

多体問題の計算科学

Computational Science for Many-Body Problems

#13 Parallelization for many-body problems
15:10-16:40 July 12, 2022

Lecture slide:

<https://github.com/compsci-alliance/many-body-problems>

1. Parallelization
2. Other numerical methods

Parallelization

Performance of computer

How many times does the computer multiply/add per second?

How much data does the computer memorize?

How much data does the computer read/write per second?

←Parallelization matters!

(Revisited) FLOP/s

Floating-point Operations Per Second

An example: Intel Xeon Phi Nights Landing

Intel Xeon Phi 7250 (1.4GHz, 68 cores, 112GB)

- 1.4×10^9 instructions per second

(instruction to perform double precision add or multiply)

-Intel AVX-512 instruction*

double precision floating point number (8byte=64bit)

8 double-precision multiply-add** operations

$\rightarrow 1.4 \times 10^9 \times 16 \times 68$ FLOP/s per processor

*Other instruction set:

SVE (for example, A64FX of Fugaku)

**Multiply-add: $a \leftarrow a + (b \times c)$

(Revisited) Increasing FLOP/s

Clock rate saturated

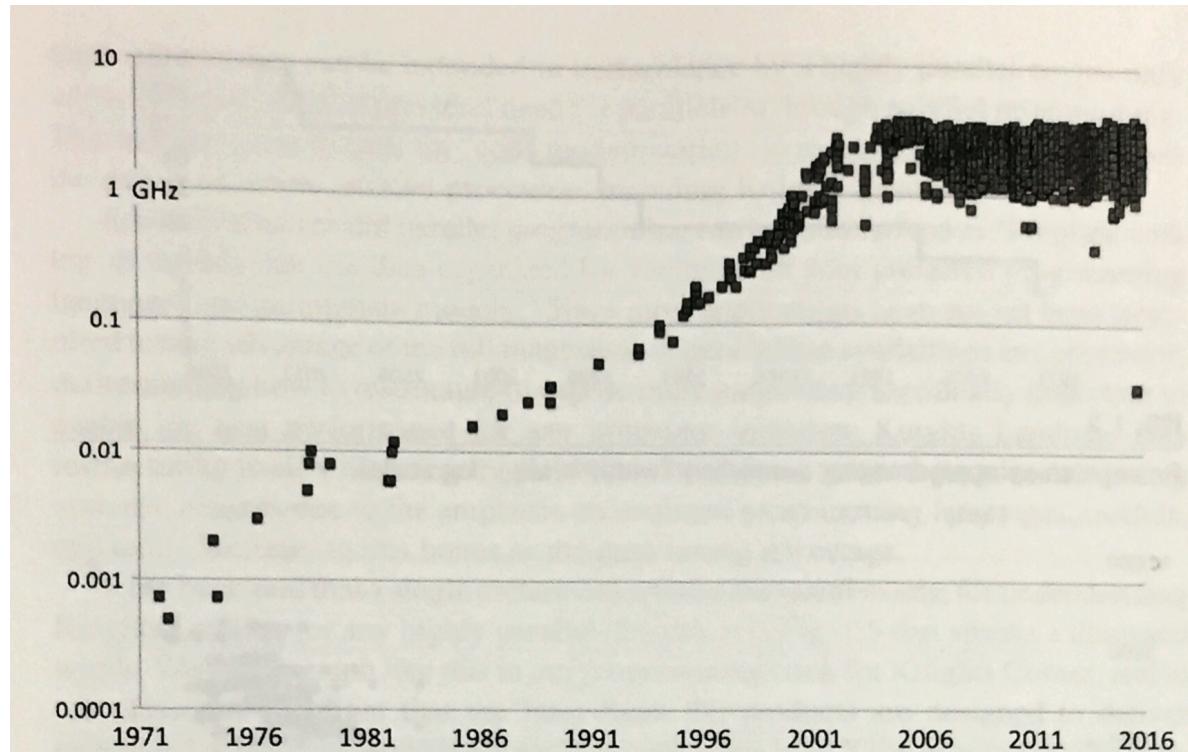


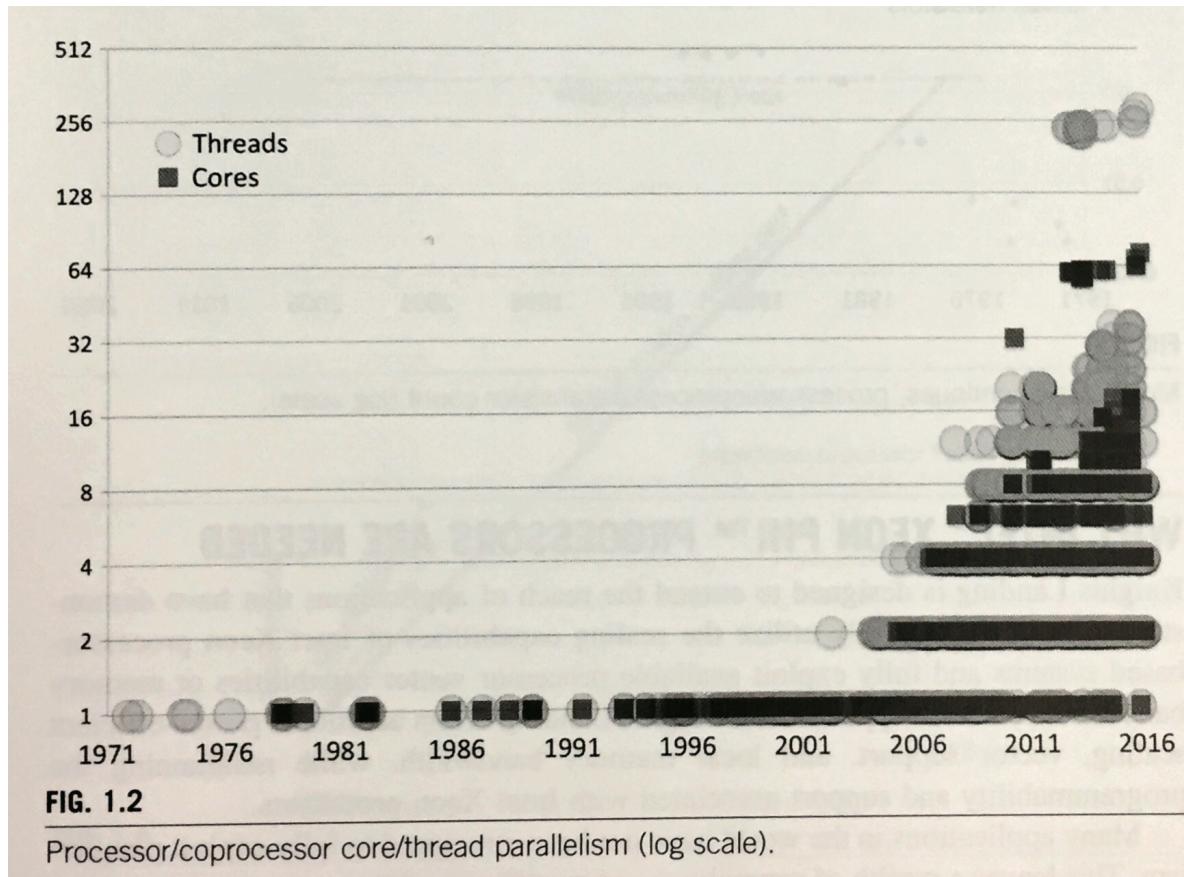
FIG. 1.1

Processor/coprocessor speed era (log scale).

J. Jeffers, J. Reinders, and A. Sodani,
Intel Xeon Phi Processor High Performance Programming

(Revisited) Increasing FLOP/s

Number of cores



J. Jeffers, J. Reinders, and A. Sodani,
Intel Xeon Phi Processor High Performance Programming

(Revisited) Supercomputers in UTokyo

Oakbridge-CX

Intel Xeon Platinum 8280
1,368 nodes

Wisteria/BDEC-01

Odyssey: A64FX 7,680 nodes
Aquarius: Intel Xeon + NVIDIA A100
45 nodes

A single CascadeLake:	4.8384 TFLOPS
A single A64FX:	3.3792 TFLOPS
A single A100:	19.5 TFLOPS

Ohtaka (CPU server)

ISSP, UTokyo@Kashiwa
AMD EPYC 7720 2.0GHz, 64 cores x 2
Memory: 258GiB
1,680 nodes



東京大学 物性研究所

THE INSTITUTE FOR SOLID STATE PHYSICS
THE UNIVERSITY OF TOKYO

(Revisited) “Fugaku” Supercomputer

Fugaku 富岳 @RIKEN, Kobe

-158,976 nodes

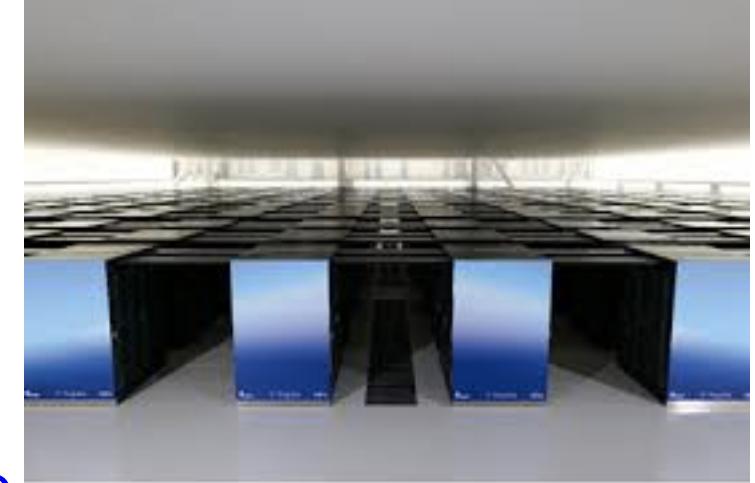
A64FX

48 cores/node

32 GiB/node



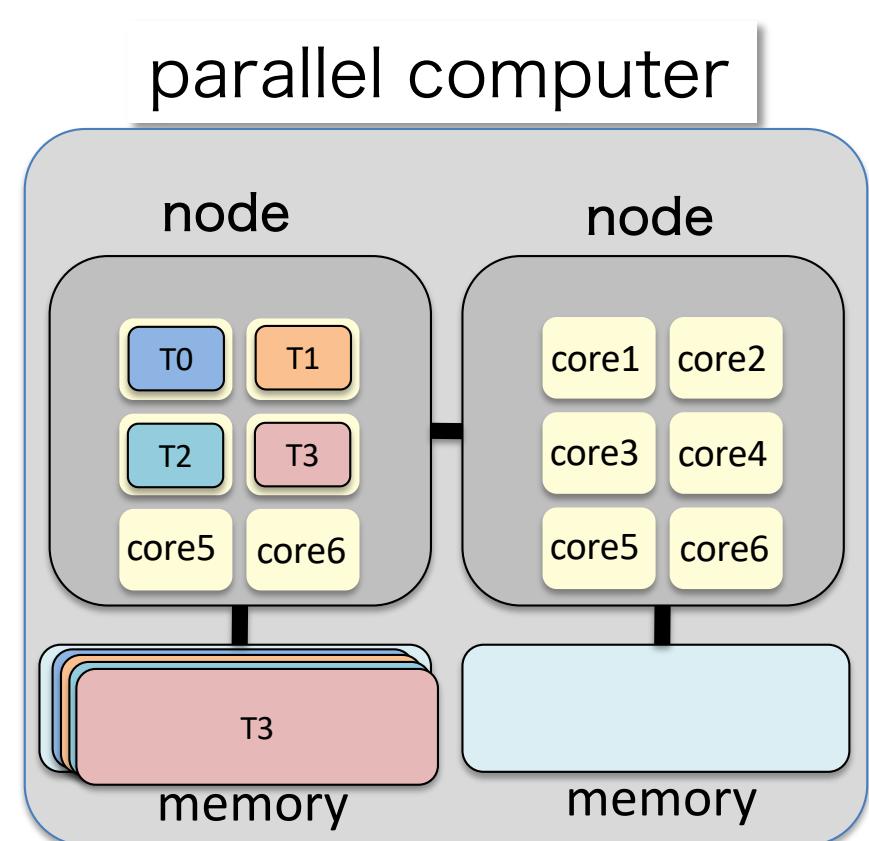
- 1st in Top500 & 25th in Green500
on November 2021



Parallelization

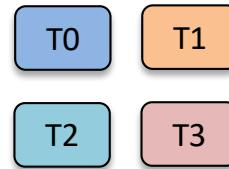
- Shared Memory Parallelization
Data on the memory of the node
is shared by the cores in the node

-Thread parallel
Realized by, for example,
OpenMP
[OpenACC](#)



Simple example in C lang: Divide a loop

```
#pragma omp parallel default(None) private(j) shared(a,b){  
#pragma omp for  
    for(j = 0; j < N; j++){  
        C[j] = a*A[j] + b;  
    }  
}
```



Dangerous example

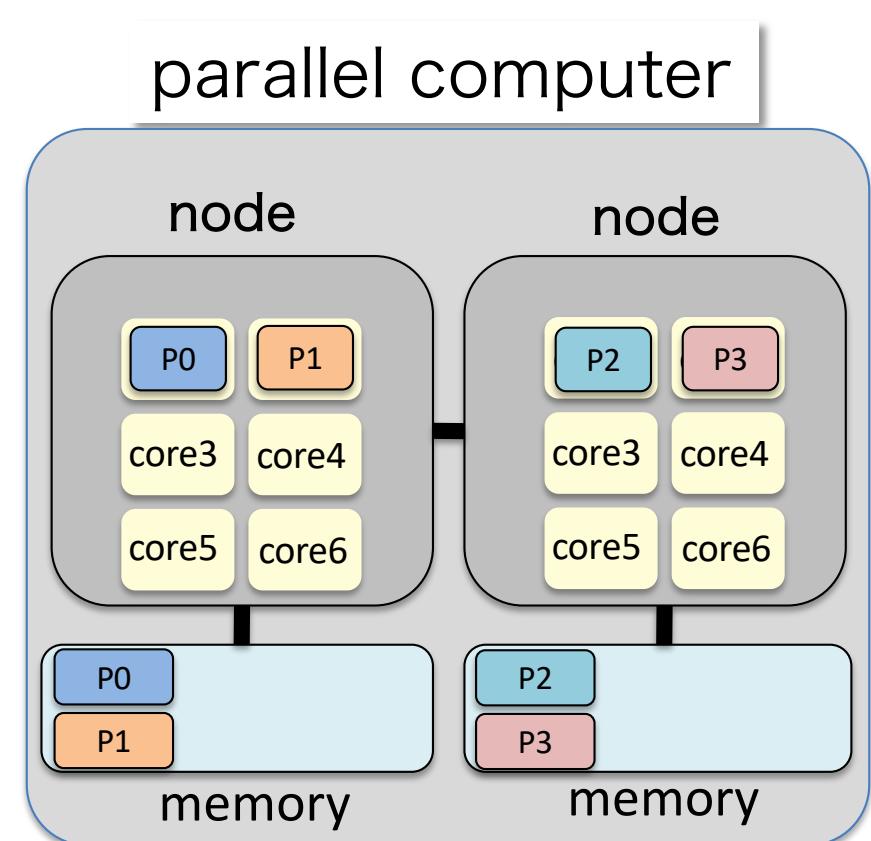
```
#pragma omp parallel default(None) private(j) shared(a,b){  
#pragma omp for  
    for(j = 0; j < N-1; j++){  
        C[j+1] = a*C[j] + b;  
    }  
}
```

Dependency on former steps

Parallelization

- Distributed Memory Parallelization
Each *process* can access its own data region in the node.

-Process parallel
Among processes,
data can be transferred
through MPI
(Message Passing Interface)



Declaration of MPI in C lang

```
ierr = MPI_Init(&argc, &argv);
ierr = MPI_Comm_size(MPI_COMM_WORLD, &nproc);
ierr = MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
```

nproc: # of processes

myrank: rank of the process, often used to generate
process-dependent random seed for MCMC

A Problem in Massively Parallel MCMC

Burn-in steps in Markov chain Monte Carlo

- Markov chain Monte Carlo (MCMC), for example, Metropolis-Hastings algorithm generates samples following a give probability distribution with *an initial state*
 - A finite sequence of steps in the initial stage of the Markov chain is *often* discarded:
Equilibration steps, burn-in or warm-up steps

cf.) Textbooks

A Problem in Massively Parallel MCMC

Extreme limit of massively parallel MCMC

- Few or few tens of warm-up steps and a single sample per process:
1 step annealed importance sampling with trivial prior distribution and no weights

of warm-up steps (> “auto correlation time”) is constant independent of # of processes

→ Total # of MC samples / # of processes will be much smaller than # of warm-up steps

Non Markov chain MC

Yukito Iba, *Population Monte Carlo algorithms*
<https://doi.org/10.1527/tjsai.16.279>

Population MC

- Diffusion MC
- Population annealing:
Annealed importance sampling+resampling

K. Hukushima and Y. Iba, AIP Conf. Proc. 690, 200 (2003)

Annealed importance sampling

$\{m_0^k, m_1^k, \dots, m_n^k\}$ D. A. Hendrix and C. Jarzynski, J. Chem. Phys. 114, 5974 (2001).
 $\{m_0^k, m_1^k, \dots, m_n^k\}$ R. M. Neal, Statistics and Computing, 11, 125 (2001)

0. Prepare replicas sampled from a prior distribution with β_0
1. Change β_j ($j=0, 1, \dots$), calculate the weight, and anneal the replica and repeat 1.

$$W_j^k = W_{j-1}^k e^{-(\beta_j - \beta_{j-1}) f(m_{j-1}^k)}$$

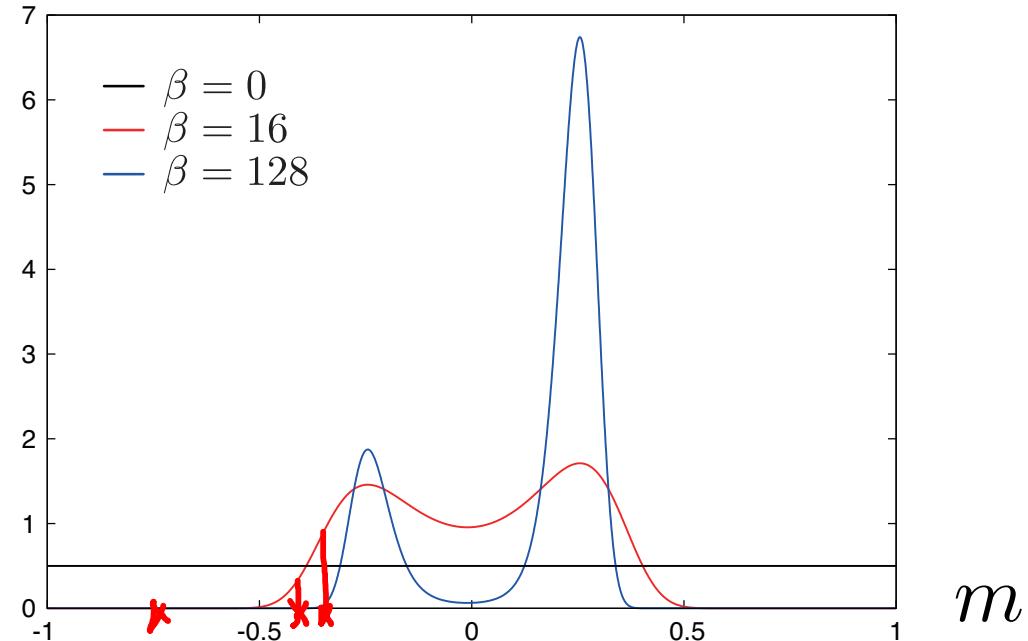
2. When $\beta_n = \beta_t$, take averages over the replicas with the weight

$$\beta_0 \leq \beta_1 \leq \dots \leq \beta_n = \beta_t$$

$$p(m) \propto e^{-\beta f(m)}$$

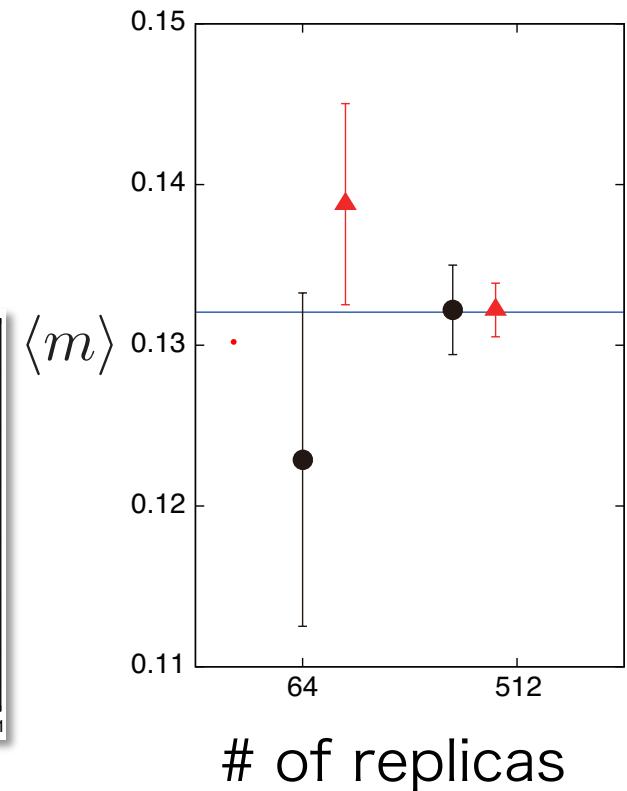
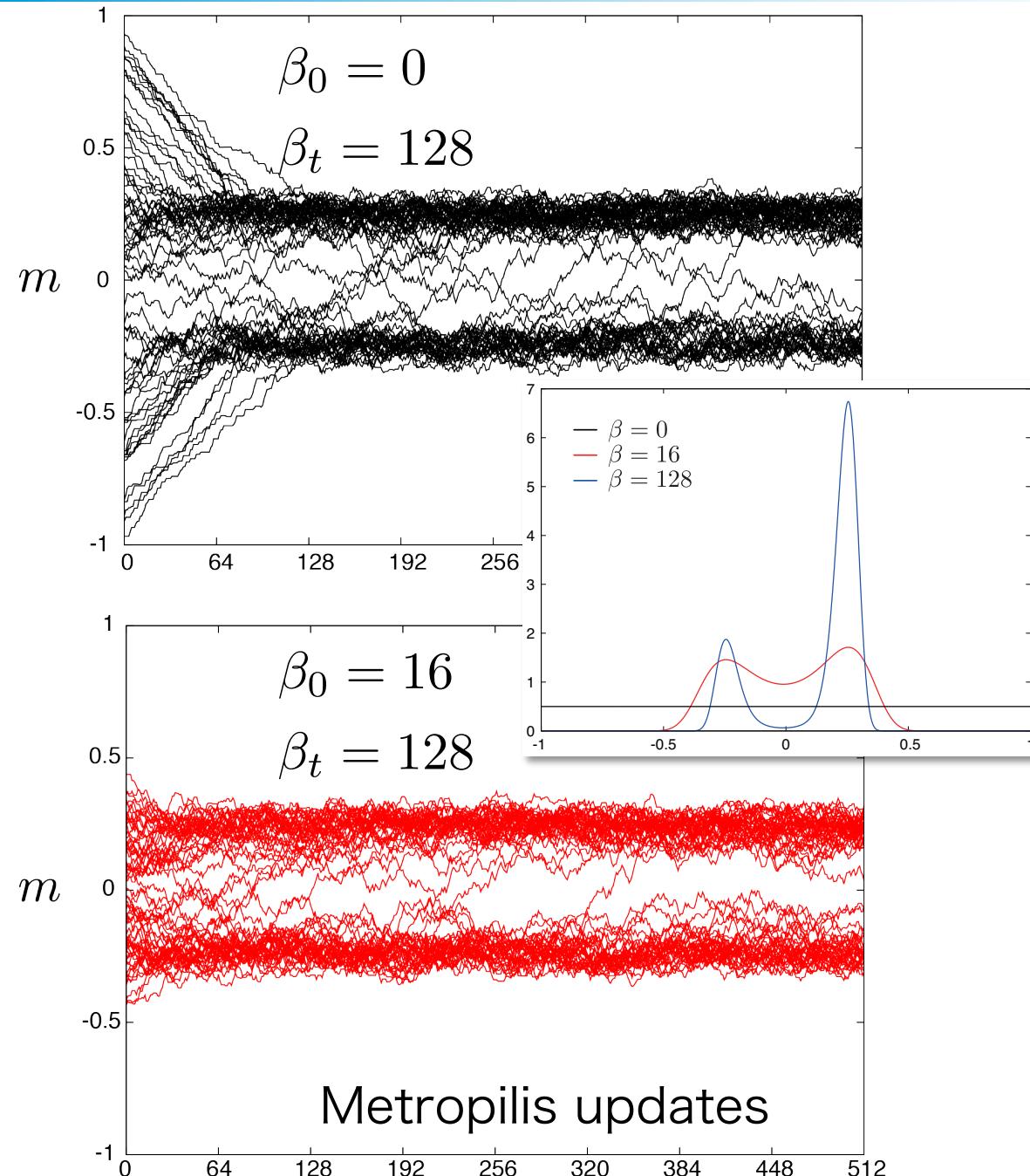
$$f(m) = -hm + rm^2 + vm^4$$

$$(h, r, v) = (0.02, -1, 8)$$



-Support condition $V_0 \supseteq V_1 \supseteq \dots \supseteq V_n$ $V_j = \{x | f_j(x) \neq 0\}$

One step annealed importance sampling



$$n = 1$$

$$W_1^k = e^{-(\beta_t - \beta_0)} f(m_0^k)$$

$$\langle m \rangle = \frac{\sum_k m_n^k W_n^k}{\sum_k W_n^k}$$

Distributed Wave Functions

Multiplication of Hamiltonian to Wave Function

Example of multiplication

-4 spins

$$(\hat{S}_1^- \hat{S}_3^+ + \hat{S}_1^+ \hat{S}_3^-) |0\textcolor{red}{1}00\rangle = |000\textcolor{red}{1}\rangle$$

$$(\hat{S}_1^- \hat{S}_3^+ + \hat{S}_1^+ \hat{S}_3^-) |000\textcolor{red}{1}\rangle = |0\textcolor{red}{1}00\rangle$$

$$\hat{S}_\ell^+ = S_\ell^x + iS_\ell^y$$

$$\hat{S}_\ell^- = S_\ell^x - iS_\ell^y$$

$$|\phi\rangle = \sum_{I_j \in \{0,1\}} C_{I_0 I_1 I_2 I_3} |I_0 I_1 I_2 I_3\rangle$$

$$(\hat{S}_1^- \hat{S}_3^+ + \hat{S}_1^+ \hat{S}_3^-) |\phi\rangle$$

$$C_{I_0 \textcolor{red}{1} I_2 0} \leftarrow C_{I_0 \textcolor{red}{0} I_2 1}$$

$$C_{I_0 \textcolor{red}{0} I_2 1} \leftarrow C_{I_0 \textcolor{red}{1} I_2 0}$$

Multiplication of Hamiltonian to Wave Function

Example of multiplication

-4 spins

-Parallel: 2 processes

(processes are labeled by their rank)

$$|I_0 I_1 I_2 I_3\rangle$$

0	$ 0000\rangle$	$\rightarrow 0$
1	$ 1000\rangle$	$\rightarrow 1$
2	$ 0100\rangle$	$\rightarrow 8$
3	$ 1100\rangle$	$\rightarrow 9$
<hr/>		
4	$ 0010\rangle$	$\rightarrow 4$
5	$ 1010\rangle$	$\rightarrow 5$
6	$ 0110\rangle$	$\rightarrow 12$
7	$ 1110\rangle$	$\rightarrow 13$
<hr/>		
8	$ 0001\rangle$	$\rightarrow 2$
9	$ 1001\rangle$	$\rightarrow 3$
10	$ 0101\rangle$	$\rightarrow 10$
11	$ 1101\rangle$	$\rightarrow 11$
<hr/>		
12	$ 0011\rangle$	$\rightarrow 6$
13	$ 1011\rangle$	$\rightarrow 7$
14	$ 0111\rangle$	$\rightarrow 14$
15	$ 1111\rangle$	$\rightarrow 15$

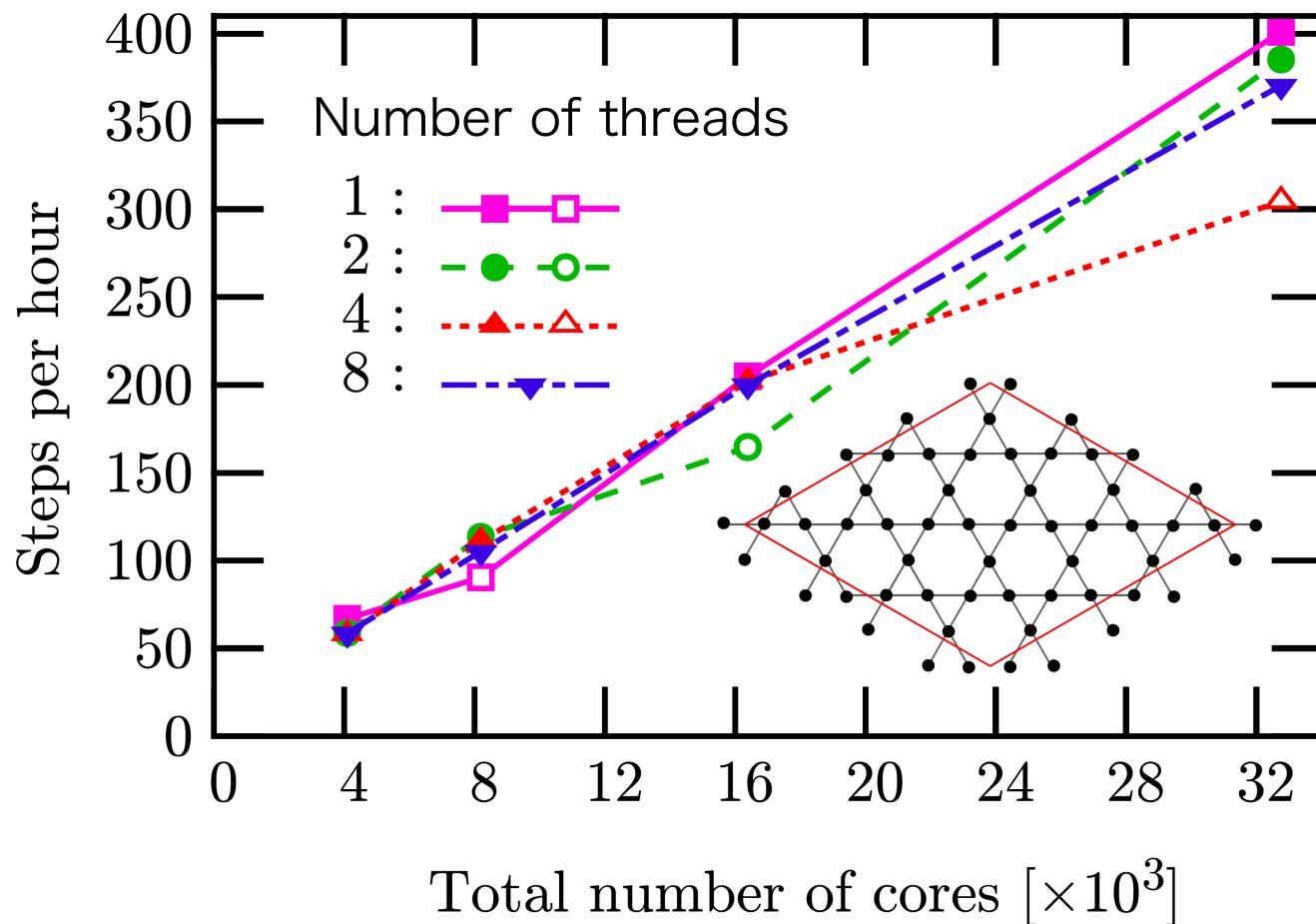
rank 0

rank 1

Speedup by Parallelization

36 spin Heisenberg model by $H\Phi$

@K computer, AICS, RIKEN



Other Numerical Methods

Other Numerical Methods

Ab initio

- Hartree-Fock theory*
- Density functional theory
 - Local density approximation*
 - Generalized gradient approximation*
 - Hybrid functional*
 - GW*
- Post Hartree-Fock (Quantum Chemistry)
 - Møller-Plesset*/Configuration interaction/Coupled cluster
- *Difficulties in describing Mott insulators
- Transcorrelated

Other Numerical Methods

Many-body

-Exact diagonalization

-Quantum Monte Carlo (QMC) method

BSS, continuous time,⋯

Variational Monte Carlo

Green's function Monte Carlo

Diffusion Monte Carlo (*also used in *ab initio* approaches*)

-Numerical renormalization group (NRG) method

K. Wilson

-Density matrix renormalization group (DMRG) method

S. White

-Matrix product and tensor network method

-Dynamical mean-field theory

Combination

(Revisited) Important Applications of Lanczos Method and Exact Wave Functions

Emergent concepts in many-body physics has been verified by using Lanczos and exact wf

Fractional quantum Hall effect

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

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

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

-Verification of Laughlin-Jastrow wave function

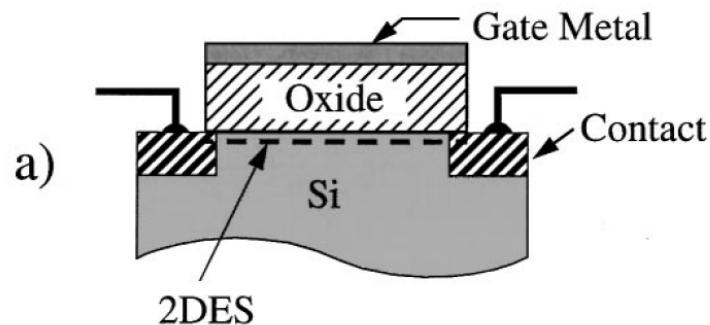
Thermalization of isolated quantum systems

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

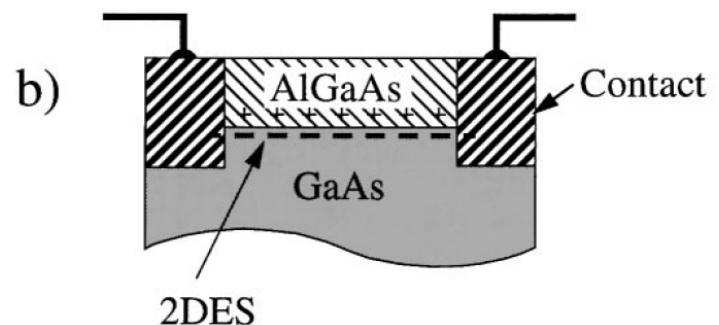
- Linear responses of strongly correlated electrons
- Frustrated magnetism
- Haldane gap

FQHE

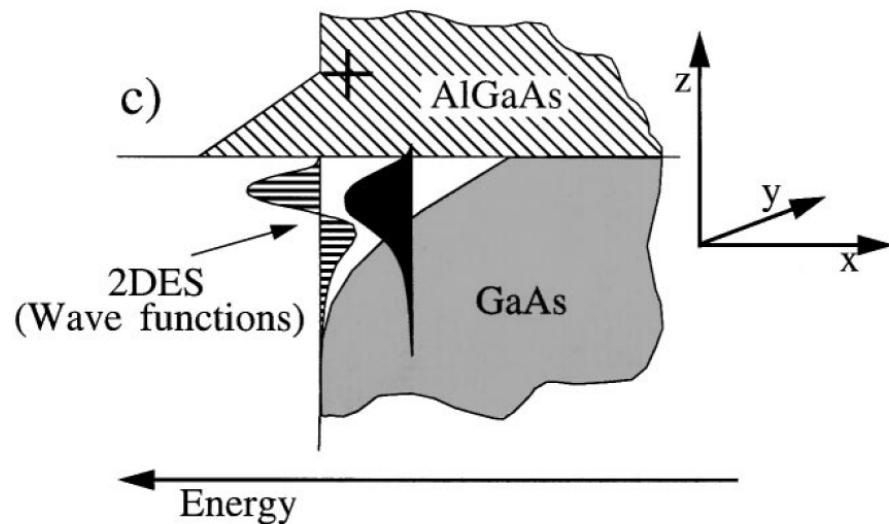
Two Dimensional Electron Gas



MOSFET
(metal-oxide-semiconductor field-effect transistor)



HEMT
(high electron mobility transistor)



H. L. Stormer,
Rev. Mod. Phys. 71, 875 (1999).

Discovery of FQHE

Hall resistance of HEMT

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

A. M. Chang, *et al.*,
Phys. Rev. Lett. 53, 997 (1984).

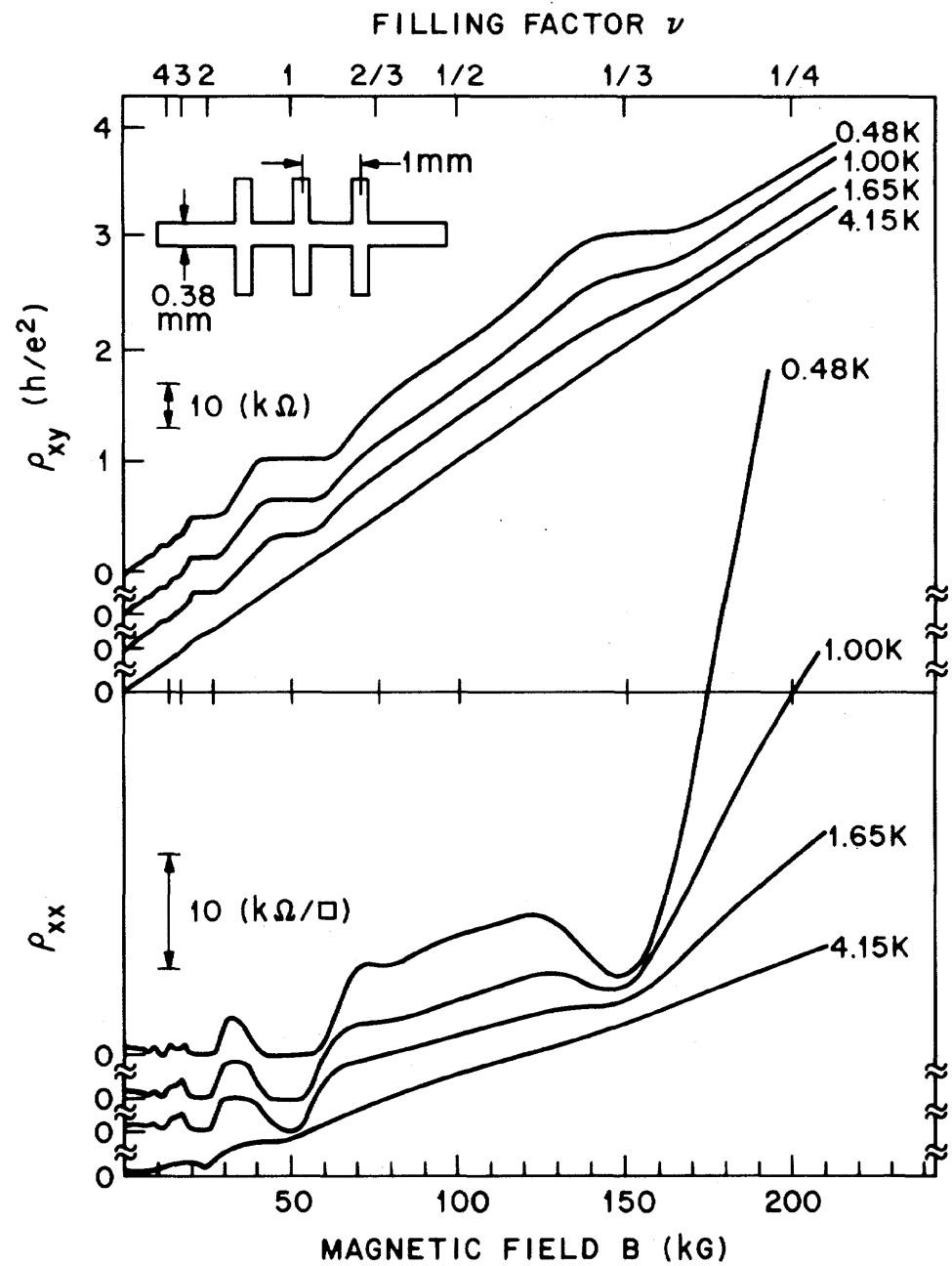
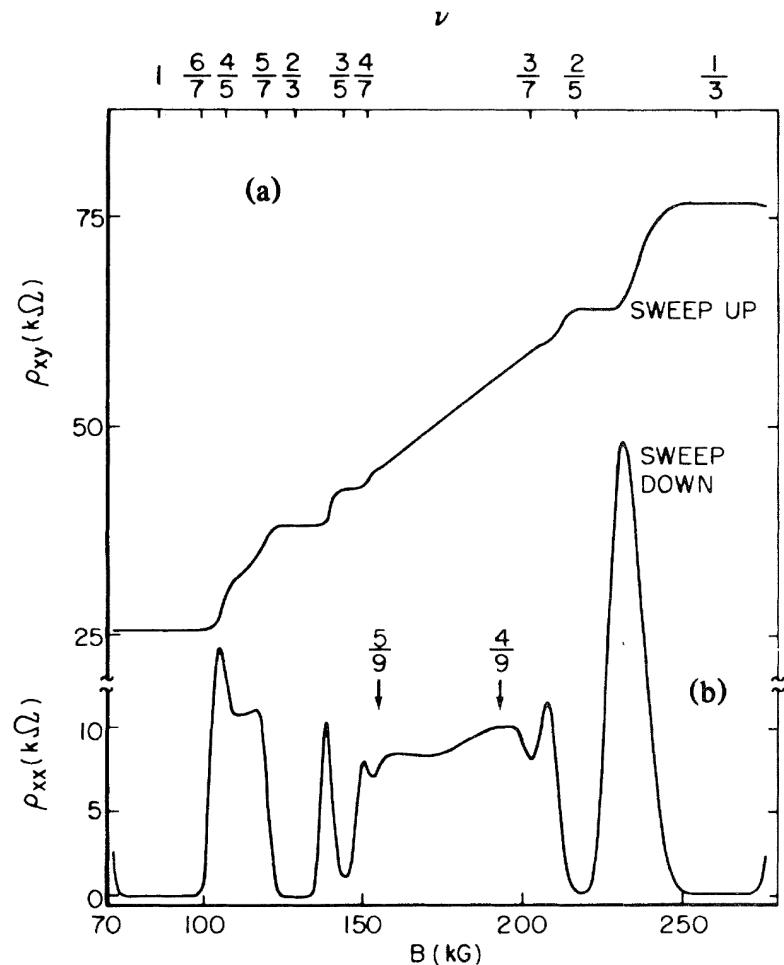


FIG. 1. ρ_{xy} and ρ_{xx} vs B , taken from a GaAs-Al_{0.3}-Ga_{0.7}As sample with $n = 1.23 \times 10^{11}/\text{cm}^2$, $\mu = 90\,000 \text{ cm}^2/\text{V sec}$, using $I = 1 \mu\text{A}$. The Landau level filling factor is defined by $\nu = nh/eB$.

Laughlin-Jastrow Trial Wave Function

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

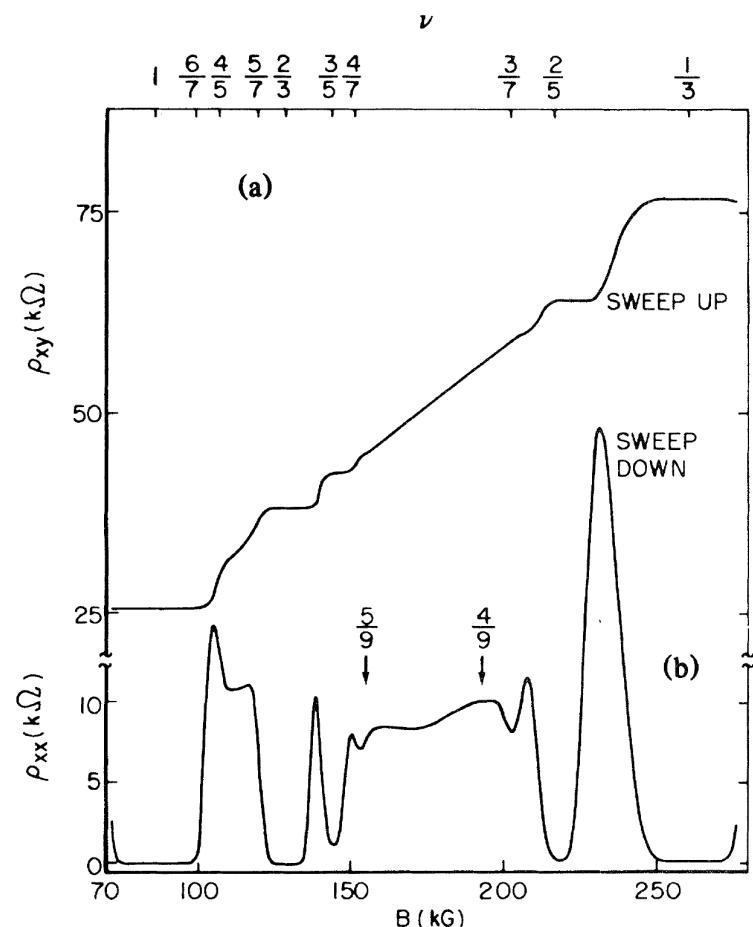
$$\psi_m(z_1, z_2, \dots, z_N) = \left[\prod_{i < j} (z_i - z_j)^m \right] \exp \left(-\frac{1}{4} \sum_k |z_k|^2 \right)$$

$$z_j = x_j - iy_j$$

$$m = 1/\nu$$

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

Exact wave function for
6 electrons in 18 states ($\nu=1/3$)
-98.81% overlap with the LJ trial w.f.



Haldane Gap

Background: Topological Phase

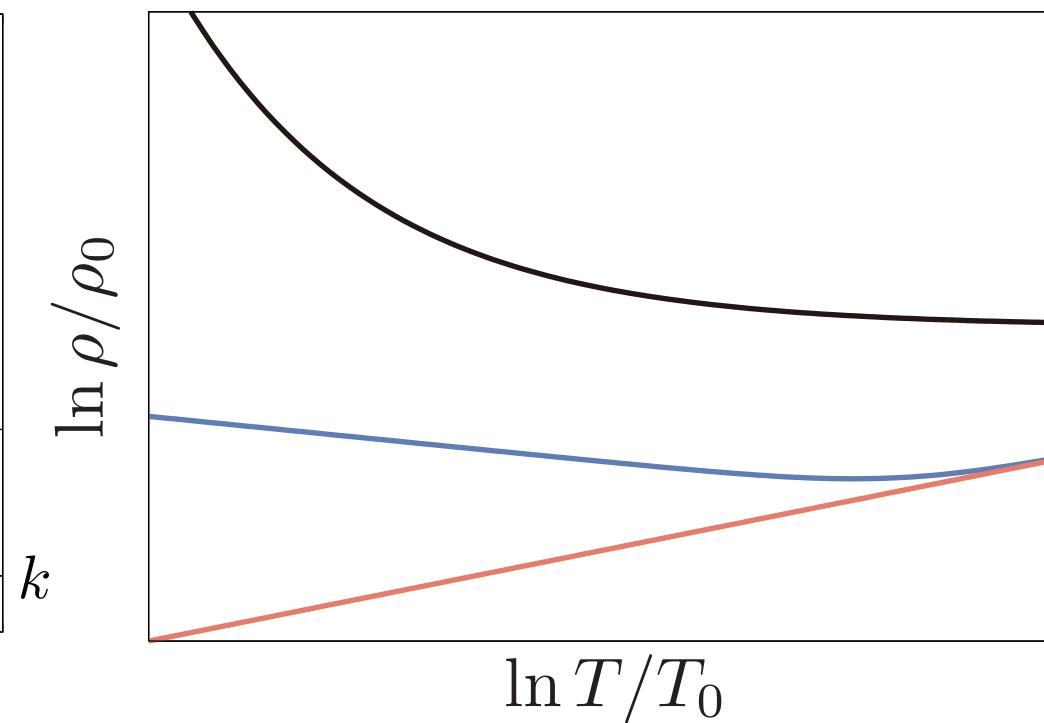
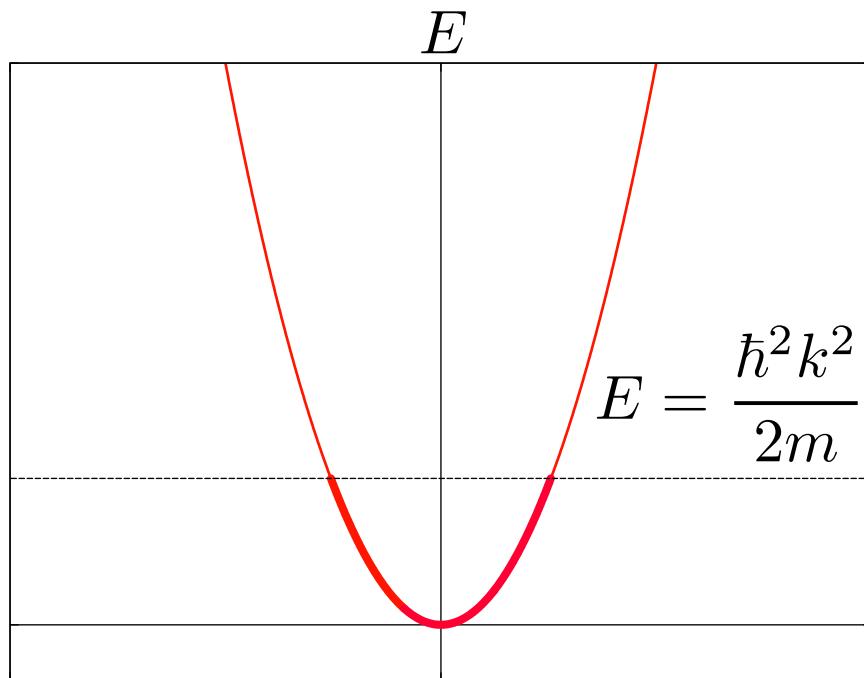
Classification of gapped quantum phases

Nobel Prize in 2016

“Topological phase transitions and
topological phases of matter”

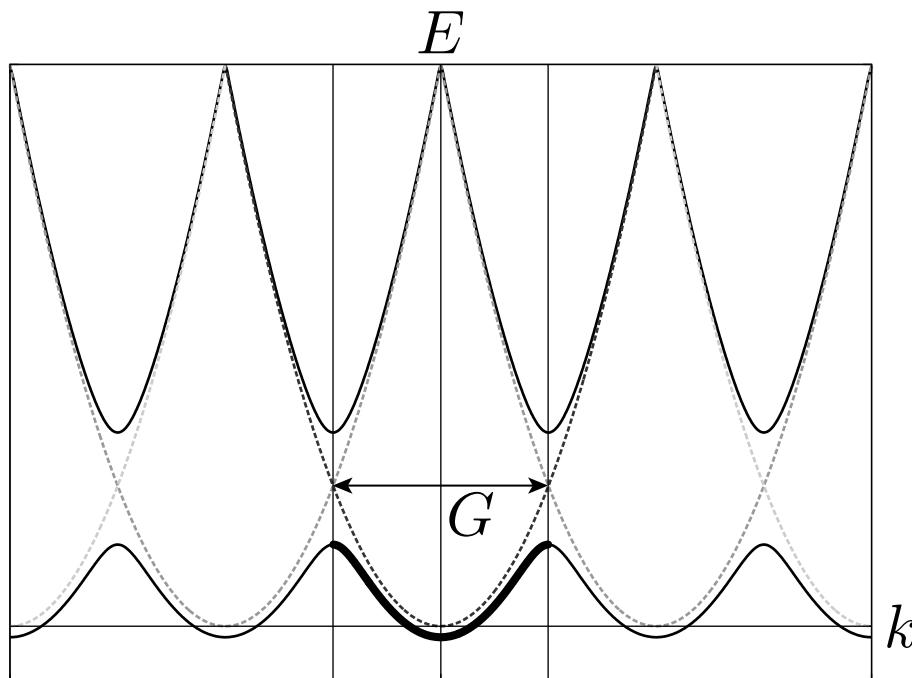
Classification of Crystalline Solids from Electric Transport

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

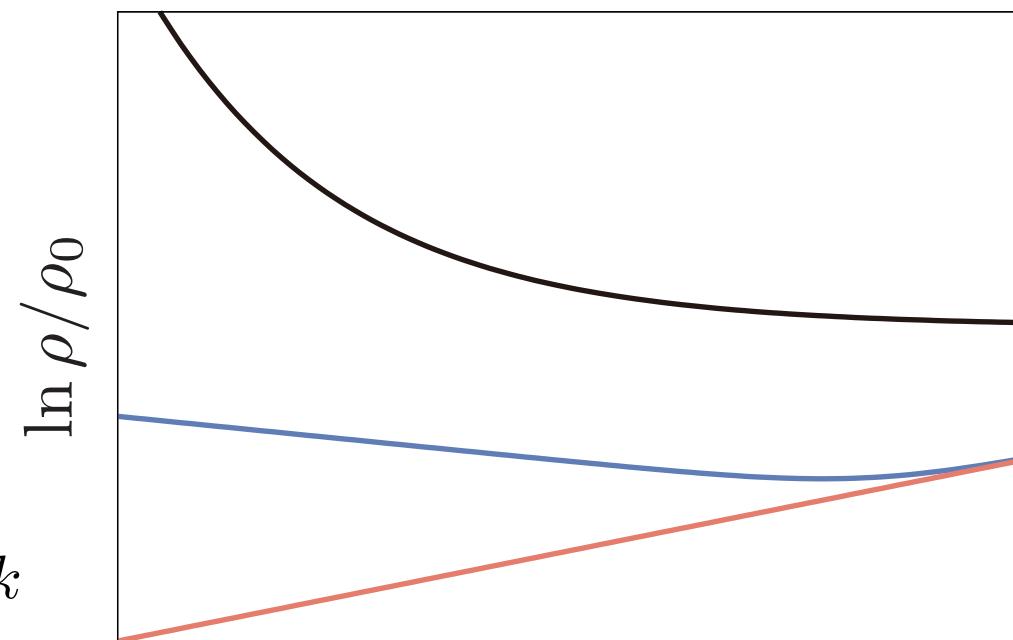


Classification of Crystalline Solids from Electric Transport

- Metal
- Zero gap semiconductor
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- Mott insulator



$$G = \frac{2\pi}{a}$$

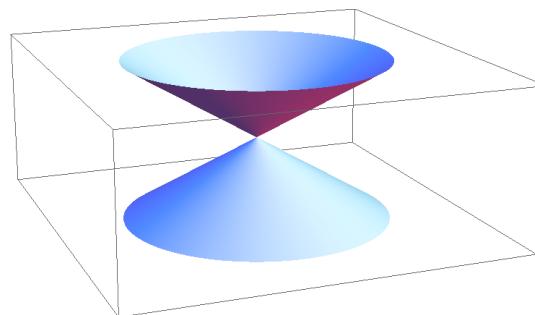
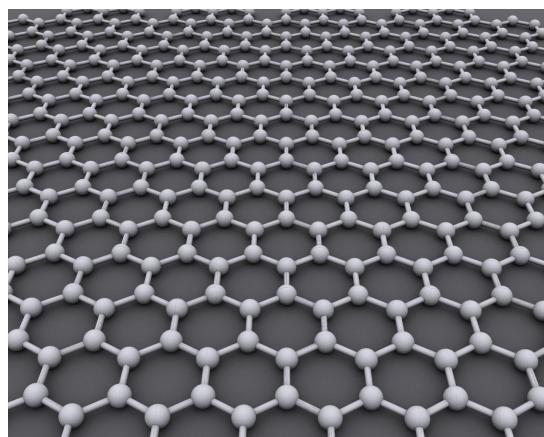


Classification of Crystalline Solids from Electric Transport

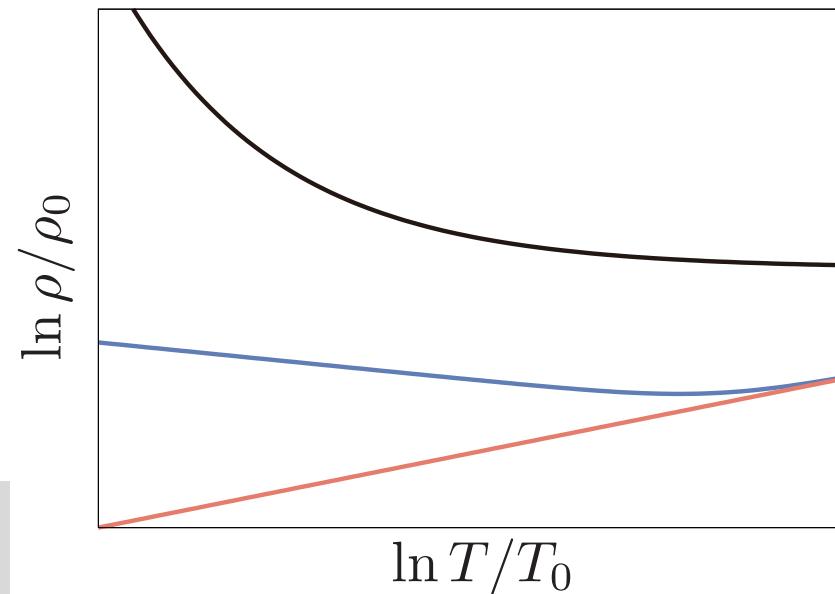
- Metal
- Zero gap semiconductor
- Band insulator
- Mott insulator

Example of zero gap semi.

2 D Dirac: Graphene

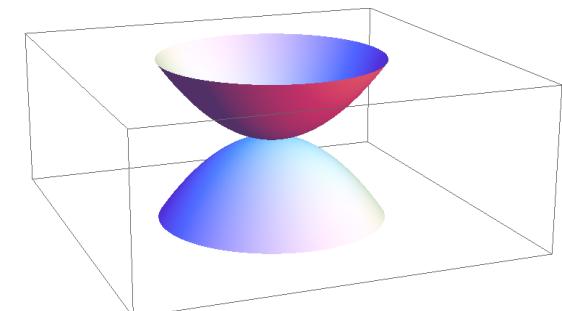


Castro Neto, Guinea, Peres, Novoselov, & Geim,
Rev. Mod. Phys. 81, 109 (2009)



3 D Dirac:
 Cd_3As_2 , Na_3Bi

HgTe , $\alpha\text{-Sn}$ (gray tin)



Classification of Crystalline Solids from Electric Transport

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

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

Trivial insulator

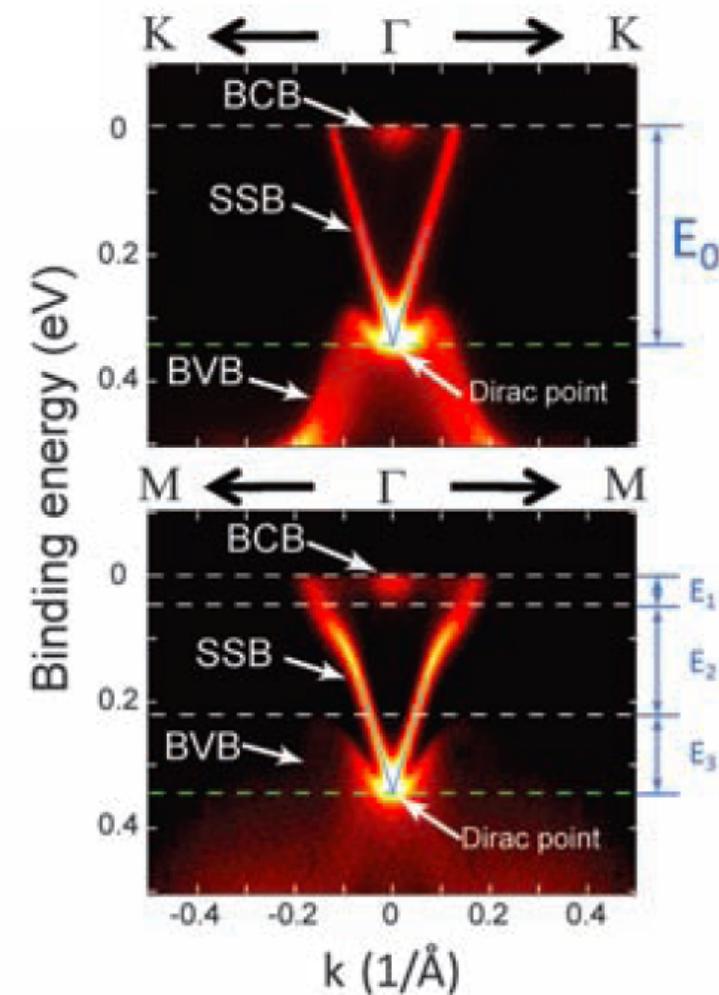
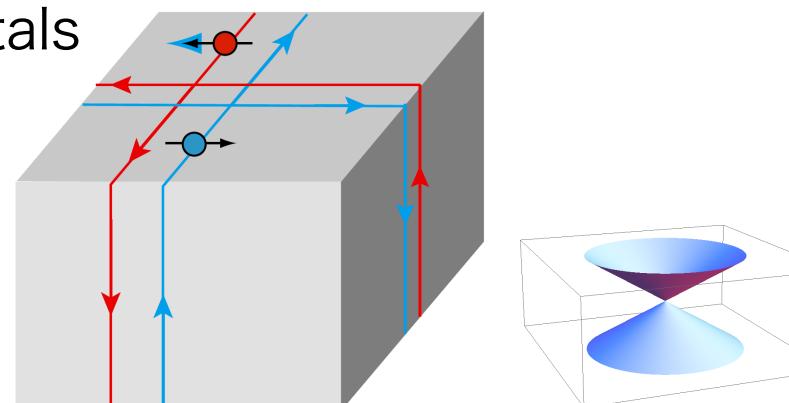
Si

Topological insulator

Bi_2Te_3

Thermoelectric

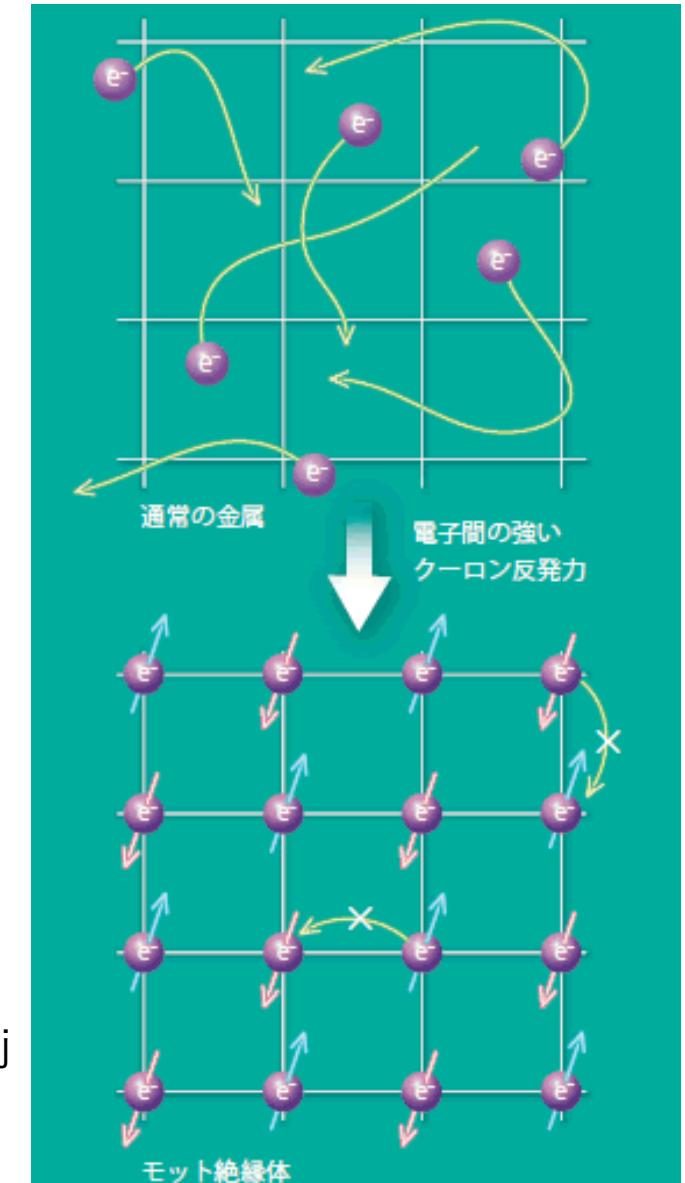
Surface metals



Classification of Crystalline Solids from Electric Transport

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

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Spin Angular Momentum Coupling

- An electron has $S=1/2$ ((spin angular momentum) = $\hbar/4\pi$)
- Origin of magnetism due to total angular momentum of many electrons in solids
- Example of spin angular momentum coupling:
Rare earth gadolinium Gd^{+3} $S=7/2$
- Classical Heisenberg spins obtained in $S \rightarrow +\infty$ limit

$S=1$ consists of two $S=1/2$

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

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

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

Spin Operators for $S=1$ Quantum Spins

Matrix representation 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

$S=1$ Heisenberg Model

Haldane gap

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

-Theoretical prediction on 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

$S=1$ Heisenberg Model

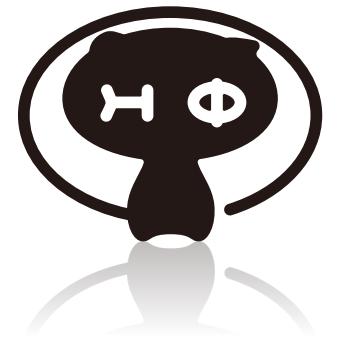
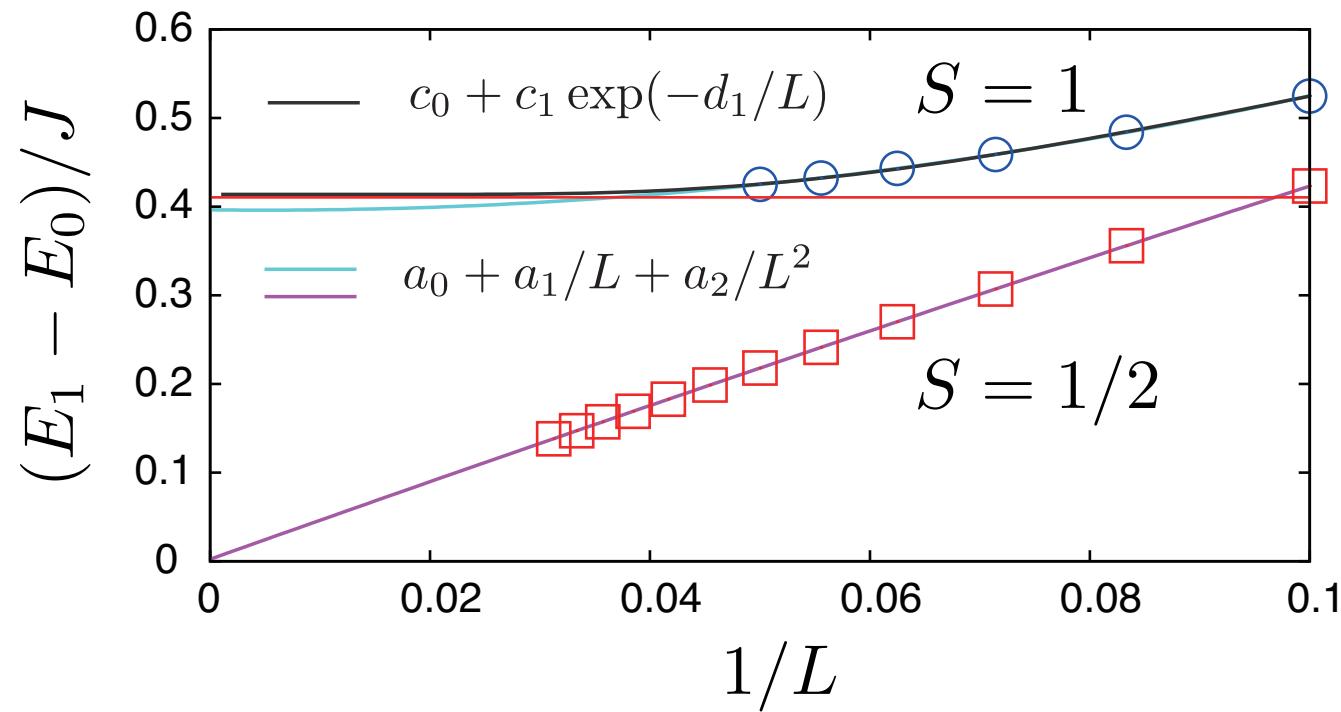
Edge states

Please see the lecture slide of Haldane

https://www.nobelprize.org/nobel_prizes/physics/laureates/2016/haldane-lecture.html

$S=1$ 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).

(Revisited) 2nd Report Problems

Please choose one of three

Report 2

Problem 1: Monte Carlo for quantum systems

1-1 (compulsory).

-Evaluate statistical errors in a 2-point distribution function $g(r)$ of liquid helium 4 at each distance r .

You may use McMillan's variational Jastrow wave function and variational parameters given in [sample_Hubbard_Helium4_v1.ipynb](#).

-Be careful about definition of the statistical errors
standard deviation of the MC averages
given by independent Markov chains (10 Markov chains may be enough)
-Obtain the relationship between the statistical errors and
numbers of Monte Carlo samples (and confirm the error is
proportional to $1/N_{MC}^{1/2}$, where N_{MC} is the number of Monte Carlo
samples).

1-2 (optional).

-Obtain 2-point distribution functions $g(r)$ of liquid helium 3
for likewise (not likewise) spin pairs at ambient pressure.

*You may use variational Jastrow-Slater wave functions and variational parameters obtained in D. Ceperley, G. V. Chester & M. H. Kalos, Phys. Rev. B 16, 3081 (1977).

Report 2

Problem 2: Krylov subspace method

2-1 (compulsory).

- Implement Lanczos method for the 1D Hubbard model and obtain the ground-state energy (the lowest eigenvalue) E_0 for 6 electrons and 6 sites at $U/t = 8$.
- Illustrate convergence of E_0 obtained at each Lanczos step.
- Obtain E_0 by Lapack and compare with the solution by Lanczos.
- Obtain U/t dependence of E_0 by Lanczos for $0 < U/t < 16$.

2-2 (Optional).

- Implement LOBCG method for the 1D Hubbard model.
- Confirm that the code can calculate E_0 and the corresponding eigenvector for 6 electrons and 6 sites at $U/t = 8$.
- Obtain the 2nd and 3rd lowest eigenvalues.
- Compare them with the solution by Lapack.

Report 2

Problem 3: Open source software

3-1 (compulsory).

-Solve the following problems. You may use HΦ.

Estimate the energy difference between the lowest and 2nd lowest eigenstates of the 1dimensional $S=1/2$ and $S=1$ Hesenberg models with periodic boundary conditions.

-Use several L (number of spins) and extrapolate the gap to thermodynamic limit ($L \rightarrow \infty$). Please compare the extrapolated values with other results in the literature.

You may use $a+b/L+c/L^2$ or $a+b \exp(-cL)$.

-Illustrate the extrapolations.

3-2 (optional). Reproduce the figures in Sec. 2.2 of the tutorials of HΦ: [https://issp-center-dev.github.io/HPhi/
manual/develop/tutorial/en/html/finite_temperature/Kitaev.html](https://issp-center-dev.github.io/HPhi/manual/develop/tutorial/en/html/finite_temperature/Kitaev.html)

-Please choose one out of the three problems

-The code should be included (a jupyter notebook is recommended).

-Deadline: 7/31

Report 1 & 2

Deadline for Report 1:

-2022/7/31

Deadline for Report 2:

-2022/7/31

Please submit your report through ITC-LMS
(web page for the reports will be opened).

If you have any trouble, please contact us via email.

*If you are interested in QMC, open source software
ALF & DSQSS would be worth trying.

Lecture Schedule

- #1 Many-body problems in physics and why they are hard to solve
- #2 Classical statistical model and numerical simulation
- #3 Classical Monte Carlo method
- #4 Applications of classical Monte Carlo method
- #5 Molecular dynamics and its application
- #6 Extended ensemble method for Monte Carlo methods
- #7 Quantum lattice models and numerical approaches
- #8 Quantum Monte Carlo methods
- #9 Applications of quantum Monte Carlo methods
- #10 Linear algebra of large and sparse matrices for quantum many-body problems
- #11 Krylov subspace methods and their applications to quantum many-body problems
- #12 Large sparse matrices and quantum statistical mechanics
- #13 Parallelization for many-body problems