i^z \hat{S}_{i+1}^z, \sum_{i=0}^{L-1} \hat{S}_i^x \right] \neq 0$$

→ 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 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

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 0 th site in `interall.def`

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

Exercise: Use Expert Mode

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

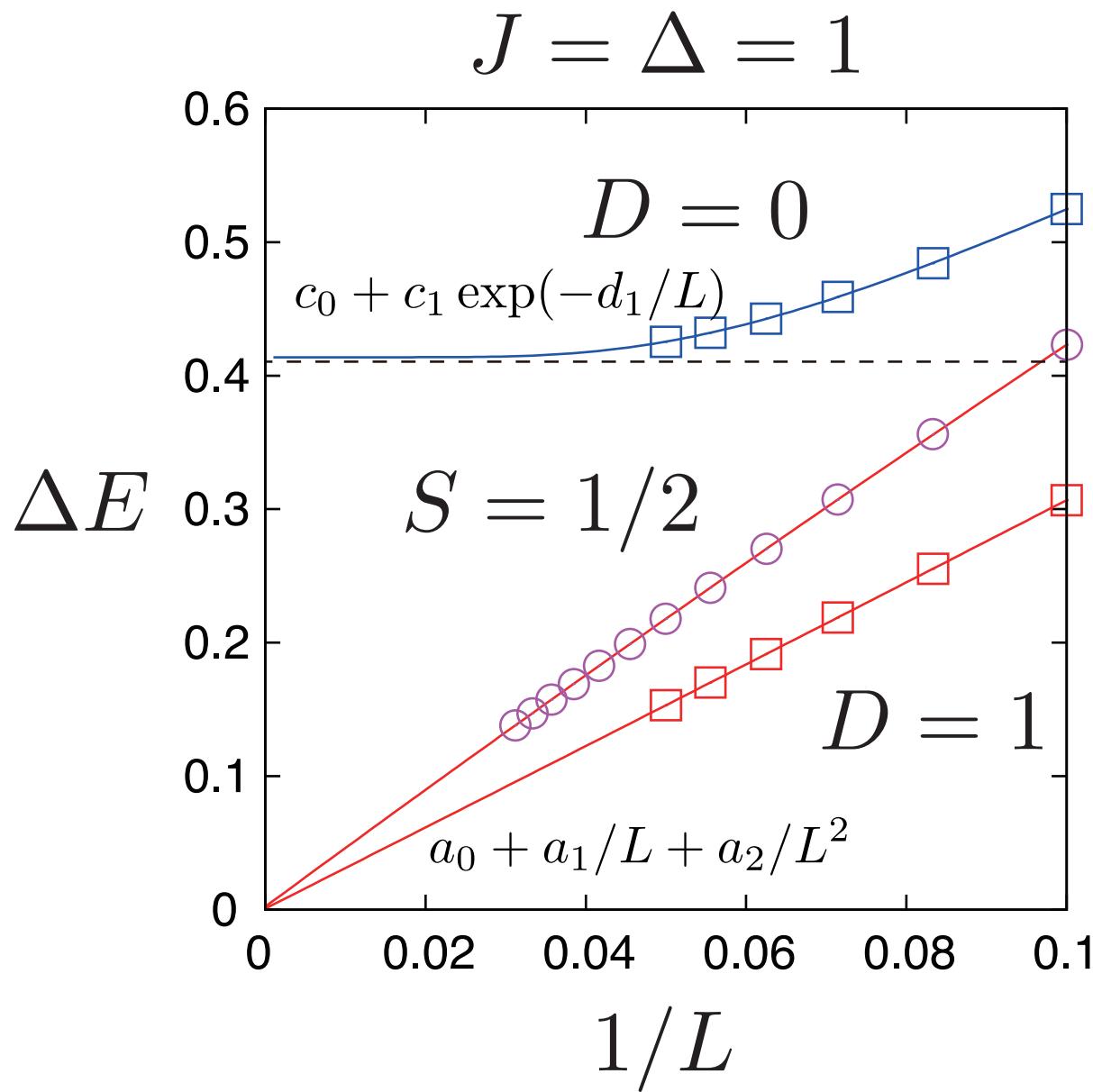
LOB(P)CG by A. V. Knyazev, SIAM j. Sci. Compt. 23, 517 (2001).

CG method is selected by CalcType in calcmod.def

modpara.def

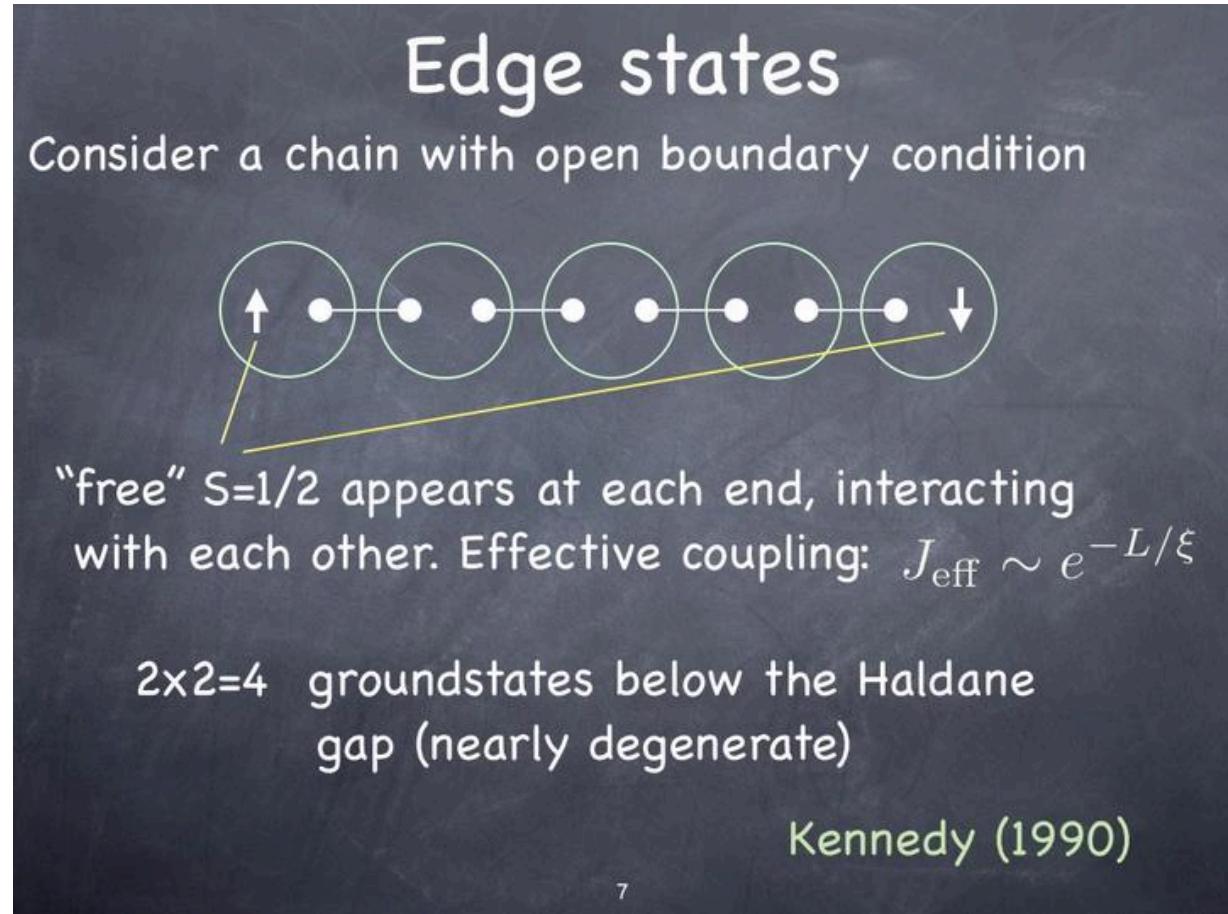
```
-----
Model_Parameters    0
-----
HPhi_Cal_Parameters
-----
CDataFileHead      zvo
CParaFileHead     zqp
-----
Nsite              12
Lanczos_max        2000
initial_iv         -1
exct               1   ← How many states you will obtain
LanczosEps          14   ← from the lowest eigenstate
LanczosTarget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

A Goal: Gap Estimate



Beyond: Open Boundary with Edge States

M. Oshikawa
From seminar @KITP



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).