特殊講義C:
量子多体問題の計算科学

1日目
2018/8/6

Special Lecture C:
Computational Science of
Quantum Many-body Problems

1. Quantum many-body physics
2. Description of quantum many-body (QMB) systems
   - -Quantum spins/qubits
   - -2nd quantization
3. From electrons in crystalline solids to lattice Hamiltonians

Lecturer

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Research:
Theoretical condensed matter physics
Computational method of many-body quantum systems

Developer of open source codes for supercomputers

Quantum lattice model solver HΦ

http://ma.cms-initiative.jp/ja/index/ja/listapps/hphi

Self-Introduction

Education

2004 B.Sc., Physics, The University of Tokyo
2006 M.Sc., Physics, The University of Tokyo
2010 Dr. Eng. Graduate School of Engineering, The University of Tokyo
Thesis Title:
"Quantum Critical Phenomena Induced by Changes in Fermi-Surface Topology"
Supervisor: Professor Masatoshi Imada

Employment

2010-2011 Post Doctoral Research Associate,
Department of Physics and Astronomy, Rutgers University
2011-2014 Research Associate,
Department of Applied Physics, The University of Tokyo
2014-2016 Project Lecturer,
Quantum-Phase Electronics Center, The University of Tokyo
2016- Project Associate Professor,
Department of Applied Physics, The University of Tokyo

Computational Science Alliance
The University of Tokyo

Many-Body Problems

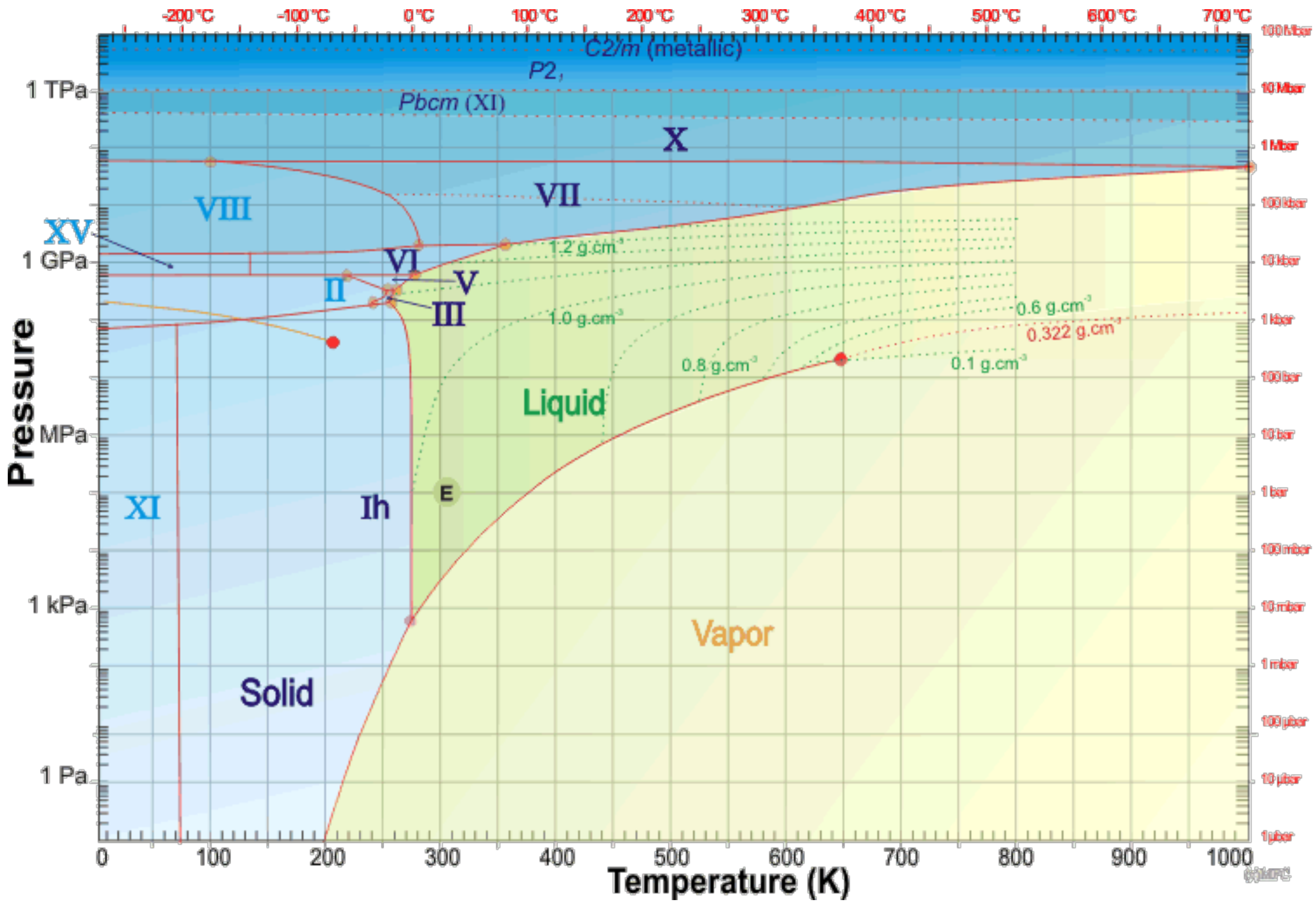
Many-body problems in Physics

Examples:
-Celestial objects
-Proteins and molecules
(molecular mechanics, quantum mechanics/molecular mechanics)
-Electrons in molecules and solids
-Quantum Chromodynamics

Principles:
・Classical mechanics
(Newtonian equation of motion, Post Newtonian, …)
・ Quantum mechanics
(Schrödinger equation, …)
・ Classical/quantum statistical mechanics

An Example of Many-Body Problems: H_2O

Phase diagram of H_2O



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

An Example of Many-Body Problems: Proteins

Proteins in water

David E. Shaw *et al*.,
D. E. Shaw Research
SC09 (2009)

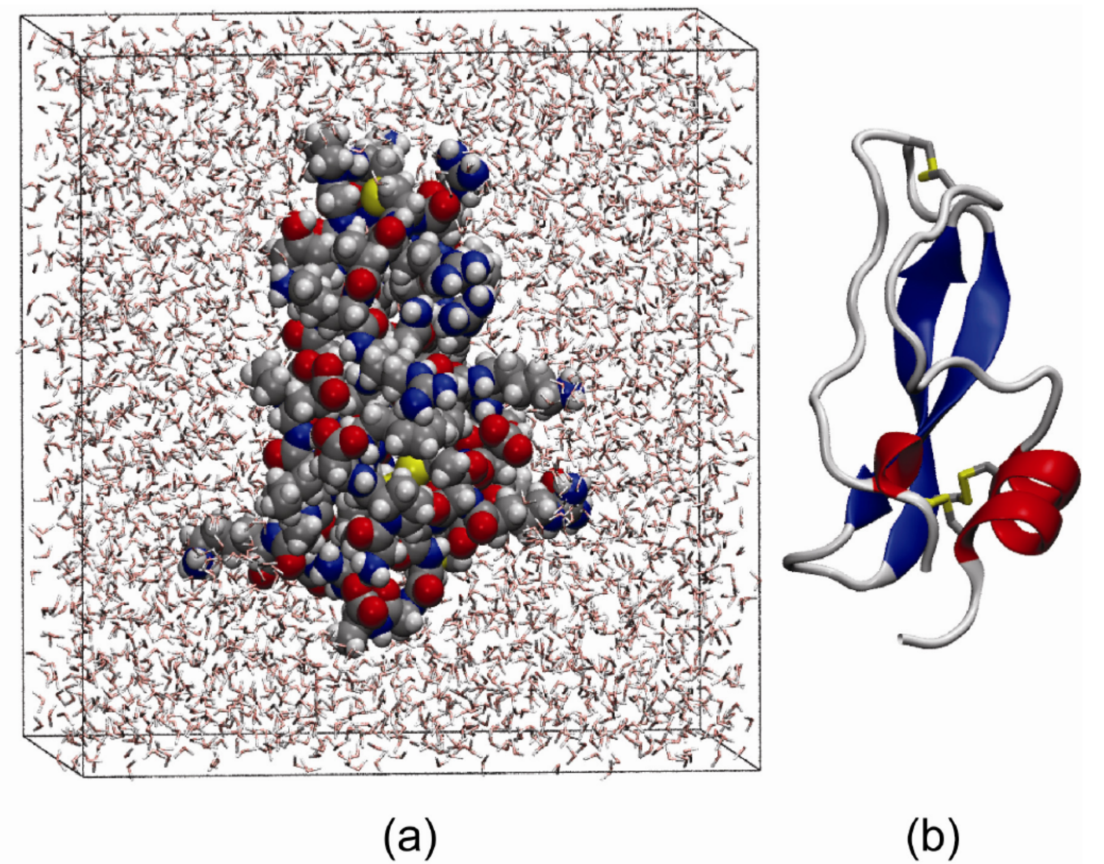
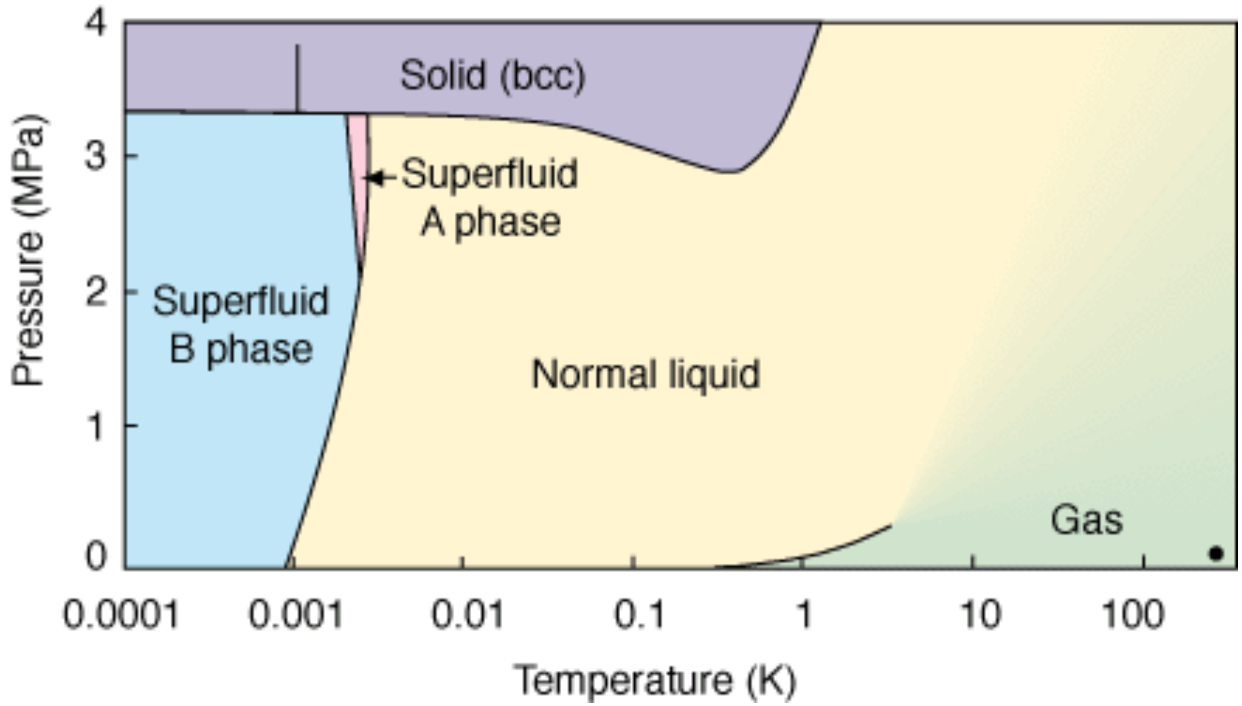


Figure 1: Two renderings of a protein (BPTI) taken from a molecular dynamics simulation on Anton. (a) The entire simulated system, with each atom of the protein represented by a sphere and the surrounding water represented by thin lines. For clarity, water molecules in front of the protein are not pictured. (b) A "cartoon" rendering showing important structural elements of the protein (secondary and tertiary structure).

An Example of Many-Body Problems: Quantum Liquids

Phase diagram of ^3He



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

Erkki Thuneberg
http://ltl.tkk.fi/research/theory/helium.html

Preliminary:
Quantum Many-Body Physics

An Example of Quantum Many-Body Systems

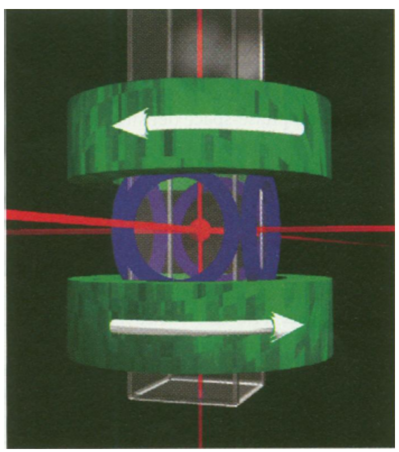
Cold atoms trapped in potential well

“Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor”
M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell,
Science 269, 198 (1995).

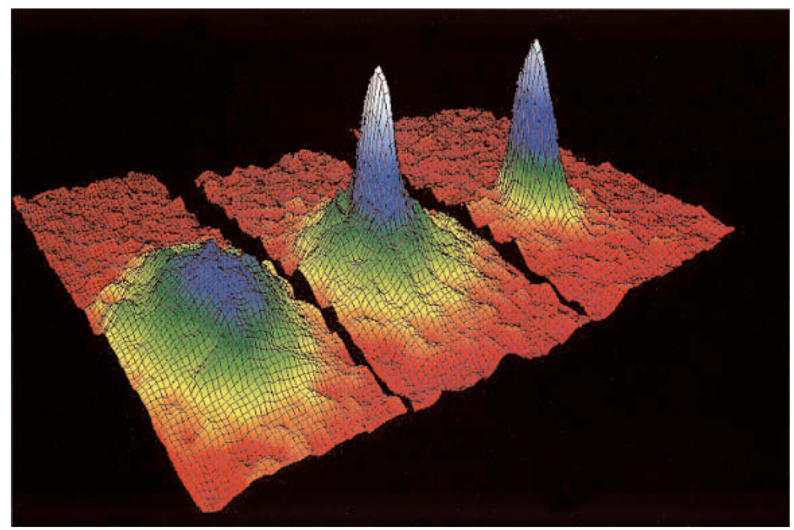
^{87}Rb

density: 2.5×10^{12} cm^{-3}
temperature: 170 nK

Magneto-optical trap



velocity distribution



“Theory of Bose-Einstein condensation in trapped gases”
F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari,
Rev. Mod. Phys. 71, 463 (1999).

A free particle in harmonic potential

-Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{k}{2}x^2$$

$$k = m\omega^2$$

-Wave function

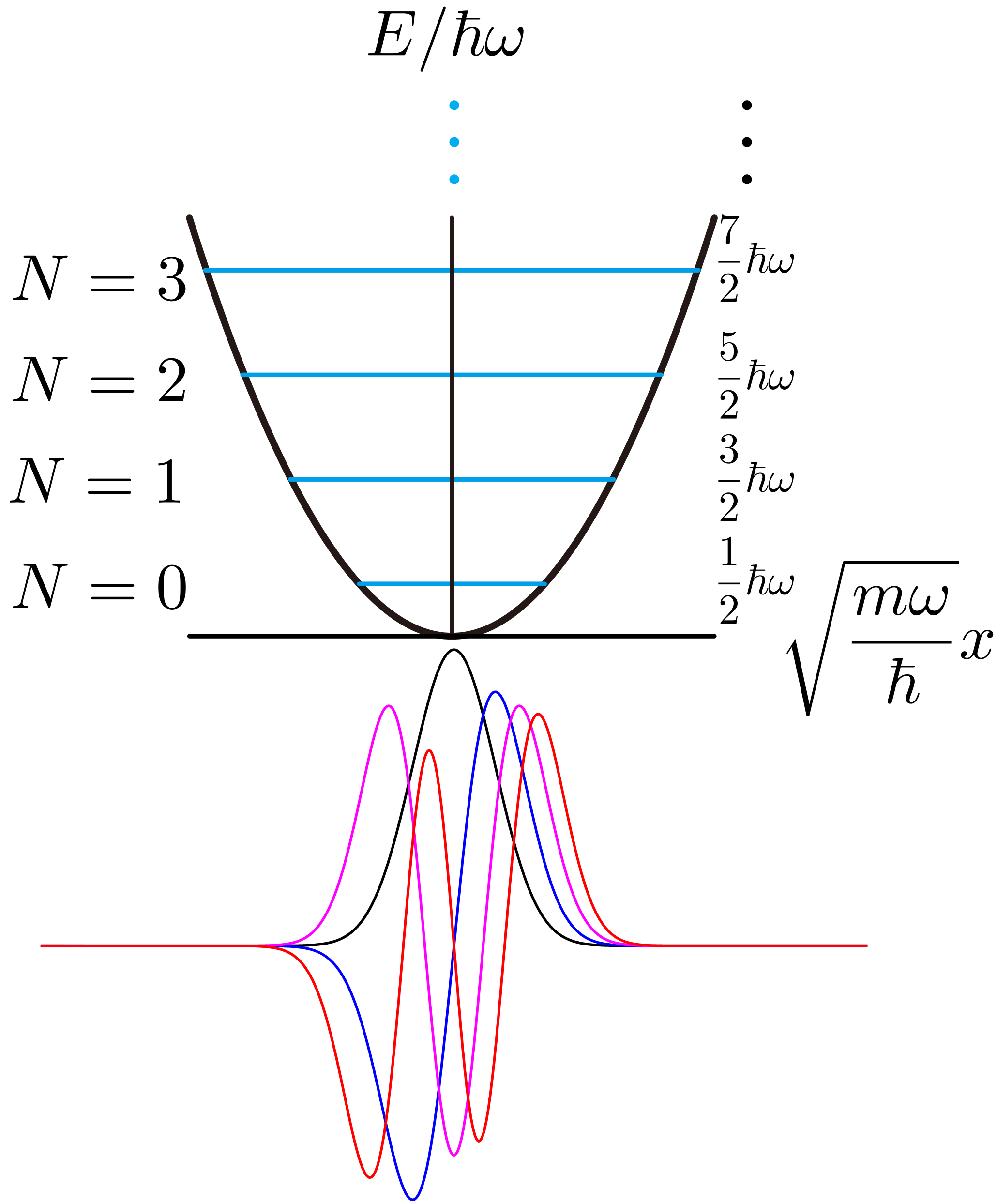
$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\phi_N(x) = \frac{1}{\sqrt{N!}}(\hat{\ell}^+)^N \phi_0(x)$$

ladder operator

$$\hat{\ell}^- = \sqrt{\frac{\hbar}{2m\omega}}\left(-\frac{\partial}{\partial x} + \frac{m\omega}{\hbar}x\right)$$

$$\hat{\ell}^+ = \sqrt{\frac{\hbar}{2m\omega}}\left(+\frac{\partial}{\partial x} + \frac{m\omega}{\hbar}x\right)$$



velocity distribution of ϕ_0 $e^{-\frac{mv^2}{2\hbar\omega}}$

Indistinguishable → Particle statistics

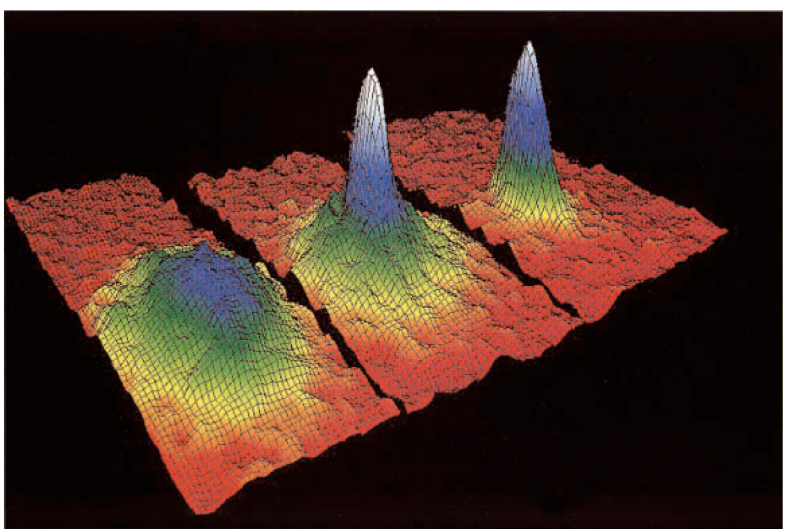
Classical: Tracking particle positions
Quantum: Tracking occupation of bases

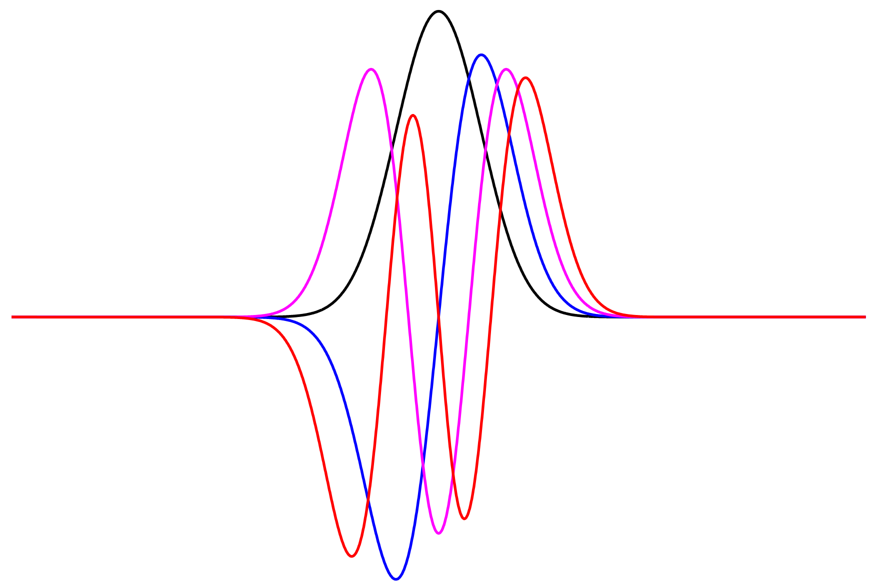
$$\hat{H} = \sum_j \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_j^2} + \frac{k}{2}x_j^2 \right)$$

The indices cannot identify the individual particle

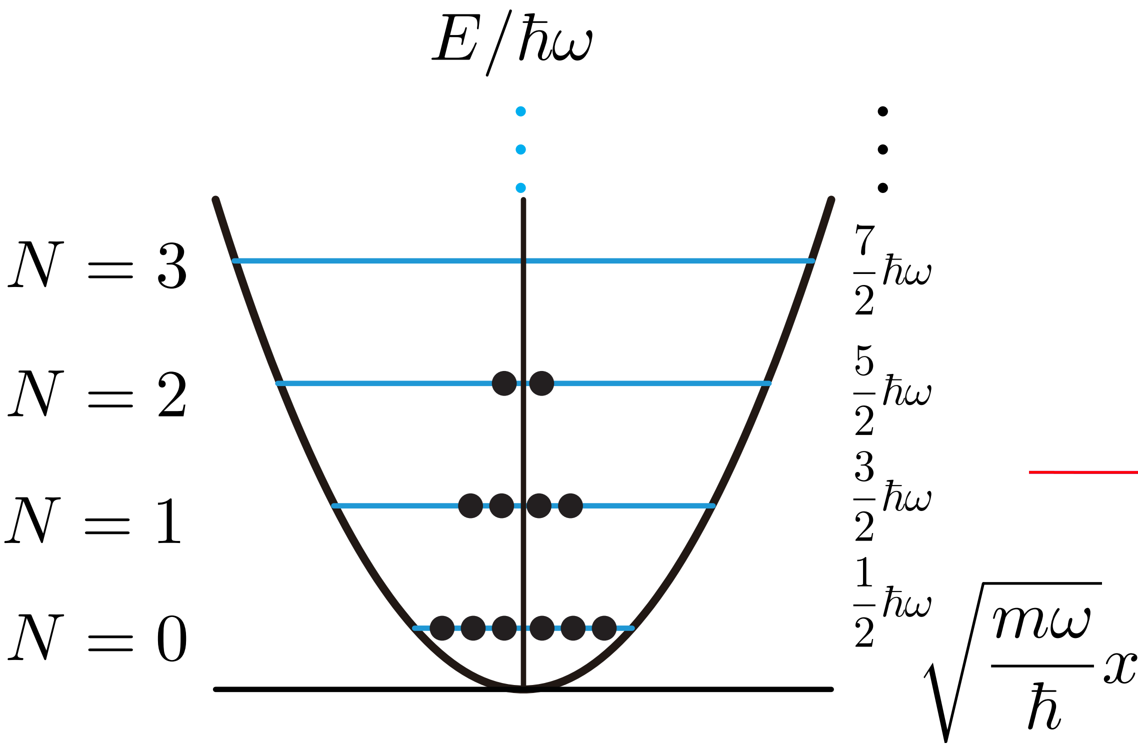
Example of Quantum phase: Bose-Einstein condensation

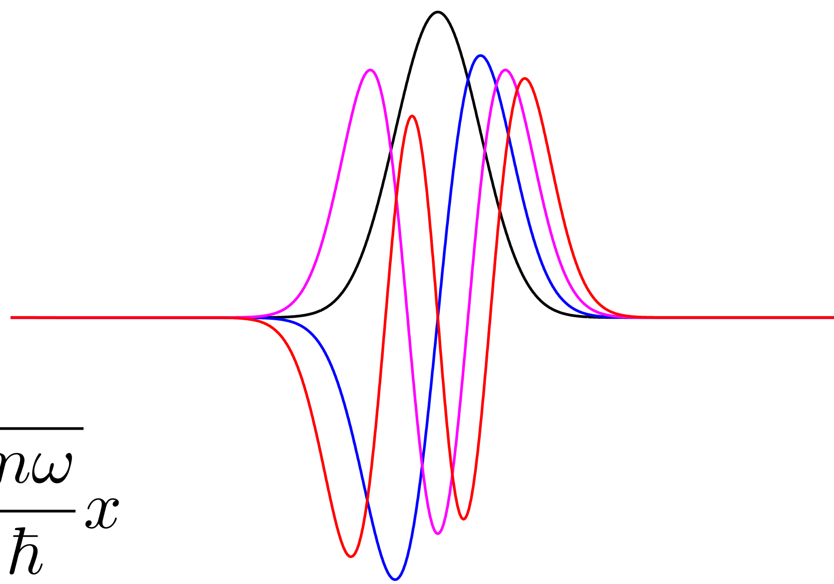
-A single state (ground state)is occupied by many bosons





Quantum: Tracking occupation of bases

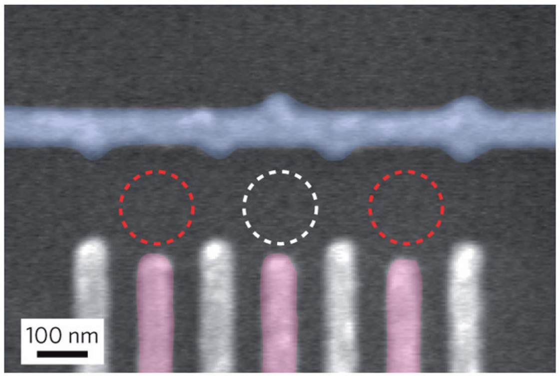




Another Quantum Many-Body Systems

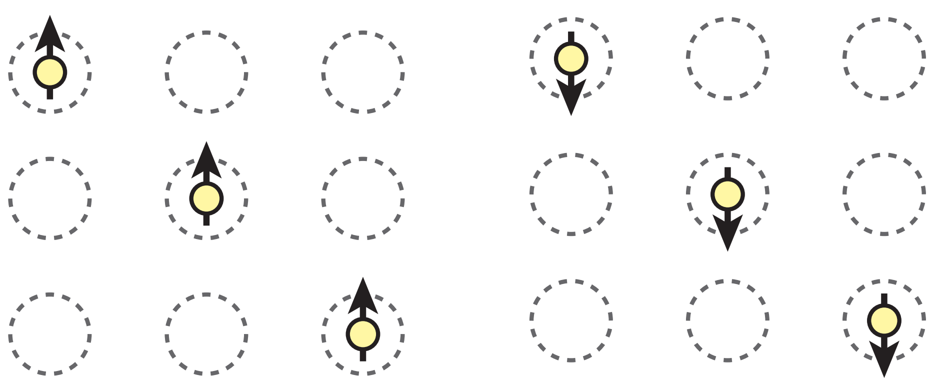
An example: 3 Quantum dots

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)



Another Quantum Many-Body Systems

An example: 3 Quantum dots

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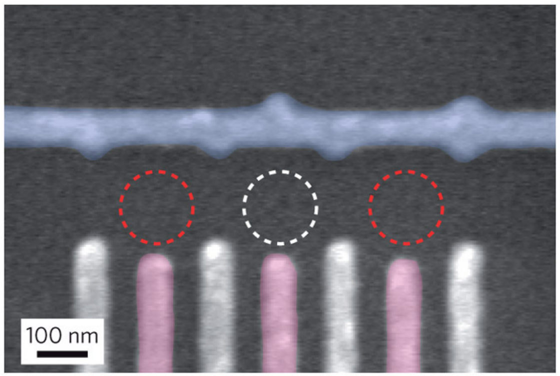
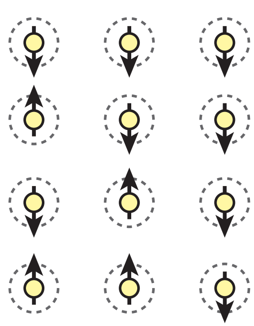


Quantum dot:
-A quantum box can confine a single electron
-Utilized for single electron transistor, quantum computers

Three-body problem:
→ Number of states = 2^3 (factor 2 from spin)

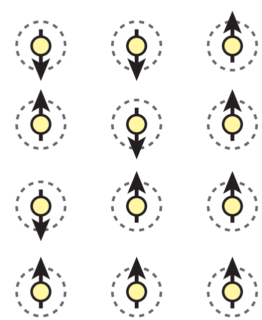


$|0\rangle \otimes |0\rangle \otimes |0\rangle$

$|1\rangle \otimes |0\rangle \otimes |0\rangle$

$|0\rangle \otimes |1\rangle \otimes |0\rangle$

$|1\rangle \otimes |1\rangle \otimes |0\rangle$



$|0\rangle \otimes |0\rangle \otimes |1\rangle$

$|1\rangle \otimes |0\rangle \otimes |1\rangle$

$|0\rangle \otimes |1\rangle \otimes |1\rangle$

$|1\rangle \otimes |1\rangle \otimes |1\rangle$

States represented by superposition

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

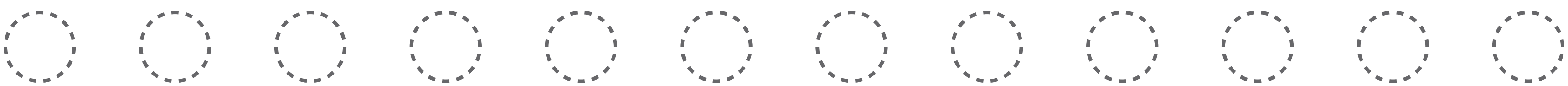
Another Quantum Many-Body Systems

N Quantum dots

One-body problem:
→ Number of states = 2×N

N-body problem:
→ Number of states = 2^N

Further example: N=12



One-body problem→ Number of states = 2×N = 24
N-body problem→ Number of states = 2^N = 4096

Extreme example: N=36

One-body→ 2×N = 72
N-body→ $2^N \sim 6.9\times10^{10}$

Quantum Many-Body Problems in Physics

Quantum Many-Body Problems in Physics

- -Quantum chromodynamics
- -Nuclear physics
- -Condensed matter physics
- -Quantum chemistry

Nucleus: Many-body systems consist of protons and neutrons

Hadrons (bryons and mesons): Quarks, antiquarks, and gluons

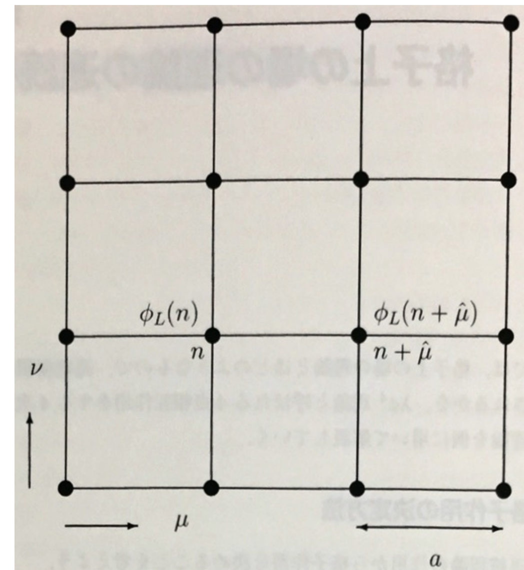
Lattice QCD: A Lattice Field Theory

Lattice QCD: Gauge & matter fields

A quantum field theory on a lattice

To define quantum field theory exactly
To regularize ultraviolet divergence

$$p/\hbar \leq \pi/a$$



Monte Carlo for guage and matter fields

SU(3) non-abelian gauge field

Applications:

-Nucleon-nucleon interaction Yukawa's pion
(Interaction among protons & neutrons)

"Nuclear Force from Lattice QCD"
N. Ishii, S. Aoki, and T. Hatsuda, Phys. Rev. Lett. 99, 022001 (2007)

-Mass of hadron consist of quark, antiquark, and gluon

"Light hadron masses from lattice QCD"
Z. Fodor and C. Hoelbling, Rev. Mod. Phys. 84, 449 (2012)

Lattice Field Theory for Condensed Matter

Lattice field theory:
Coulomb fields and massless Dirac electrons

Monte Carlo for guage and matter fields

Application to condensed matter physics:

-Mass generation due to chiral symmetry breakings
in Dirac electrons in graphene

"Lattice field theory simulations of graphene"
J. E. Drut and T. A. Lähde, Phys. Rev. B 79, 165425 (2009)

Coulomb gauge field

Field theory: Massless to massive
Condensed matter: Semimetal to insulator

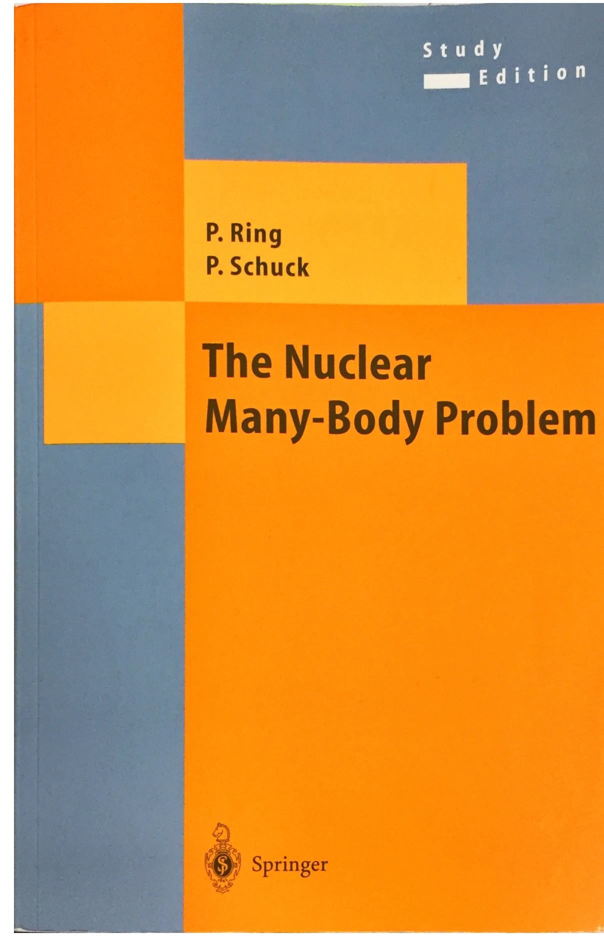
Nuclear Physics

Many-body systems with finite number of nucleons

-No derivation for the nucleon-nucleon force other than lattice QCD
-Models have been used

Effective Hamiltonian approach is common to condensed matter physics

Numerical technique common to condensed matter physics:
-Hartree-Fock/Hartree-Fock-Bogoliubov
-Time-dependent HF/HFB
-Random phase approximation
-Quantum number projection



Condensed Matter Physics and Quantum Chemistry

Many-body electrons and ions

Not feasible to simulate in general

- Born-Oppenheimer approximation:
  Decoupling electrons and ions

→Many-body electrons

cf.) *ab initio* MD

Note that density functional theory *captures* many-body physics (will be explained in the Quantum Monte Carlo part)

P. Hohenberg & W. Kohn, Phys. Rev. 136, B864 (1964).
W. Kohn & L. J. Sham, Phys. Rev. 140, A1133 (1965).

Other many-body systems: Cold atoms, qubits,…

"Density functional theory for atomic Fermi gases"
P. N. Ma, S. Pilati, M. Troyer, & X. Dai, Nat. Phys. 8, 601 (2012).

Why Many-Body Problem is Hard to Solve

Why Many-Body Problem Is Hard to Solve

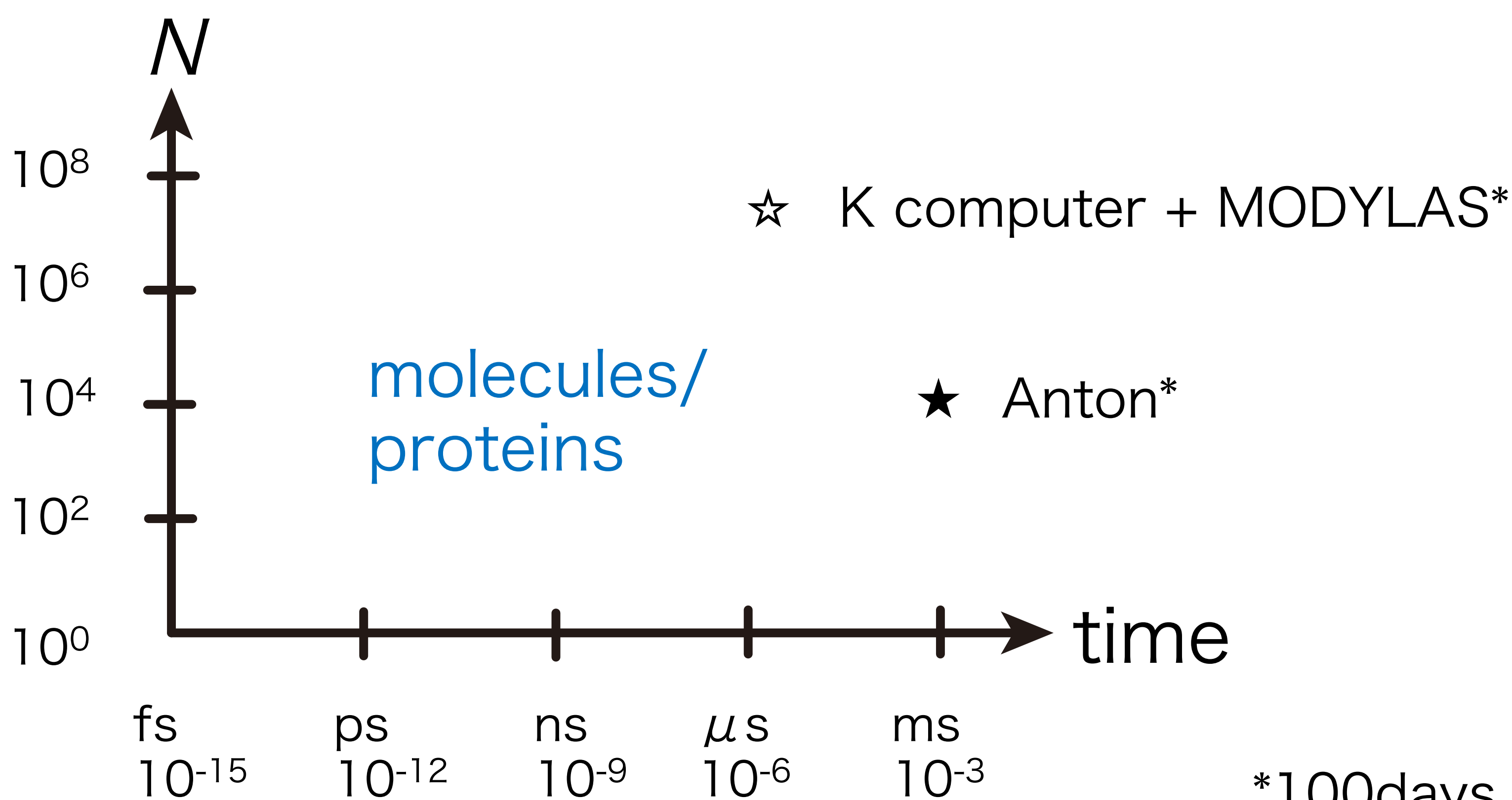
Example of many-body problems:

1. N-body Newtonian equation of motion
2. N-body classical statistical mechanics
3. N-body Schrödinger equation
4. N-body quantum statistical mechanics

Why Many-Body Problem Is Hard to Solve

1. N-body Newtonian equation of motion
-Time evolution of 6N degrees of freedom

parallelization



*100days

An Example of Many-Body Problems: Proteins

Proteins in water

David E. Shaw *et al*.,
D. E. Shaw Research
SC09 (2009)

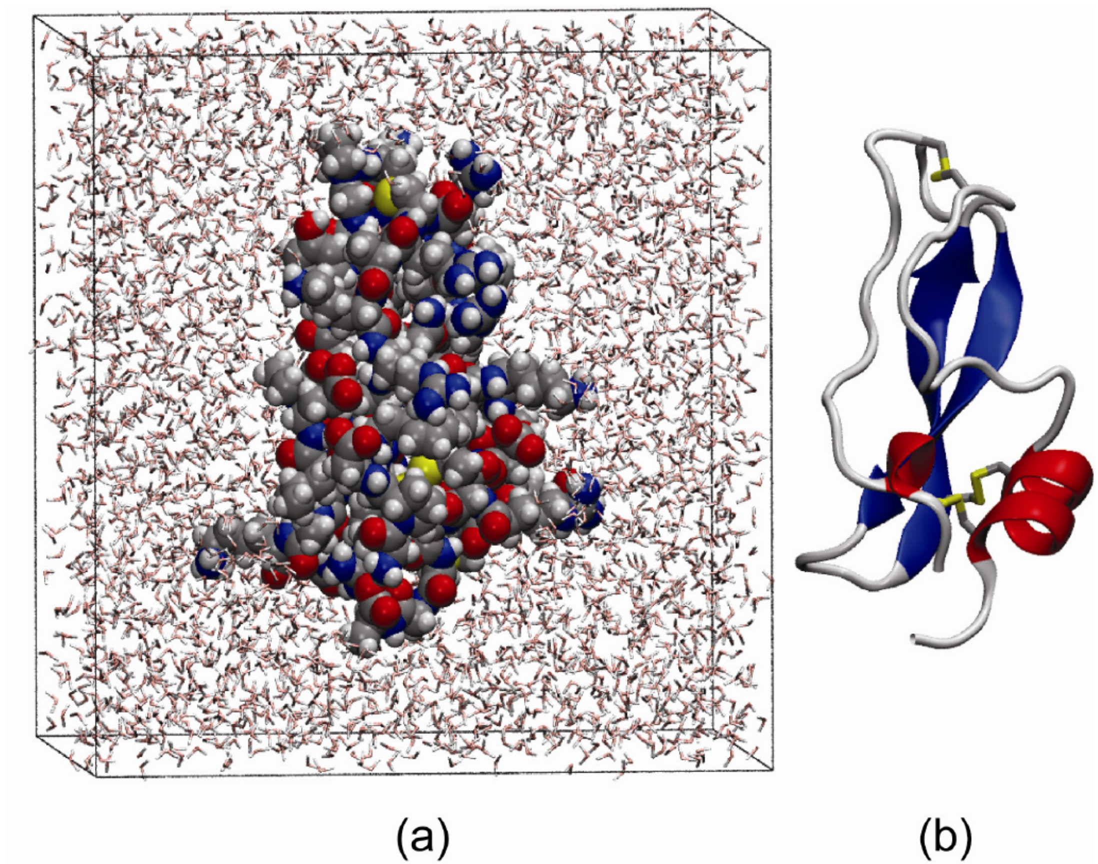


Figure 1: Two renderings of a protein (BPTI) taken from a molecular dynamics simulation on Anton. (a) The entire simulated system, with each atom of the protein represented by a sphere and the surrounding water represented by thin lines. For clarity, water molecules in front of the protein are not pictured. (b) A "cartoon" rendering showing important structural elements of the protein (secondary and tertiary structure).

Why Many-Body Problem Is Hard to Solve

1. *N*-body Newtonian equation of motion
-Time evolution of 6*N* degrees of freedom:
*Larger Δt is desirable

$\Delta t = 1\text{–}2$ fs
For hydrogen atom 0.1fs

*If the system can be divided into independent subsystems, it is easy to treat the system in parallel

However, ions interact each other through long-range Coulomb repulsion

First Principle of Molecular Mechanics: Newtonian/Hamiltonian Mechanics

Brief summary of Hamiltonian mechanics

Hamilton's eqs.

$$\frac{d}{dt}\begin{bmatrix} q \\ p \end{bmatrix} = \begin{bmatrix} +\partial H/\partial p \\ -\partial H/\partial q \end{bmatrix}$$

Operator representation

$$\rightarrow \frac{d}{dt}\begin{bmatrix} q \\ p \end{bmatrix} = \hat{D}_H \begin{bmatrix} q \\ p \end{bmatrix}$$

* Poisson braket

$$\hat{D}_g f = \{f, g\} = \frac{\partial f}{\partial q}\frac{\partial g}{\partial p} - \frac{\partial g}{\partial q}\frac{\partial f}{\partial p}$$

$$\frac{d}{dt} f\left(q(t), p(t)\right) = \{f, H\}\left(q(t), p(t)\right)$$

linear

$$\hat{D}_{g+h} f = \hat{D}_g f + \hat{D}_h f$$

Difference Equation for Hamiltonian Mechanics

Formal solution (Not easy to calulate)

$$\begin{bmatrix} q(t+\Delta t) \\ p(t+\Delta t) \end{bmatrix} = \exp\left[\Delta t \hat{D}_H\right] \begin{bmatrix} q(t) \\ p(t) \end{bmatrix}$$

Forward difference

$$\begin{aligned} \begin{bmatrix} q(t+\Delta t) \\ p(t+\Delta t) \end{bmatrix} &= \exp\left[\Delta t \hat{D}_H\right] \begin{bmatrix} q(t) \\ p(t) \end{bmatrix} \\ &= \underbrace{\begin{bmatrix} q(t) \\ p(t) \end{bmatrix} + \Delta t \hat{D}_H \begin{bmatrix} q(t) \\ p(t) \end{bmatrix}}_{\text{Euler method}} + \frac{(\Delta t)^2}{2!} \hat{D}_H^2 \begin{bmatrix} q(t) \\ p(t) \end{bmatrix} + \mathcal{O}(\Delta t^3) \end{aligned}$$

Do not use Euler!

Difference Equation for Hamiltonian Mechanics

Another formulation of forward difference

Hamiltonian split into kinetic energy *T* and potential *V*

$$H = T(p) + V(q)$$

$$\exp\left[\Delta t \hat{D}_H\right] \simeq \exp\left[\frac{\Delta t}{2}\hat{D}_T\right]\exp\left[\Delta t \hat{D}_V\right]\exp\left[\frac{\Delta t}{2}\hat{D}_T\right]$$

$$\boxed{\begin{aligned} \exp\left[\Delta t \hat{D}_T\right]\begin{bmatrix} q(t) \\ p(t) \end{bmatrix} &= \begin{bmatrix} q(t) + \Delta t \left.\frac{\partial T}{\partial p}\right|_{p=p(t)} \\ p(t) \end{bmatrix} \\ \exp\left[\Delta t \hat{D}_V\right]\begin{bmatrix} q(t) \\ p(t) \end{bmatrix} &= \begin{bmatrix} q(t) \\ p(t) - \Delta t \left.\frac{\partial V}{\partial q}\right|_{q=q(t)} \end{bmatrix} \end{aligned}}$$

No series expansion !

Why Many-Body Problem Is Hard to Solve

2. *N*-body classical statistical mechanics

Example: 1 D Ising Model

$$H = J\sum_{i=0}^{L-1}\sigma_i\sigma_{i+1} - B\sum_{i=0}^{L-1}\sigma_i$$

Ising spin: $\sigma_i = \pm 1$

Periodic boundary: $i+1 \rightarrow \mathrm{mod}(i+1, L)$

Ising Model 1

History of the Lenz-Ising Model, S. G. Brush, Rev. Mod. Phys. 39, 883 (1967)

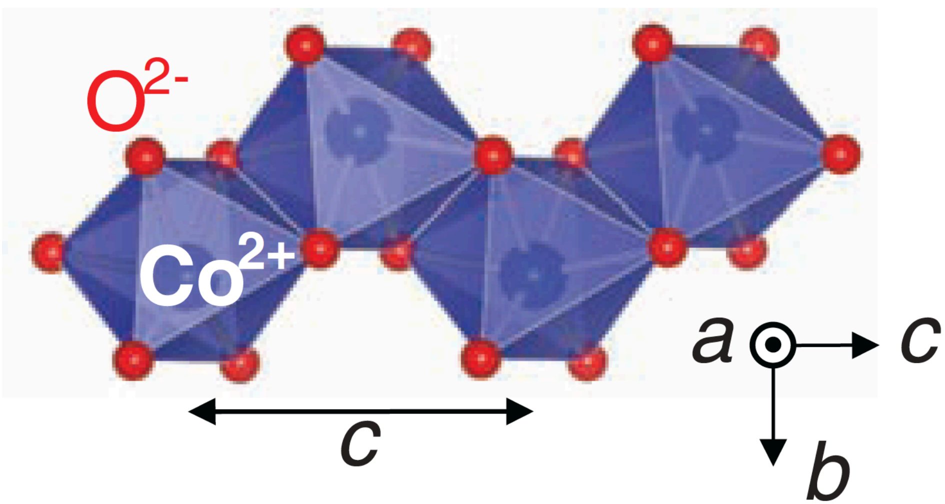
Many physico-chemical systems can be represented more or less accurately by a lattice arrangement of molecules with nearest-neighbor interactions.
The simplest and most popular version of this theory is the so-called “Ising model,” discussed by Ernst Ising in 1925 but suggested earlier (1920) by Wilhelm Lenz.

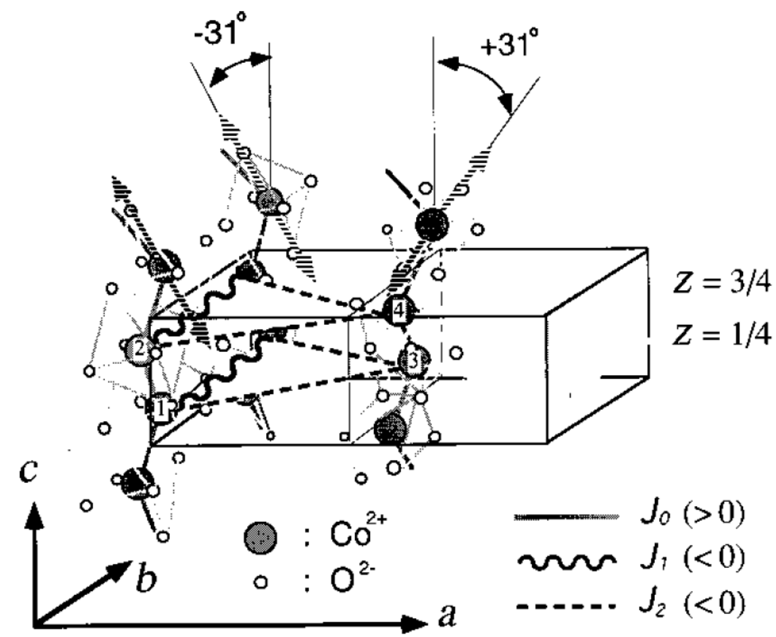
After many years of being scorned or ignored by most scientists, the so-called “Ising model” has recently enjoyed increased popularity and may, if present trends continue, take its place as the preferred basic theory of all cooperative phenomena.

Ising Model 2

A realization of Ising models

Quasi-1D Ising Ferromagnet: $CoNb_2O_6$





S. Kobayashi, *et al.*,
Phys. Rev. B 60, 3331 (1999)

Recent progress, *i.e.*,
R. Coldea, *et al.*,
Science 327, 177 (2010)

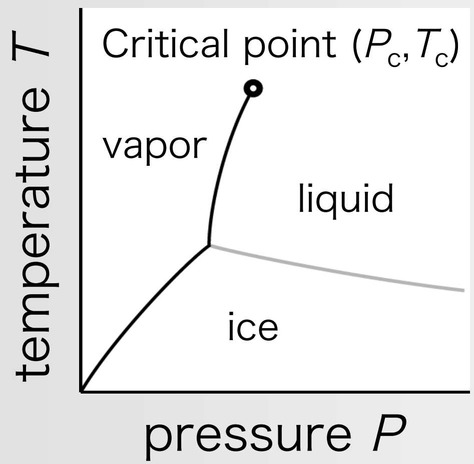
Ising Model 3

The archetype of critical phenomena

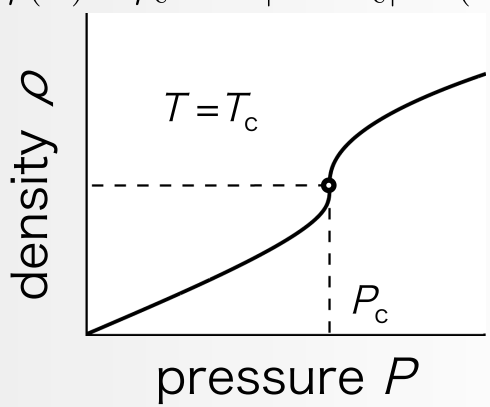
Critical phenomena of liquid/vapor water is characterized by 3D Ising universarity although *prediction* of T_c and P_c requires QM/MM

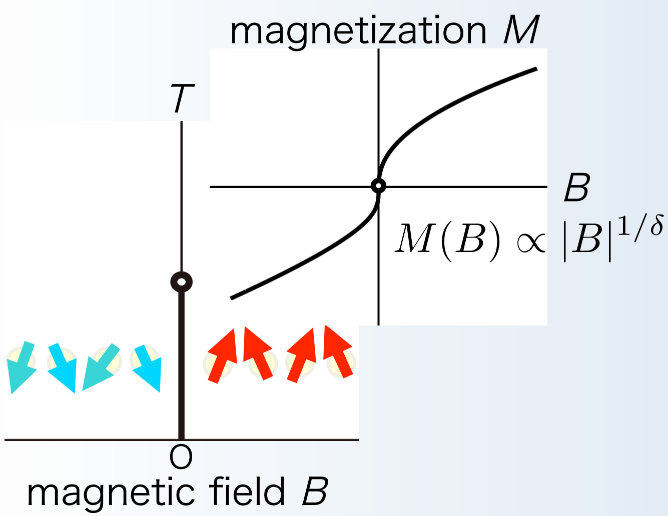
Water

3D Ising



$$\rho(P) = \rho_c + \alpha_+ |P - P_c|^{1/\delta} \ (P > P_c)$$
$$\rho(P) = \rho_c - \alpha_- |P - P_c|^{1/\delta} \ (P < P_c)$$





Why Many-Body Problem Is Hard to Solve

2. *N*-body classical statistical mechanics

Example: 1 D Ising Model

$$H = J\sum_{i=0}^{L-1}\sigma_i\sigma_{i+1} - B\sum_{i=0}^{L-1}\sigma_i$$

Ising spin: $\sigma_i = \pm 1$

Periodic boundary: $i+1 \to \mathrm{mod}(i+1, L)$

Partition function: Summation over 2^L configurations

$$Z = \sum_{\sigma_0=\pm 1}\sum_{\sigma_1=\pm 1}\cdots\sum_{\sigma_{L-1}=\pm 1}\exp\left(-H[\{\sigma\}]/k_{\mathrm{B}}T\right)$$

$$\{\sigma\} = \{\sigma_0, \sigma_1, \ldots, \sigma_{L-1}\}$$

Why Many-Body Problem Is Hard to Solve

3&4. *N*-body Schrödinger equation & quantum statistical mechanics

Example: 1 D Transverse Field Ising Model (TFIM)

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

Quantum Spin 1/2 or Qubit

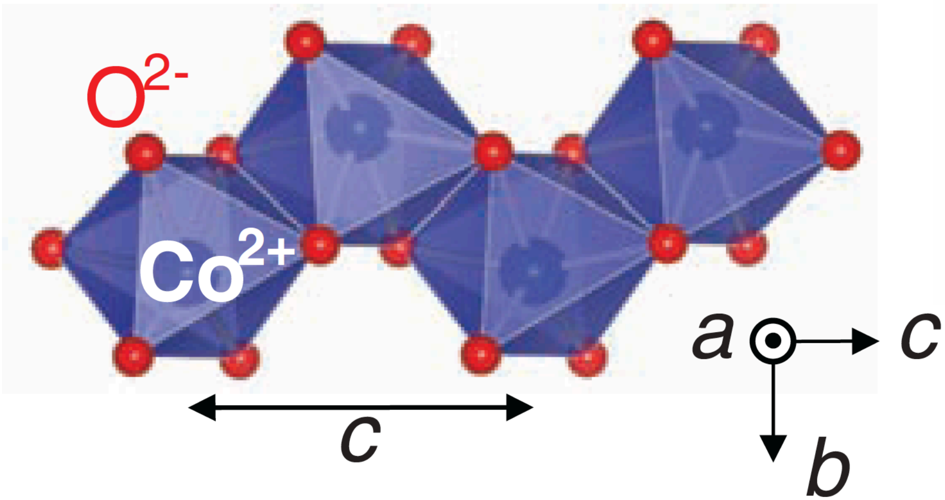
$$|\uparrow\rangle, \ |\downarrow\rangle$$

$$|1\rangle, \ |0\rangle$$

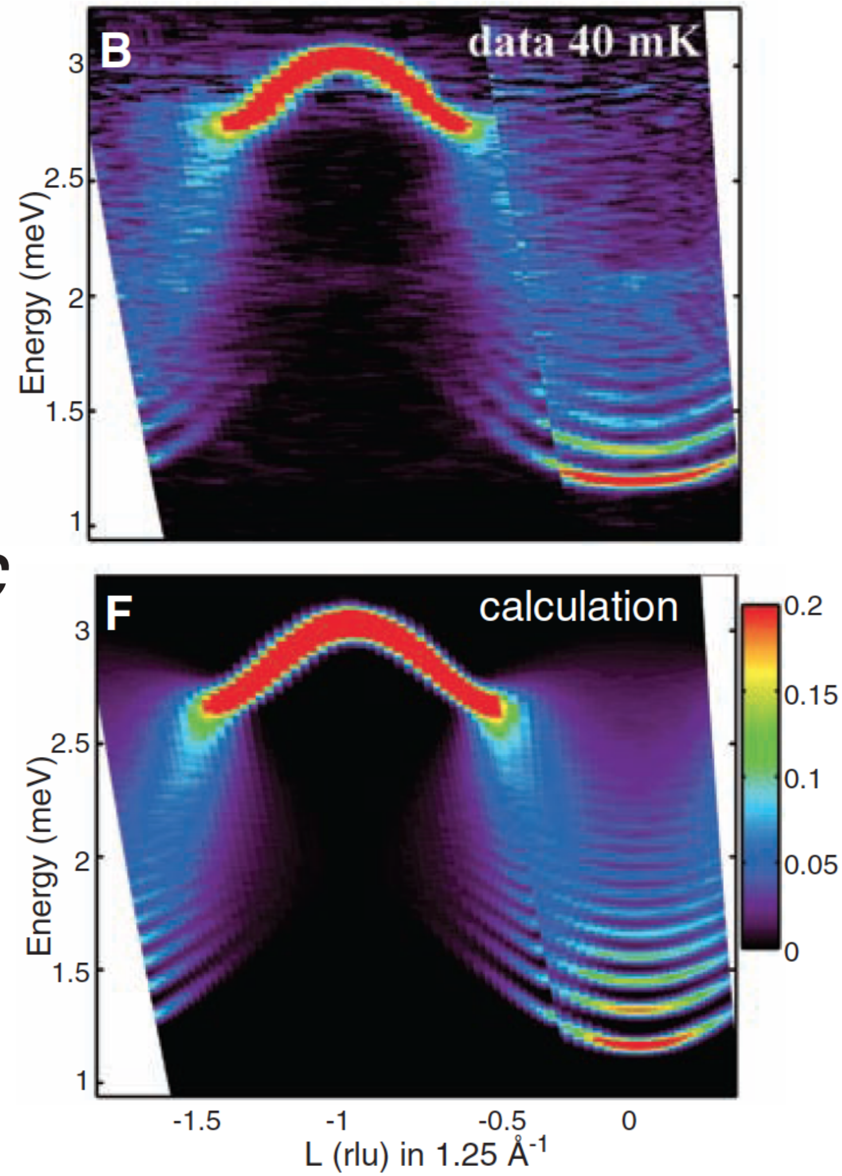
Periodic boundary: $i+1 \rightarrow \mathrm{mod}(i+1, L)$

Transverse Field Ising Model

A realization of TFIM:
$CoNb_2O_6$



R. Coldea, *et al.*,
Science 327, 177 (2010)



Mathematical Description of Quantum Many-Body Systems

Operators and Hilbert space

Operator $\hat{O} \in \mathcal{O}$ $\quad \hat{O}: \ \mathcal{F} \to \mathcal{F}$ (square matrix)

$$\text{If } \hat{O}_1, \hat{O}_2 \in \mathcal{O}, \hat{O}_1\hat{O}_2 \in \mathcal{O}$$

$$\text{If } \hat{O}_1, \hat{O}_2 \in \mathcal{O}, \ c_1\hat{O}_1 + c_2\hat{O}_2 \in \mathcal{O} \ (c_1, c_2 \in \mathbb{C})$$

Hilbert space/Fock space (vector space)

$$\text{If } |\alpha_1\rangle, |\alpha_2\rangle \in \mathcal{F}, \ c_1|\alpha_1\rangle + c_2|\alpha_2\rangle \in \mathcal{F} \ (c_1, c_2 \in \mathbb{C})$$

$$\text{Hermitian conjugate}: (|\alpha\rangle)^\dagger = \langle\alpha|$$

(complex conjugate + transpose)

$$\text{Inner product}: \langle\alpha_1| \cdot |\alpha_2\rangle = \langle\alpha_1|\alpha_2\rangle \in \mathbb{C}$$

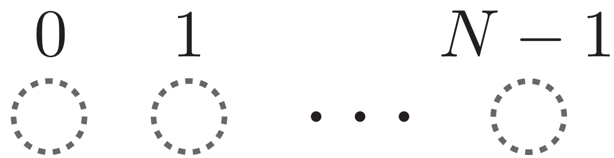
$$\cdot : \mathcal{F} \times \mathcal{F} \to \mathbb{C}$$

$$\text{If } \hat{O} \in \mathcal{O} \text{ and } |\alpha\rangle \in \mathcal{F}, \hat{O}|\alpha\rangle \in \mathcal{F}$$

$$(\hat{O}|\alpha\rangle)^\dagger = \langle\alpha|\hat{O}^\dagger$$

An Example: N Qubits

N Qubits



Hilbert space of N qubits:

$$\mathcal{F} = \{ \sum_{n_0=0,1} \sum_{n_1=0,1} \cdots \sum_{n_{N-1}=0,1} C_{n_0 n_1 \cdots n_{N-1}} |n_0\rangle \otimes |n_1\rangle \otimes \cdots \otimes |n_{N-1}\rangle \}$$

$$(C_{n_0 n_1 \cdots n_{N-1}} \in \mathbb{C})$$

Inner product:

$$\langle n_0'| \otimes \langle n_1'| \otimes \cdots \otimes \langle n_{N-1}'| \cdot |n_0\rangle \otimes |n_1\rangle \otimes \cdots \otimes |n_{N-1}\rangle$$

$$= \langle n_0'|n_0\rangle \times \langle n_1'|n_1\rangle \times \cdots \langle n_{N-1}'|n_{N-1}\rangle$$

$$\langle n'|n\rangle = \delta_{n',n} \ (n, n' = 0, 1)$$

Operators acting on N qubits: $\hat{S}_j^a, \hat{S}_j^a \hat{S}_{j+1}^a : \mathcal{F} \to \mathcal{F}$

$$\hat{S}_j^a \doteq \overbrace{1 \otimes \cdots \otimes 1}^{j-1} \otimes \hat{S}_j^a \otimes \overbrace{1 \otimes \cdots \otimes 1}^{N-j}$$

$$\hat{S}_j^a \hat{S}_{j+1}^a \doteq \overbrace{1 \otimes \cdots \otimes 1}^{j-1} \otimes \hat{S}_j^a \otimes \hat{S}_{j+1}^a \otimes \overbrace{1 \otimes \cdots \otimes 1}^{N-j-1}$$

Quantum Spin S=1/2 or Qubit

Operators acting on a single qubit

$$|1\rangle = |\uparrow\rangle, \quad |0\rangle = |\downarrow\rangle$$

A two dimensional representation of Lie algebra SU(2)

$$[\hat{S}_j^x, \hat{S}_j^y] = i\hat{S}_j^z$$
$$[\hat{S}_j^y, \hat{S}_j^z] = i\hat{S}_j^x$$
$$[\hat{S}_j^z, \hat{S}_j^x] = i\hat{S}_j^y$$

$$\hat{S}_j^x|1\rangle = +\frac{1}{2}|0\rangle$$
$$\hat{S}_j^x|0\rangle = +\frac{1}{2}|1\rangle$$
$$\hat{S}_j^y|1\rangle = +i\frac{1}{2}|0\rangle$$
$$\hat{S}_j^y|0\rangle = -i\frac{1}{2}|1\rangle$$
$$\hat{S}_j^z|1\rangle = +\frac{1}{2}|1\rangle$$
$$\hat{S}_j^z|0\rangle = -\frac{1}{2}|0\rangle$$

Quantum Spin S=1/2 or Qubit

$$|\phi\rangle = c_\uparrow |1\rangle + c_\downarrow |0\rangle$$

$$\hat{S}_j^\alpha |\phi\rangle = c'_\uparrow |1\rangle + c'_\downarrow |0\rangle$$

$$\begin{pmatrix} c'_\uparrow \\ c'_\downarrow \end{pmatrix} = \frac{1}{2}\hat{\sigma}^\alpha \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$$

$$\hat{\sigma}^x = \begin{pmatrix} 0 & +1 \\ +1 & 0 \end{pmatrix}$$

$$\hat{\sigma}^y = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}$$

$$\hat{\sigma}^z = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}$$

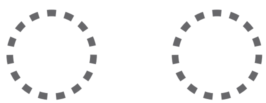
$$\hat{S}_j^\alpha \doteq \frac{1}{2}\hat{\sigma}^\alpha$$

An Example of Many-Body States

Entangled states (量子もつれ状態)

-重ね合わせで作られる
-量子テレポーテーションに用いられる
cf.) EPR“パラドクス”

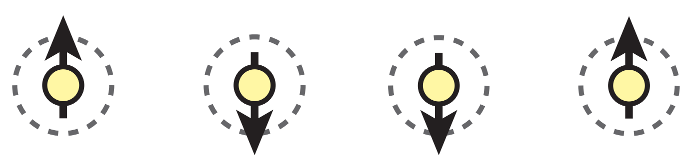
2 qubits



Inter bit interaction

$$\hat{H} = J \sum_{a=x,y,z} \hat{S}_0^a \hat{S}_1^a \qquad (J \in \mathbb{R}, J > 0)$$

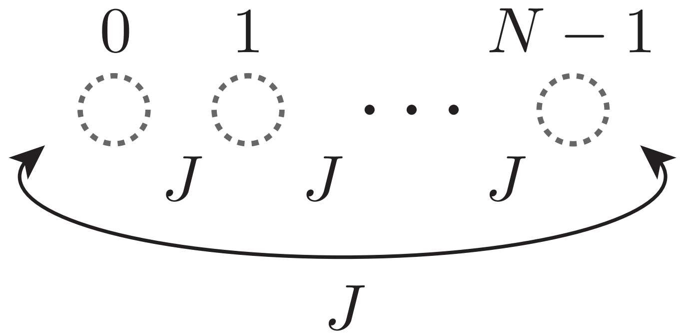
→Entangled state



$$|1\rangle \otimes |0\rangle - |0\rangle \otimes |1\rangle$$

Hamiltonian

N qubits



N qubit Hilbert space:

$$\mathcal{F} = \{ \sum_{n_0=0,1} \sum_{n_1=0,1} \cdots \sum_{n_{N-1}=0,1} C_{n_0 n_1 \cdots n_{N-1}} |n_0\rangle \otimes |n_1\rangle \otimes \cdots \otimes |n_{N-1}\rangle \}$$

$$(C_{n_0 n_1 \cdots n_{N-1}} \in \mathbb{C})$$

Inter qubit interaction/Hamiltonian operator $\hat{H} : \mathcal{F} \to \mathcal{F}$

$$\hat{H} = J \sum_{j=0}^{N-1} \sum_{a=x,y,z} \hat{S}_j^a \hat{S}_{\mathrm{mod}(j+1,N)}^a$$

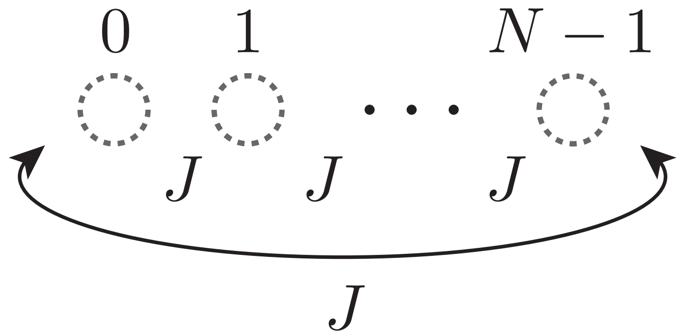
Heisenberg model

-Effective description of insulating magnets

-Example: $KCuF_3$, La_2CuO_4 (2D)

Hamiltonian

N qubits



N qubit Hilbert space:

$$\mathcal{F} = \{ \sum_{n_0=0,1} \sum_{n_1=0,1} \cdots \sum_{n_{N-1}=0,1} C_{n_0 n_1 \cdots n_{N-1}} |n_0\rangle \otimes |n_1\rangle \otimes \cdots \otimes |n_{N-1}\rangle \}$$

$$(C_{n_0 n_1 \cdots n_{N-1}} \in \mathbb{C})$$

Inter qubit interaction/Hamiltonian operator $\hat{H} : \mathcal{F} \to \mathcal{F}$

$$\hat{H} = J \sum_{j=0}^{N-1} \sum_{a=x,y,z} \hat{S}_j^a \hat{S}_{\mathrm{mod}(j+1,N)}^a$$

Orthonormal bases: $|I\rangle, |I'\rangle \in \mathcal{F}$ $\quad \langle 0| = (|0\rangle)^\dagger$

$\langle I|I'\rangle = \delta_{I,I'}$ $\quad \langle 1| = (|1\rangle)^\dagger$

Hamiltonian matrix $\quad H_{II'} = \langle I|\hat{H}|I'\rangle$

量子多体問題の最も簡単な例: 固体物理学から

N-body quantum statistical mechanics

Example: 1 D Transverse Field Ising Model (TFIM)

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

Quantum Spin 1/2
or Qubit

$$|\uparrow\rangle, \ |\downarrow\rangle$$
$$|1\rangle, \ |0\rangle$$

Periodic boundary: $i + 1 \to \mathrm{mod}(i + 1, L)$

Quantum Spins: Two Site TFIM

Decimal representation of orthonormalized basis

		0 th site		1 st site
$\vert 0\rangle_{\mathrm{d}}$	$=$	$\vert\downarrow\rangle$	$\otimes$	$\vert\downarrow\rangle$
$\vert 1\rangle_{\mathrm{d}}$	$=$	$\vert\uparrow\rangle$	$\otimes$	$\vert\downarrow\rangle$
$\vert 2\rangle_{\mathrm{d}}$	$=$	$\vert\downarrow\rangle$	$\otimes$	$\vert\uparrow\rangle$
$\vert 3\rangle_{\mathrm{d}}$	$=$	$\vert\uparrow\rangle$	$\otimes$	$\vert\uparrow\rangle$

$$L = 2 \qquad \hat{H} = J\sum_{i=0}^{L-1}\hat{S}_i^z\hat{S}_{i+1}^z - \Gamma\sum_{i=0}^{L-1}\hat{S}_i^x$$

$$\hat{H} \doteq \begin{pmatrix} +J/2 & -\Gamma/2 & -\Gamma/2 & 0 \\ -\Gamma/2 & -J/2 & 0 & -\Gamma/2 \\ -\Gamma/2 & 0 & -J/2 & -\Gamma/2 \\ 0 & -\Gamma/2 & -\Gamma/2 & +J/2 \end{pmatrix} \quad {}_{\mathrm{d}}\langle i|\hat{H}|j\rangle_{\mathrm{d}}$$

Larger TFIM

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

-Non-commutative

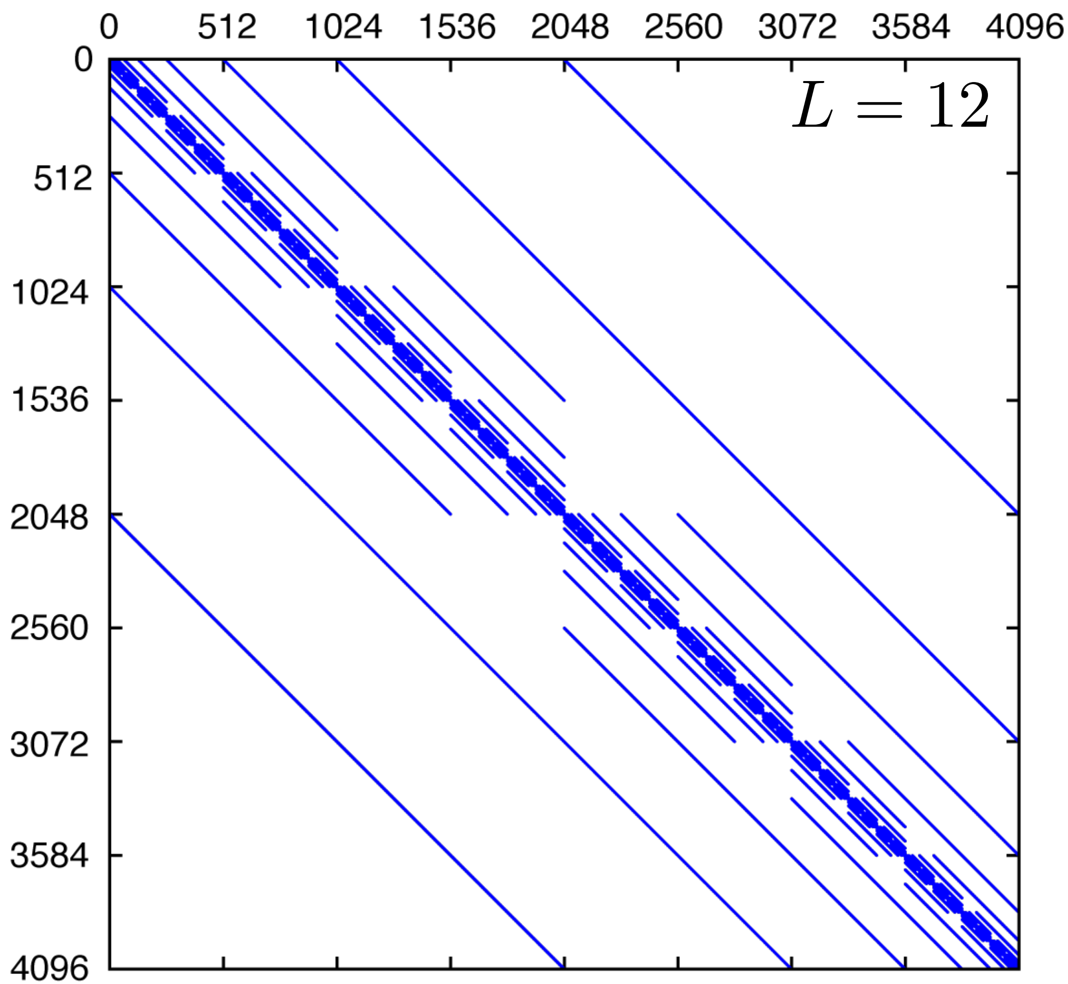
$$\left[\sum_{i=0}^{L-1}\hat{S}_i^z\hat{S}_{i+1}^z, \sum_{i=0}^{L-1}\hat{S}_i^x\right] \neq 0$$

→Quantum fluctuations
or Zero point motion

-Sparse
\# of elements ∝ $O(2^L)$

-Solvable

-Hierarchical matrix?

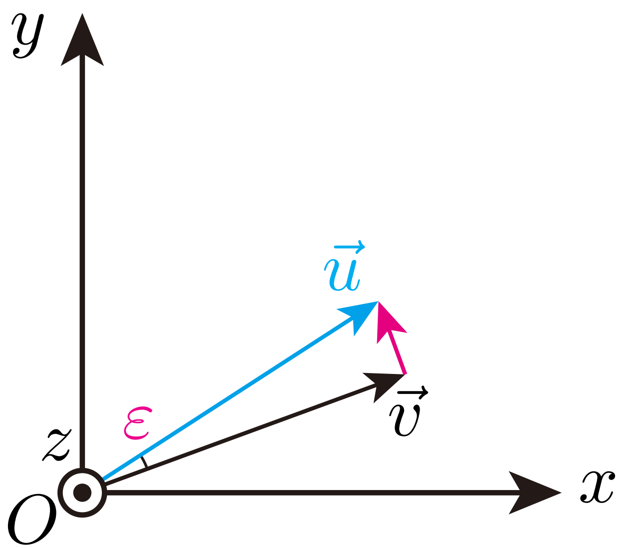


Appendix: S=1/2 Spins

Appendix: Rotation of Vector

Infinitesimal rotation ε :

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} 1 & -\varepsilon & 0 \\ +\varepsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$



$$\begin{pmatrix} 1 & -\varepsilon & 0 \\ +\varepsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - i\varepsilon \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\simeq e^{-i\varepsilon \ell_z}$$

$$\ell_z \equiv \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\ell_x \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & +i & 0 \end{pmatrix}$$

$$\ell_y \equiv \begin{pmatrix} 0 & 0 & +i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

Appendix: Finite Angle Rotation

Finite rotation

$$\vec{u} = e^{-i\theta\vec{n}\cdot\vec{\ell}}\vec{v}$$

$$\lim_{N\to+\infty}\left(1 - i\frac{\theta}{N}\vec{n}\cdot\vec{\ell}\right)^N = e^{-i\theta\vec{n}\cdot\vec{\ell}}$$

Rotations are not commutable:

$$e^{-i\theta_1\ell_z} = \begin{pmatrix} +\cos\theta_1 & -\sin\theta_1 & 0 \\ +\sin\theta_1 & +\cos\theta_1 & 0 \\ 0 & 0 & +1 \end{pmatrix}$$

$$e^{-i\theta_2\ell_x} = \begin{pmatrix} +1 & 0 & 0 \\ 0 & +\cos\theta_2 & -\sin\theta_2 \\ 0 & +\sin\theta_2 & +\cos\theta_2 \end{pmatrix}$$

$$e^{-i\theta_1\ell_z}e^{-i\theta_2\ell_x} \neq e^{-i\theta_2\ell_x}e^{-i\theta_1\ell_z}$$

Infinitesimal Rotation: An Example of Lie Algebra

SU(2) $$[\ell_\alpha, \ell_\beta] = i\epsilon_{\alpha\beta\gamma}\ell_\gamma$$

$[\ell_\alpha, \ell_\beta] \equiv \ell_\alpha\ell_\beta - \ell_\beta\ell_\alpha$ $\quad \alpha, \beta, \gamma = x, y, z$

Antisymmetric tensor: $$\epsilon_{\alpha\beta\gamma} = \begin{cases} +1 & \text{for } (\alpha,\beta,\gamma) = (x,y,z),(y,z,x),(z,x,y) \\ -1 & \text{for } (\alpha,\beta,\gamma) = (x,z,y),(y,x,z),(z,y,x) \\ 0 & \text{others} \end{cases}$$

3 D representation:

$$\ell_z \equiv \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\ell_x \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & +i & 0 \end{pmatrix}$$

$$\ell_y \equiv \begin{pmatrix} 0 & 0 & +i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

2 D representation:

$$s_z = \frac{1}{2}\begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$s_x = \frac{1}{2}\begin{pmatrix} 0 & +1 \\ +1 & 0 \end{pmatrix}$$

$$s_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}$$

有限回転はSO(3)と呼ばれるリー群

$$e^{-i\theta\vec{n}\cdot\vec{\ell}}$$

Appendix: 群(Group)の定義

群Gとは, 任意の一対の元に対して, 以下の性質を満たす第３の元を割り当てる規則をもった集合である:

1) $f, g \in G$ ならば $h = fg \in G$
2) $f, g, h \in G$ に対して, $f(gh) = (fg)h$
3) 単位元 e が存在し, 全ての元 $f \in G$ に対して, $ef = fe = f$
4) 任意の元 $f \in G$ に, 逆元f^{-1}が存在し, $f f^{-1} = f^{-1} f = e$

参考書:
ジョージャイ
『物理学におけるリー代数』
(吉岡書店, 2010)

例: 正方行列の部分集合で, 逆行列が存在する行列の集合
例: 任意軸まわりの回転行列の集合

Rep. & Basis of Rotation Group

"Wave function" Double rep.

$$e^{-i\phi s_z} e^{-i\theta s_y} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\vec{u} = \begin{pmatrix} \cos\frac{\theta}{2} e^{-i\frac{\phi}{2}} \\ \sin\frac{\theta}{2} e^{+i\frac{\phi}{2}} \end{pmatrix}$$

Spin

$$e^{-i\phi \ell_z} e^{-i\theta \ell_y} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\vec{s} = \frac{1}{2} \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}$$

Appendix: 2D Rep. to 3D Rep.

Wave function to spin components

$$\vec{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$$

$$\langle s_z \rangle \equiv \vec{u}^\dagger s_z \vec{u}$$

$$\langle s_x \rangle \equiv \vec{u}^\dagger s_x \vec{u}$$

$$\langle s_y \rangle \equiv \vec{u}^\dagger s_y \vec{u}$$

$$\vec{s} = \begin{pmatrix} \langle s_x \rangle \\ \langle s_y \rangle \\ \langle s_z \rangle \end{pmatrix}$$

Exercise: Wave Function of Spin

1. Obtain a wave function describing a spin that is parallel & antiparallel to x axis

2. Obtain a wave function describing a spin that is parallel & antiparallel to y axis

3. Rotate a wave function of a spin parallel to x axis by 180° around z axis

4. Rotate a wave function of a spin parallel to x axis by 360° around z axis

Exercise: 2 Site Heisenberg Model

$$\hat{H} = J \sum_{a=x,y,z} \hat{S}_0^a \hat{S}_1^a \qquad (J \in \mathbb{R}, J > 0)$$

1. Obtain a Hamiltonian matrix of the 2 site Heisenberg model

2. Diagonalize the Hamiltonian matrix obtained in 1. and obtain eigenvalues and eigenvectors

How about bosonic and fermionic particles?

2nd Quantization: Boson

-Basis

$$\frac{e^{+i\vec{k}\cdot\vec{r}}}{\sqrt{L^3}} \ \left(\vec{k}^T = \left(\frac{2\pi\ell_x}{L}, \frac{2\pi\ell_y}{L}, \frac{2\pi\ell_z}{L}\right),\ \ell_{x,y,z} \in \mathbb{Z}\right)$$

Boson

$$\left[\ \hat{a}_{\vec{k}},\ \hat{a}^\dagger_{\vec{k}'}\ \right] = \hat{a}_{\vec{k}}\hat{a}^\dagger_{\vec{k}'} - \hat{a}^\dagger_{\vec{k}'}\hat{a}_{\vec{k}} = \delta_{\vec{k},\vec{k}'}$$

$$\left[\ \hat{a}_{\vec{k}},\ \hat{a}_{\vec{k}'}\ \right] = \left[\ \hat{a}^\dagger_{\vec{k}},\ \hat{a}^\dagger_{\vec{k}'}\ \right] = 0$$

-Commutation rule

$$\hat{a}_{\vec{k}'}\hat{a}^\dagger_{\vec{k}} = \hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}'} + \delta_{\vec{k},\vec{k}'}$$

$$\hat{a}_{\vec{k}'}\hat{a}_{\vec{k}} = \hat{a}_{\vec{k}}\hat{a}_{\vec{k}'}$$

$$\hat{a}^\dagger_{\vec{k}'}\hat{a}^\dagger_{\vec{k}} = \hat{a}^\dagger_{\vec{k}}\hat{a}^\dagger_{\vec{k}'}$$

-Fock state

$$\hat{a}_{\vec{k}}|\mathrm{vac}\rangle = 0\cdot|\mathrm{vac}\rangle = 0 \ (\text{zero vector})$$

$$\hat{a}^\dagger_{\vec{k}}|\mathrm{vac}\rangle \ (\text{a particle with } \vec{k})$$

$$\left(\hat{a}^\dagger_{\vec{k}}\right)^N |\mathrm{vac}\rangle \ (N \ \text{ particles with } \vec{k})$$

2nd Quantization: Fermion

-Basis

$$\frac{e^{+i\vec{k}\cdot\vec{r}}}{\sqrt{L^3}} \quad \left(\vec{k}^T = \left(\frac{2\pi\ell_x}{L}, \frac{2\pi\ell_y}{L}, \frac{2\pi\ell_z}{L}\right),\ \ell_{x,y,z} \in \mathbb{Z}\right)$$

Fermion

$$\left\{\hat{c}_{\vec{k}\sigma},\ \hat{c}^\dagger_{\vec{k}'\sigma'}\right\} = \hat{c}_{\vec{k}\sigma}\hat{c}^\dagger_{\vec{k}'\sigma'} + \hat{c}^\dagger_{\vec{k}'\sigma'}\hat{c}_{\vec{k}\sigma} = \delta_{\vec{k},\vec{k}'}\delta_{\sigma,\sigma'}$$

$$\left\{\hat{c}_{\vec{k}\sigma},\ \hat{c}_{\vec{k}'\sigma'}\right\} = \left\{\hat{c}^\dagger_{\vec{k}\sigma},\ \hat{c}^\dagger_{\vec{k}'\sigma'}\right\} = 0$$

-Commutation rule

$$\hat{c}_{\vec{k}'\sigma'}\hat{c}^\dagger_{\vec{k}\sigma} = -\hat{c}^\dagger_{\vec{k}\sigma}\hat{c}_{\vec{k}'\sigma'} + \delta_{\vec{k},\vec{k}'}\delta_{\sigma,\sigma'}$$

$$\hat{c}_{\vec{k}'\sigma'}\hat{c}_{\vec{k}\sigma} = -\hat{c}_{\vec{k}\sigma}\hat{c}_{\vec{k}'\sigma'}$$

$$\hat{c}^\dagger_{\vec{k}'\sigma'}\hat{c}^\dagger_{\vec{k}\sigma} = -\hat{c}^\dagger_{\vec{k}\sigma}\hat{c}^\dagger_{\vec{k}'\sigma'}$$

2nd Quantization: Fermion

-Basis $\dfrac{e^{+i\vec{k}\cdot\vec{r}}}{\sqrt{L^3}} \left(\vec{k}^T = \left(\dfrac{2\pi\ell_x}{L}, \dfrac{2\pi\ell_y}{L}, \dfrac{2\pi\ell_z}{L}\right),\ \ell_{x,y,z} \in \mathbb{Z}\right)$

Fermion

$$\left\{\hat{c}_{\vec{k}\sigma},\ \hat{c}^\dagger_{\vec{k}'\sigma'}\right\} = \hat{c}_{\vec{k}\sigma}\hat{c}^\dagger_{\vec{k}'\sigma'} + \hat{c}^\dagger_{\vec{k}'\sigma'}\hat{c}_{\vec{k}\sigma} = \delta_{\vec{k},\vec{k}'}\delta_{\sigma,\sigma'}$$

$$\left\{\hat{c}_{\vec{k}\sigma},\ \hat{c}_{\vec{k}'\sigma'}\right\} = \left\{\hat{c}^\dagger_{\vec{k}\sigma},\ \hat{c}^\dagger_{\vec{k}'\sigma'}\right\} = 0$$

-Fock state

$$\hat{c}^\dagger_{\vec{k}\sigma}|\mathrm{vac}\rangle \text{ (a particle with } \vec{k} \text{ and } \sigma)$$

$$\hat{c}_{\vec{k}\sigma}|\mathrm{vac}\rangle = 0 \cdot |\mathrm{vac}\rangle = 0 \text{ (zero vector)}$$

$$\hat{c}^\dagger_{\vec{k}\sigma} \cdot \hat{c}^\dagger_{\vec{k}\sigma}|\mathrm{vac}\rangle = -\hat{c}^\dagger_{\vec{k}\sigma} \cdot \hat{c}^\dagger_{\vec{k}\sigma}|\mathrm{vac}\rangle = 0$$

Pauli principle

Description of Quantum Many-Body Systems 1.

Building blocks of many-body quantum theory

-Complete orthonormal basis set of 1-body wave functions

An example:
Plane wave

$$\frac{e^{+i\vec{k}\cdot\vec{r}}}{\sqrt{L^3}} \left(\vec{k}^T = \left(\frac{2\pi\ell_x}{L}, \frac{2\pi\ell_y}{L}, \frac{2\pi\ell_z}{L}\right), \ \ell_{x,y,z} \in \mathbb{Z}\right)$$

-Creation & annihilation operators

Non-commutative
→ Quantum fluctuations

boson

$$\left[\ \hat{a}_{\vec{k}},\ \hat{a}^{\dagger}_{\vec{k}'}\ \right] = \hat{a}_{\vec{k}}\hat{a}^{\dagger}_{\vec{k}'} - \hat{a}^{\dagger}_{\vec{k}'}\hat{a}_{\vec{k}} = \delta_{\vec{k},\vec{k}'}$$

$$\left[\ \hat{a}_{\vec{k}},\ \hat{a}_{\vec{k}'}\ \right] = \left[\ \hat{a}^{\dagger}_{\vec{k}},\ \hat{a}^{\dagger}_{\vec{k}'}\ \right] = 0$$

fermion

$$\left\{\hat{c}_{\vec{k}\sigma},\ \hat{c}^{\dagger}_{\vec{k}'\sigma'}\right\} = \hat{c}_{\vec{k}\sigma}\hat{c}^{\dagger}_{\vec{k}'\sigma'} + \hat{c}^{\dagger}_{\vec{k}'\sigma'}\hat{c}_{\vec{k}\sigma} = \delta_{\vec{k},\vec{k}'}\delta_{\sigma,\sigma'}$$

$$\left\{\hat{c}_{\vec{k}\sigma},\ \hat{c}_{\vec{k}'\sigma'}\right\} = \left\{\hat{c}^{\dagger}_{\vec{k}\sigma},\ \hat{c}^{\dagger}_{\vec{k}'\sigma'}\right\} = 0$$

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$$

-Vacuum (kernel of annihilation operators)

$$\hat{a}_{\vec{k}}|\mathrm{vac}\rangle = 0$$

$$\hat{c}_{\vec{k}\sigma}|\mathrm{vac}\rangle = 0$$

Description of Quantum Many-Body Systems 2.

Hilbert/Fock space (Revisited):

-Vector space expanded by
 products of operators and vacuum

ket vectors $|\Psi\rangle = |\mathrm{vac}\rangle, \hat{A}|\mathrm{vac}\rangle, \hat{A}\hat{B}|\mathrm{vac}\rangle, \ldots$

-Inner product $\langle \mathrm{vac}|\hat{D}^\dagger \hat{C}^\dagger \cdot \hat{A}\hat{B}|\mathrm{vac}\rangle \in \mathbb{C}$

bra vectors $\left(\hat{A}\hat{B}|\mathrm{vac}\rangle\right)^\dagger = \langle \mathrm{vac}|\hat{B}^\dagger \hat{A}^\dagger$

Hermitian conjugate $\left(\hat{A}^\dagger\right)^\dagger = \hat{A}$

Usually we normalize the vacuum $\langle \mathrm{vac}| \cdot |\mathrm{vac}\rangle = \langle \mathrm{vac}|\mathrm{vac}\rangle = 1$

2-norm of $|\Psi\rangle = \hat{A}\hat{B}|\mathrm{vac}\rangle$ $\sqrt{\langle \mathrm{vac}|\hat{B}^\dagger \hat{A}^\dagger \hat{A}\hat{B}|\mathrm{vac}\rangle}$

Description of Quantum Many-Body Systems 3.

Many-body bosons

Exercise 1. Particle number operator $\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}$

Confirm the following identity:

$$\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}\left(\hat{a}^\dagger_{\vec{k}}\right)^N|\mathrm{vac}\rangle = N\left(\hat{a}^\dagger_{\vec{k}}\right)^N|\mathrm{vac}\rangle$$

Exercise 2. Norm of a *N* boson wave function

Evaluate the following inner product:

$$\langle\mathrm{vac}|\left(\hat{a}_{\vec{k}}\right)^N\left(\hat{a}^\dagger_{\vec{k}}\right)^N|\mathrm{vac}\rangle$$

$$\left(\left(\hat{a}^\dagger_{\vec{k}}\right)^N|\mathrm{vac}\rangle\right)^\dagger = \langle\mathrm{vac}|\left(\hat{a}_{\vec{k}}\right)^N$$

Answer to the exercises

Exercise 1. Particle number operator $\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}$

Confirm the following identity:

$$\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}\left(\hat{a}^\dagger_{\vec{k}}\right)^N|\mathrm{vac}\rangle = N\left(\hat{a}^\dagger_{\vec{k}}\right)^N|\mathrm{vac}\rangle$$

$$\begin{aligned}
\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}\left(\hat{a}^\dagger_{\vec{k}}\right)^N|\mathrm{vac}\rangle &= \hat{a}^\dagger_{\vec{k}}\cdot\hat{a}_{\vec{k}}\hat{a}^\dagger_{\vec{k}}\cdot\left(\hat{a}^\dagger_{\vec{k}}\right)^{N-1}|\mathrm{vac}\rangle \\
&= \hat{a}^\dagger_{\vec{k}}\left(\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}+1\right)\left(\hat{a}^\dagger_{\vec{k}}\right)^{N-1}|\mathrm{vac}\rangle \\
&= \left(\hat{a}^\dagger_{\vec{k}}\right)^2\hat{a}_{\vec{k}}\left(\hat{a}^\dagger_{\vec{k}}\right)^{N-1}|\mathrm{vac}\rangle + \left(\hat{a}^\dagger_{\vec{k}}\right)^N|\mathrm{vac}\rangle \\
&= \left(\hat{a}^\dagger_{\vec{k}}\right)^3\hat{a}_{\vec{k}}\left(\hat{a}^\dagger_{\vec{k}}\right)^{N-2}|\mathrm{vac}\rangle + 2\left(\hat{a}^\dagger_{\vec{k}}\right)^N|\mathrm{vac}\rangle \\
&\vdots \\
&= N\left(\hat{a}^\dagger_{\vec{k}}\right)^N|\mathrm{vac}\rangle
\end{aligned}$$

Answer to the exercises

Exercise 2. Norm of a N boson wave function

Evaluate the following inner product:

$$\langle \mathrm{vac}| \left(\hat{a}_{\vec{k}}\right)^N \left(\hat{a}^\dagger_{\vec{k}}\right)^N |\mathrm{vac}\rangle$$

$$\left(\left(\hat{a}^\dagger_{\vec{k}}\right)^N |\mathrm{vac}\rangle\right)^\dagger = \langle \mathrm{vac}| \left(\hat{a}_{\vec{k}}\right)^N$$

$$\begin{aligned}
\langle \mathrm{vac}| \left(\hat{a}_{\vec{k}}\right)^N \left(\hat{a}^\dagger_{\vec{k}}\right)^N |\mathrm{vac}\rangle &= \langle \mathrm{vac}| \left(\hat{a}_{\vec{k}}\right)^{N-1} \left(\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}} + 1\right) \left(\hat{a}^\dagger_{\vec{k}}\right)^{N-1} |\mathrm{vac}\rangle \\
&= N \langle \mathrm{vac}| \left(\hat{a}_{\vec{k}}\right)^{N-1} \left(\hat{a}^\dagger_{\vec{k}}\right)^{N-1} |\mathrm{vac}\rangle \\
&= N(N-1) \langle \mathrm{vac}| \left(\hat{a}_{\vec{k}}\right)^{N-2} \left(\hat{a}^\dagger_{\vec{k}}\right)^{N-2} |\mathrm{vac}\rangle \\
&\vdots \\
&= N!
\end{aligned}$$

Description of Quantum Many-Body Systems 4.

1st quantization and 2nd quantization in bosons

Field operator $\hat{\phi}(\vec{r}) = \sum_{\vec{k}} \frac{e^{+i\vec{k}\cdot\vec{r}}}{\sqrt{L^3}} \hat{a}_{\vec{k}}$

A non-interacting many-body wave function

$$|\Psi\rangle = \prod_{\nu} \frac{1}{\sqrt{N_\nu !}} \left(\hat{a}^{\dagger}_{\vec{k}_\nu} \right)^{N_\nu} |\mathrm{vac}\rangle \quad \langle \Psi | \Psi \rangle = 1$$

A 2-body wave function:

2nd quantization $|\Psi\rangle = \hat{a}^{\dagger}_{\vec{k}_1} \hat{a}^{\dagger}_{\vec{k}_2} |\mathrm{vac}\rangle$

1st quantization $\psi(\vec{r}_1, \vec{r}_2) = \langle \mathrm{vac} | \hat{\phi}(\vec{r}_2) \hat{\phi}(\vec{r}_1) | \Psi \rangle$

Exercise: Evaluate $\langle \mathrm{vac} | \hat{\phi}(\vec{r}_2) \hat{\phi}(\vec{r}_1) | \Psi \rangle$

Indistinguishable particles $\psi(\vec{r}_1, \vec{r}_2) = +\psi(\vec{r}_2, \vec{r}_1)$

Description of Quantum Many-Body Systems 5.

1st quantization and 2nd quantization in fermions

Field operator $\hat{\phi}_\sigma(\vec{r}) = \sum_{\vec{k}} \frac{e^{+i\vec{k}\cdot\vec{r}}}{\sqrt{L^3}} \hat{c}_{\vec{k}\sigma}$

A non-interacting many-body wave function

$$|\Psi\rangle = \prod_\mu \hat{c}^\dagger_{\vec{k}_\mu\uparrow} \prod_\nu \hat{c}^\dagger_{\vec{k}_\nu\downarrow} |\mathrm{vac}\rangle \qquad \langle\Psi|\Psi\rangle = 1$$

A 2-body wave function:

2nd quantization $\quad |\Psi\rangle = \hat{c}^\dagger_{\vec{k}_1\sigma} \hat{c}^\dagger_{\vec{k}_2\sigma} |\mathrm{vac}\rangle$

1st quantization $\quad \psi(\vec{r}_1\sigma, \vec{r}_2\sigma) = \langle\mathrm{vac}|\hat{\phi}_\sigma(\vec{r}_2)\hat{\phi}_\sigma(\vec{r}_1)|\Psi\rangle$

Exercise: Evaluate $\langle\mathrm{vac}|\hat{\phi}_\sigma(\vec{r}_2)\hat{\phi}_\sigma(\vec{r}_1)|\Psi\rangle$

Indistinguishable particles $\quad \psi(\vec{r}_1\sigma, \vec{r}_2\sigma) = -\psi(\vec{r}_2\sigma, \vec{r}_1\sigma)$

Description of Quantum Many-Body Systems 6.

Hamiltonian in 2nd quantization form

Spin independent

$$\hat{H} = \int d^3r \hat{\phi}^\dagger(\vec{r}) \left(-\frac{\hbar^2}{2m}\nabla^2 + v(\vec{r}) \right) \hat{\phi}(\vec{r})$$
$$+ \frac{1}{2} \int d^3r \int d^3r' \hat{\phi}^\dagger(\vec{r}) \hat{\phi}(\vec{r}) V(|\vec{r} - \vec{r}'|) \hat{\phi}^\dagger(\vec{r}') \hat{\phi}(\vec{r}')$$

Spin dependent

$$\hat{H} = \sum_{\sigma,\sigma'} \int d^3r \hat{\phi}_\sigma^\dagger(\vec{r}) \left(-\delta_{\sigma,\sigma'} \frac{\hbar^2}{2m}\nabla^2 + v_{\sigma\sigma'}(\vec{\nabla}, \vec{r}) \right) \hat{\phi}_{\sigma'}(\vec{r})$$
$$+ \frac{1}{2} \sum_{\sigma,\sigma'} \int d^3r \int d^3r' \hat{\phi}_\sigma^\dagger(\vec{r}) \hat{\phi}_\sigma(\vec{r}) V(|\vec{r} - \vec{r}'|) \hat{\phi}_{\sigma'}^\dagger(\vec{r}') \hat{\phi}_{\sigma'}(\vec{r}')$$

Wave Function of Non-Interacting Fermions (S=1/2): Slater Determinant

1st quantization

$$\psi(\vec{r}_1 \uparrow, \vec{r}_2 \uparrow, \cdots, \vec{r}_{N_\uparrow} \uparrow; \vec{r}_{N_\uparrow+1} \downarrow, \vec{r}_{N_\uparrow+2} \downarrow, \cdots, \vec{r}_{N_\uparrow+N_\downarrow} \downarrow)$$
$$= (L^3)^{-(N_\uparrow+N_\downarrow)/2} D_\uparrow D_\downarrow$$

$$D_\uparrow = \det \begin{bmatrix} e^{i\vec{k}_1\cdot\vec{r}_1} & e^{i\vec{k}_2\cdot\vec{r}_1} & \cdots & e^{i\vec{k}_{N_\uparrow}\cdot\vec{r}_1} \\ e^{i\vec{k}_1\cdot\vec{r}_2} & e^{i\vec{k}_2\cdot\vec{r}_2} & \cdots & e^{i\vec{k}_{N_\uparrow}\cdot\vec{r}_2} \\ \vdots & \vdots & & \vdots \\ e^{i\vec{k}_1\cdot\vec{r}_{N_\uparrow}} & e^{i\vec{k}_2\cdot\vec{r}_{N_\uparrow}} & \cdots & e^{i\vec{k}_{N_\uparrow}\cdot\vec{r}_{N_\uparrow}} \end{bmatrix}$$

$$D_\downarrow = \det \begin{bmatrix} e^{i\vec{k}_{N_\uparrow+1}\cdot\vec{r}_{N_\uparrow+1}} & e^{i\vec{k}_{N_\uparrow+2}\cdot\vec{r}_{N_\uparrow+1}} & \cdots & e^{i\vec{k}_{N_\uparrow+N_\downarrow}\cdot\vec{r}_{N_\uparrow+1}} \\ e^{i\vec{k}_{N_\uparrow+1}\cdot\vec{r}_{N_\uparrow+2}} & e^{i\vec{k}_{N_\uparrow+2}\cdot\vec{r}_{N_\uparrow+2}} & \cdots & e^{i\vec{k}_{N_\uparrow+N_\downarrow}\cdot\vec{r}_{N_\uparrow+2}} \\ \vdots & \vdots & & \vdots \\ e^{i\vec{k}_{N_\uparrow+1}\cdot\vec{r}_{N_\uparrow+N_\downarrow}} & e^{i\vec{k}_{N_\uparrow+2}\cdot\vec{r}_{N_\uparrow+N_\downarrow}} & \cdots & e^{i\vec{k}_{N_\uparrow+N_\downarrow}\cdot\vec{r}_{N_\uparrow+N_\downarrow}} \end{bmatrix}$$

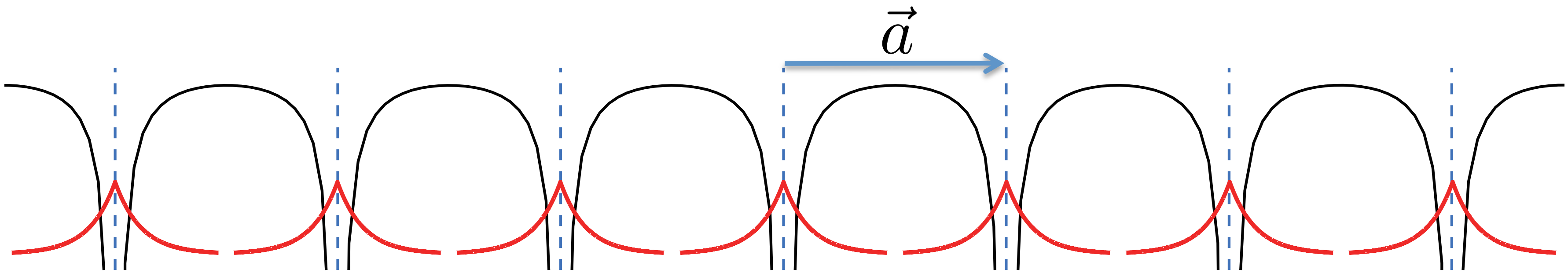
2nd quantization

$$|\Psi\rangle = \prod_{\mu=1}^{N_\uparrow} \hat{c}^\dagger_{\vec{k}_\mu\uparrow} \prod_{\nu=N_\uparrow+1}^{N_\uparrow+N_\downarrow} \hat{c}^\dagger_{\vec{k}_\nu\downarrow} |\mathrm{vac}\rangle$$

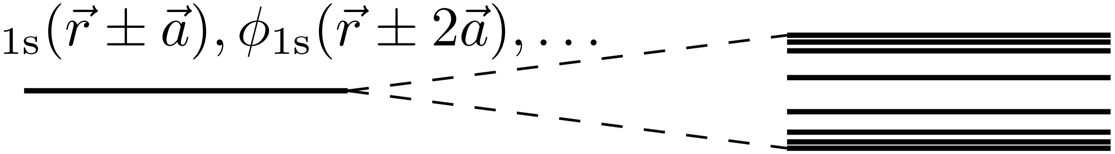
From Electrons in Crystalline Solids to Lattice Hamiltonians

Model of Many-Body Electrons

One of the simplest many-body electrons in Crystalline solids: Hydrogen solid

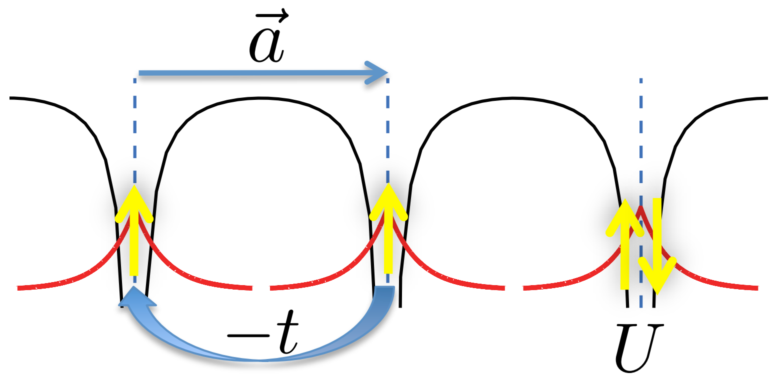


$\phi_{1\mathrm{s}}(\vec{r}), \phi_{1\mathrm{s}}(\vec{r} \pm \vec{a}), \phi_{1\mathrm{s}}(\vec{r} \pm 2\vec{a}), \ldots$



Gedankenexperiment of F. N. Mott

One of the Simplest Model: 1D Hubbard Model



$$\phi_{1\mathrm{s}}(\vec{r}), \phi_{1\mathrm{s}}(\vec{r} \pm \vec{a}), \phi_{1\mathrm{s}}(\vec{r} \pm 2\vec{a}), \ldots$$

-Tunnelling among neighboring 1s orbitals

$$-t = \int d^3 r \phi_{1\mathrm{s}}^*(\vec{r}) \frac{-\hbar^2}{2m} \nabla^2 \phi_{1\mathrm{s}}(\vec{r} - \vec{a})$$

-Intra-atomic Coulomb in 1s orbitals

$$U = \int d^3 r \int d^3 r' \phi_{1\mathrm{s}}^*(\vec{r}) \phi_{1\mathrm{s}}^*(\vec{r'}) \frac{e^2}{\left|\vec{r} - \vec{r'}\right|} \phi_{1\mathrm{s}}(\vec{r'}) \phi_{1\mathrm{s}}(\vec{r})$$

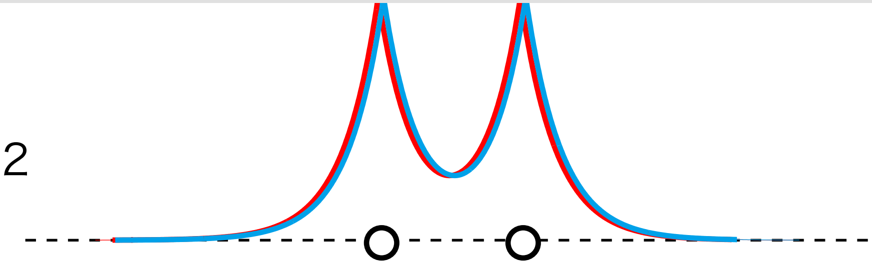
1D Hubbard model (periodic boundary condition, *L* site)

$$\hat{H} = -t \sum_{i=0}^{L-1} \sum_{\sigma=\uparrow,\downarrow} \left[\hat{c}_{i\sigma}^\dagger \hat{c}_{\mathrm{mod}(i+1,L)\sigma} + \hat{c}_{\mathrm{mod}(i+1,L)\sigma}^\dagger \hat{c}_{i\sigma} \right] + U \sum_{i=0}^{L-1} \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}$$

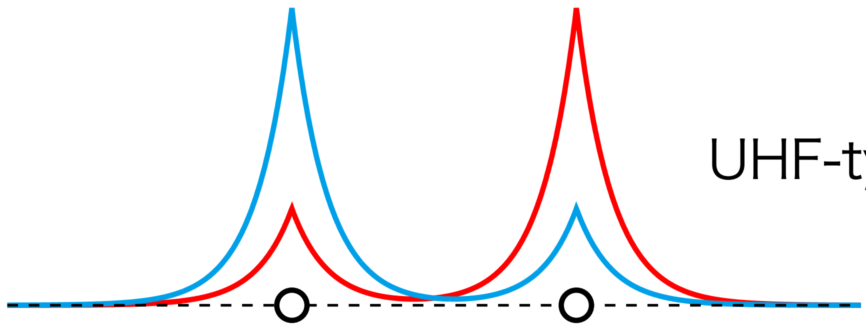
cf.) Bethe ansatz, Tomonaga-Luttinger liquid

Hydrogen Molecule

H_2



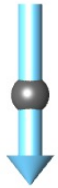
UHF-type wave function



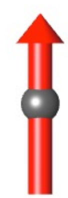
Hubbard model   cf.) Chiappe *et al.*, Phys. Rev. B 75, 195104 (2007)

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} \left(\hat{c}^{\dagger}_{0\sigma} \hat{c}_{1\sigma} + \hat{c}^{\dagger}_{1\sigma} \hat{c}_{0\sigma} \right) + U \sum_{j=0,1} \hat{c}^{\dagger}_{j\uparrow} \hat{c}_{j\uparrow} \hat{c}^{\dagger}_{j\downarrow} \hat{c}_{j\downarrow}$$

Heisenberg model or *J*-coupling $\hat{H} = J \left(\hat{S}^x_0 \hat{S}^x_1 + \hat{S}^y_0 \hat{S}^y_1 + \hat{S}^z_0 \hat{S}^z_1 \right)$



$$J = 4t^2/U$$



Singlet ground state

Model Hamiltonians

- Ising model
  -Rare earth magnets
- Heisenberg model
  -Transition-metal oxides
- Hubbard model (Gutzwiller, Kanamori)
  -Itinerant magnets, Mott insulators
- $t-J$ model
  -Cuprate superconductors
- Kondo model and Anderson model
  -Magnetic inpurities in alloys
  -Rare earth alloys

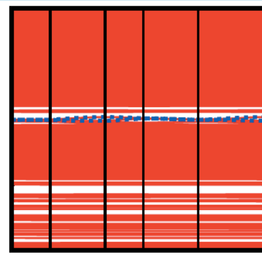
Quantitative Construction of Effective Hamiltonians

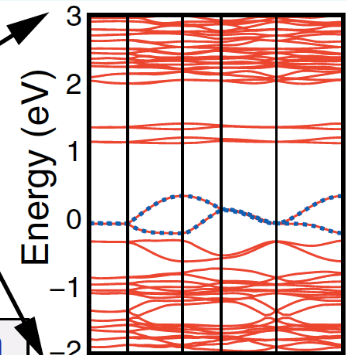
Schematic procedure of three–stage scheme thanks to energy hierarchy structure

1. Global electronic structure by DFT

far from Fermi level

tens eV

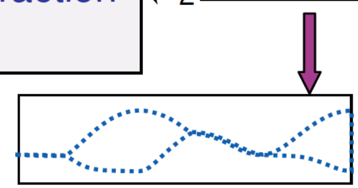




2. downfolding

constrained RPA

(1) Screened Coulomb interaction
(2) Self–energy



"target band"

Low–energy effective Hamiltonian

1/10-1/100 eV

3. Low-energy solver

variational Monte Carlo (VMC),
path-integral renormalization group (PIRG) ,
(cluster) dynamical mean-field theory (DMFT),
....

Model Hamiltonian derived by DFT+DMFT, Wannier+cRPA

G. Kotliar, et al., RMP 78, 865 (2006)

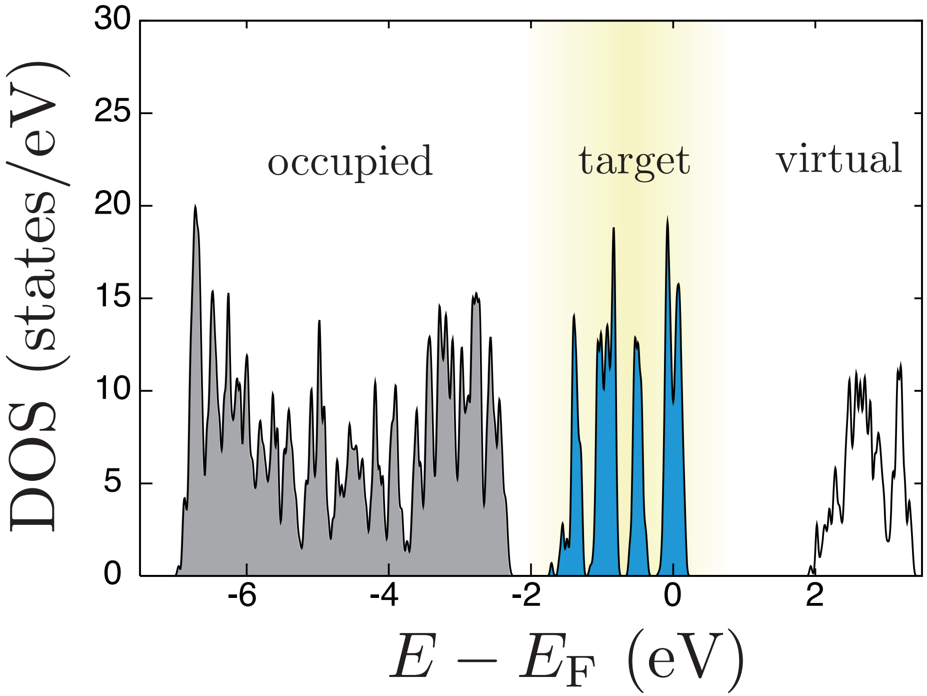
M. Imada & T. Miyake, JPSJ 79, 112001 (2010)

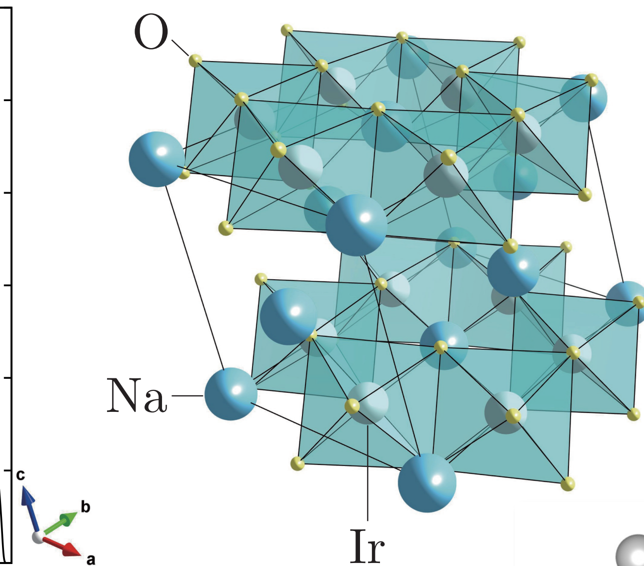
Construction of Effective Hamiltonians: An Example

- Target Hilbert space expanded by localized Wannier orbitals

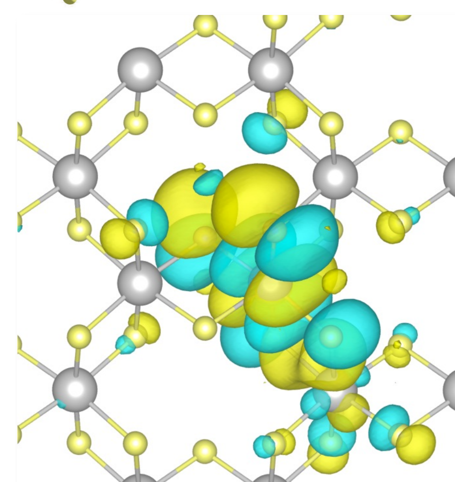
DFT result for energy spectrum

Souza-Marzari-Vanderbilt





Na_2IrO_3



- Effective Coulomb interactions in target space

  Renormalization due to
  infinite virtual particle-hole excitations

  ← Constrained random phase approximation

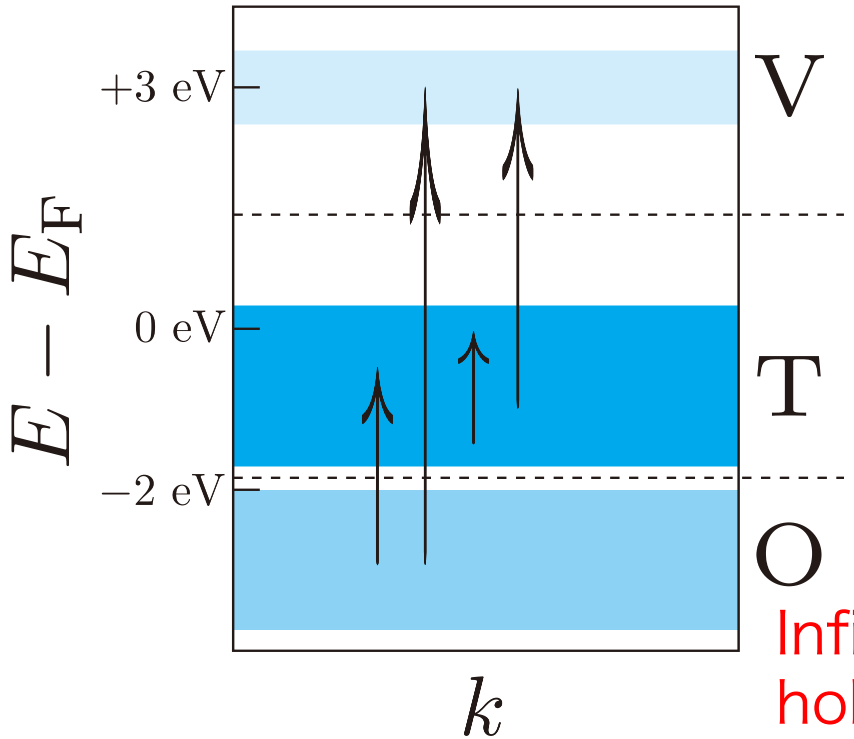
Imada & Miyake, J. Phys. Soc. Jpn. **79**, 112001 (2010)

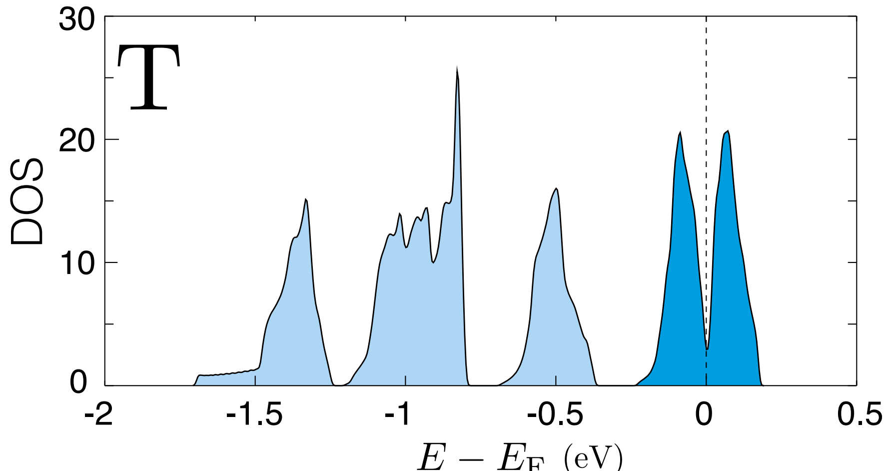
Constrained RPA Estimate on Coulomb Interaction of t_{2g}-Hubbard

$$W^{\mathrm{cRPA}} = \frac{V}{1 + V\chi^{\mathrm{cRPA}}}$$ ←Dielectric constant

$$\chi^{\mathrm{RPA}} = \chi_{\mathrm{O}\to\mathrm{T}} + \chi_{\mathrm{O}\to\mathrm{V}} + \chi_{\mathrm{T}\to\mathrm{T}} + \chi_{\mathrm{T}\to\mathrm{V}}$$

$$\chi^{\mathrm{cRPA}} = \chi_{\mathrm{O}\to\mathrm{T}} + \chi_{\mathrm{O}\to\mathrm{V}} + \cancel{\chi_{\mathrm{T}\to\mathrm{T}}} + \chi_{\mathrm{T}\to\mathrm{V}}$$





Infinite number of RPA-type particle-hole excitations

Ab initio t_{2g}-Hubbard Model: cRPA+Wannier

Hopping

$$\hat{H}_0 = \sum_{\ell \neq m} \sum_{a,b=xy,yz,zx} \sum_{\sigma,\sigma'} t^{\sigma\sigma'}_{\ell,m;a,b} \left[\hat{c}^{\dagger}_{\ell a \sigma} \hat{c}_{m b \sigma'} + \text{h.c.} \right]$$

Trigonal+orbital-dependent μ

$$\hat{H}_{\text{tri}} = \sum_{\ell} \hat{\vec{c}}^{\,\dagger}_{\ell} \begin{bmatrix} -\mu_{yz} & \Delta & \Delta \\ \Delta & -\mu_{zx} & \Delta \\ \Delta & \Delta & -\mu_{xy} \end{bmatrix} \hat{\sigma}_0 \hat{\vec{c}}_{\ell}$$

SOC

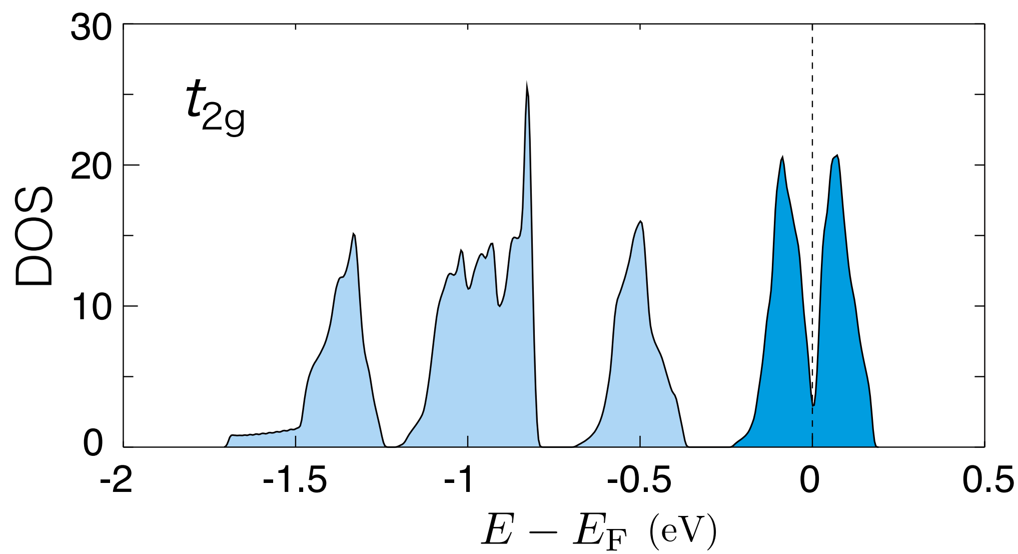
$$\hat{H}_{\text{SOC}} = \frac{\zeta_{\text{so}}}{2} \sum_{\ell} \hat{\vec{c}}^{\,\dagger}_{\ell} \begin{bmatrix} 0 & +i\hat{\sigma}_z & -i\hat{\sigma}_y \\ -i\hat{\sigma}_z & 0 & +i\hat{\sigma}_x \\ +i\hat{\sigma}_y & -i\hat{\sigma}_x & 0 \end{bmatrix} \hat{\vec{c}}_{\ell}$$

$$\hat{\vec{c}}^{\,\dagger}_{\ell} = (\hat{c}^{\dagger}_{\ell yz\uparrow}, \hat{c}^{\dagger}_{\ell yz\downarrow}, \hat{c}^{\dagger}_{\ell zx\uparrow}, \hat{c}^{\dagger}_{\ell zx\downarrow}, \hat{c}^{\dagger}_{\ell xy\uparrow}, \hat{c}^{\dagger}_{\ell xy\downarrow})$$

Coulomb

$$\hat{H}_U = U \sum_{\ell} \sum_{a=yz,zx,xy} \hat{n}_{\ell a\uparrow} \hat{n}_{\ell a\downarrow}$$
$$+ \sum_{\ell \neq m} \sum_{a,b} \frac{V_{\ell,m}}{2} (\hat{n}_{\ell a\uparrow} + \hat{n}_{\ell a\downarrow})(\hat{n}_{mb\uparrow} + \hat{n}_{mb\downarrow})$$
$$+ \sum_{\ell} \sum_{a<b} \sum_{\sigma} [U' \hat{n}_{\ell a\sigma} \hat{n}_{\ell b\overline{\sigma}} + (U' - J_{\text{H}}) \hat{n}_{\ell a\sigma} \hat{n}_{\ell b\sigma}]$$
$$+ J_{\text{H}} \sum_{\ell} \sum_{a\neq b} \left[\hat{c}^{\dagger}_{\ell a\uparrow} \hat{c}^{\dagger}_{\ell b\downarrow} \hat{c}_{\ell a\downarrow} \hat{c}_{\ell b\uparrow} + \hat{c}^{\dagger}_{\ell a\uparrow} \hat{c}^{\dagger}_{\ell a\downarrow} \hat{c}_{\ell b\downarrow} \hat{c}_{\ell b\uparrow} \right]$$

F. Aryasetiawan, *et al.*,
Phys. Rev. B 70, 195104 (2004)
M. Imada & T. Miyake, JPSJ 79, 112001 (2010)



DFT: Elk (FLAPW)
http://elk.sourceforge.net
Vxc: Perdew-Wang 1992

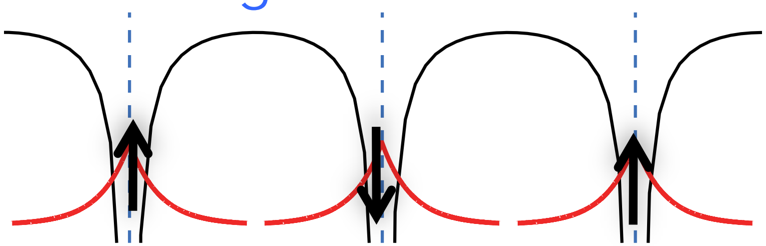
One-body parameters (eV)	t	$\mu_{xy} - \mu_{yz,zx}$	ζ_{so}	Δ
	0.27	0.035	0.39	−0.028
Two-body parameters (eV)	U	U'	J_H	V
	2.72	2.09	0.23	1.1

Strong Coupling Expansion: 2nd Order Perturbation

Unperturbed hamiltonian:

$$\hat{H}_{\mathrm{tri}} + \hat{H}_{\mathrm{SOC}} + \hat{H}_{U}$$

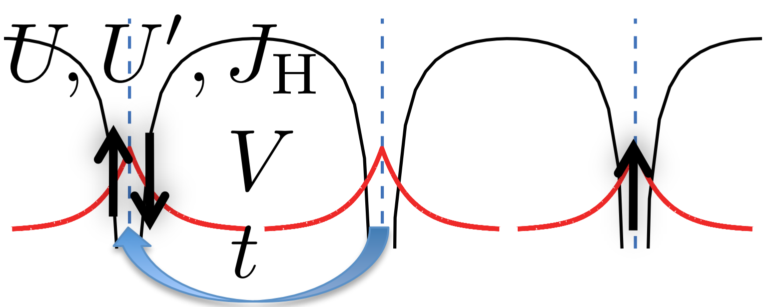
2^N degenerated states

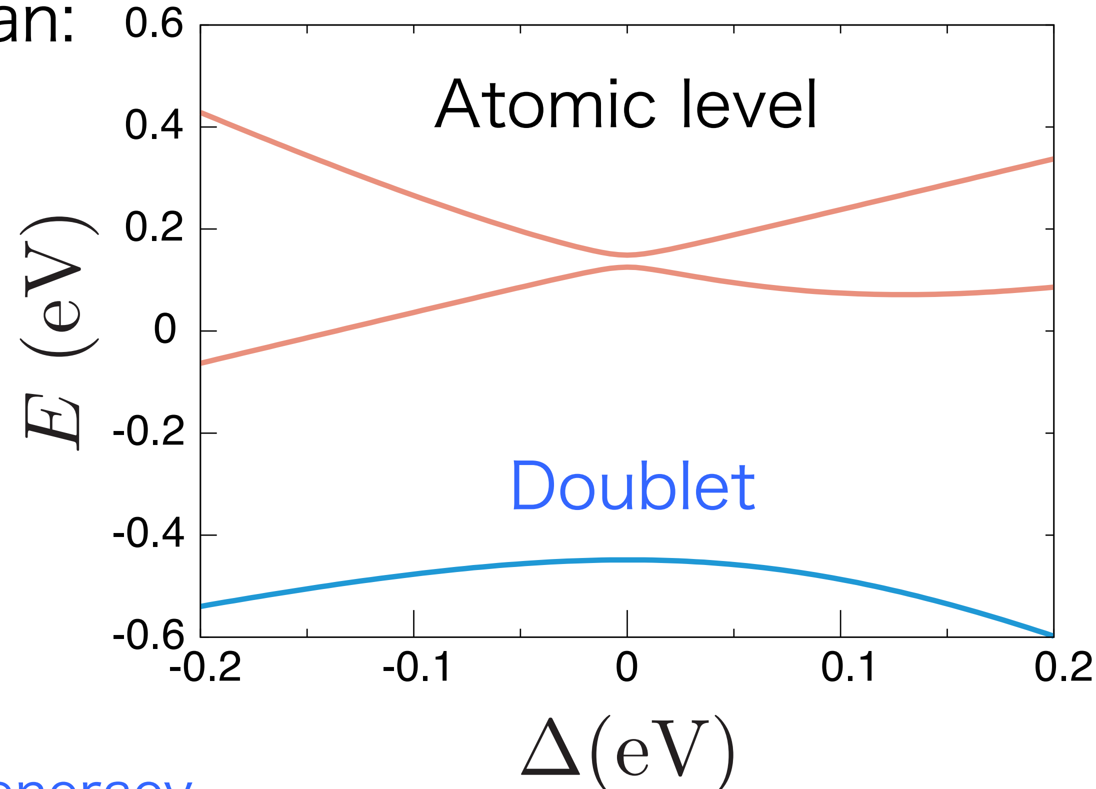


Perturbation:

$$\hat{H}_0$$

virtual states lift the degeneracy





Spin Hamiltonian

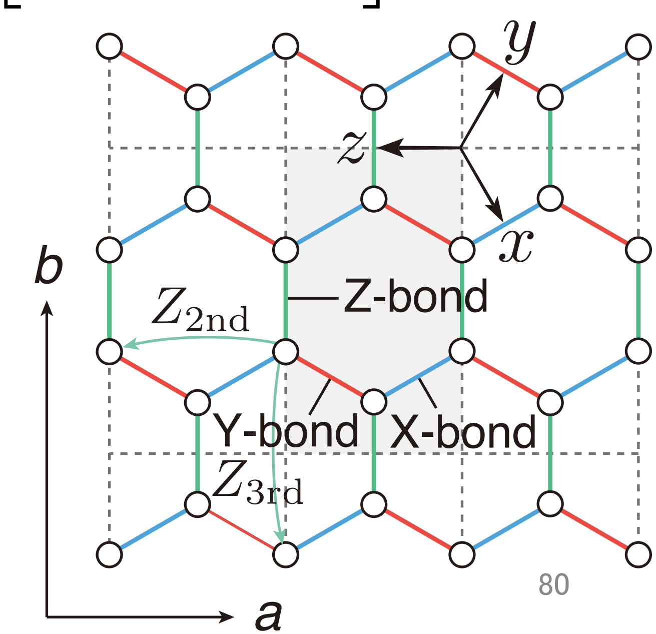
Y. Yamaji, Y. Nomura, M. Kurita, R. Arita, & M. Imada, Phys. Rev. Lett. 113, 107201 (2014).

$$\hat{H} = \sum_{\Gamma = X, Y, Z, Z_{2\mathrm{nd}}, 3} \sum_{\langle \ell, m \rangle \in \Gamma} \hat{\vec{S}}_\ell^T \mathcal{J}_\Gamma \hat{\vec{S}}_m \qquad \hat{\vec{S}}_\ell^T = (\hat{S}_\ell^x, \hat{S}_\ell^y, \hat{S}_\ell^z)$$

$$\mathcal{J}_X = \begin{bmatrix} \mathbf{-23.9} & -3.1 & -8.4 \\ -3.1 & 3.2 & 1.8 \\ -8.4 & 1.8 & 2.0 \end{bmatrix} (\mathrm{meV}) \qquad \mathcal{J}_{Z_{2\mathrm{nd}}} = \begin{bmatrix} -0.8 & 1.0 & -1.4 \\ 1.0 & -0.8 & -1.4 \\ -1.4 & -1.4 & -1.2 \end{bmatrix} (\mathrm{meV})$$

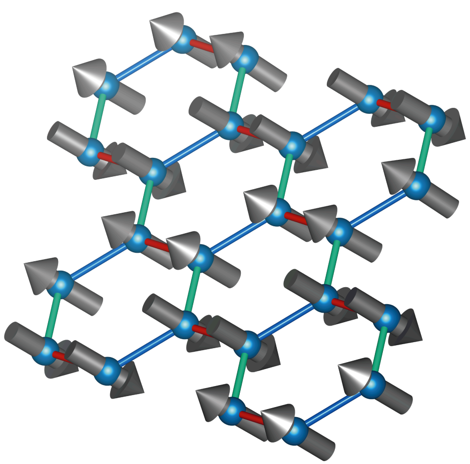
$$\mathcal{J}_Y = \begin{bmatrix} 3.2 & -3.1 & 1.8 \\ -3.1 & \mathbf{-23.9} & -8.4 \\ 1.8 & -8.4 & 2.0 \end{bmatrix} (\mathrm{meV}) \qquad \mathcal{J}_3 = \begin{bmatrix} 1.7 & 0.0 & 0.0 \\ 0.0 & 1.7 & 0.0 \\ 0.0 & 0.0 & 1.7 \end{bmatrix} (\mathrm{meV})$$

$$\mathcal{J}_Z = \begin{bmatrix} 4.4 & -0.4 & 1.1 \\ -0.4 & 4.4 & 1.1 \\ 1.1 & 1.1 & \mathbf{-30.7} \end{bmatrix} (\mathrm{meV})$$



Ground state:
Zigzag order
agrees with experiments

iPEPS, 2D DMRG, & ED:
T. Okubo, K. Shinjo, Y. Yamaji, *et al.*, arXiv:1611.03614.



宿題

VirtualBoxの最新版を各自のノートPCに
インストールしてください:
https://www.virtualbox.org/wiki/Downloads

講義資料: https://github.com/yyamaji/lectures
ＨΦ関連: http://issp-center-dev.github.io/HPhi/index.html