多体問題の計算科学
Computational Science for Many-Body Problems

#1 Many-body problems in physics and why they are hard to solve

14:55-16:40 April 5, 2021

1. Background of the lecture
2. Many-body problems in physics
3. Finite size and discretization
4. Why many-body problems is hard to solve
5. (Super)computers
6. Details and exercises

Lecture Materials

You will find our lecture materials at ITC-LMS or Github

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

Background of This Lecture

Computational
Science
Alliance
The University of Tokyo

UTokyo
Computational Science Alliance

Fugaku project

Program for Promoting Researches on the Supercomputer Fugaku
Basic Science for Emergence and Functionality in Quantum Matter
— Innovative Strongly-Correlated Electron Science by
Integration of “Fugaku” and Frontier Experiments —

富岳

Lecturer

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Senior Researcher
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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

Background of This Lecture
Computational Science

1st Experimental Science
2nd Theoretical Science
3rd Computational Science
4th Data Science

Computational Science 計算科学
Computer Science 計算機科学

Background of This Lecture

Computational Science Education

Computational
Science
Alliance

The University of Tokyo

Background of This Lecture
Computational Science Education

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This lecture is in Category F Computational Science
計算科学の各分野におけるシミュレーション手法と
その研究成果について学ぶ。
電子状態計算、分子動力学、量子多体計算、数値流体力学、
構造計算、ゲノム解析など、さらには社会科学や経済分野
における最先端手法を学習する。
また、実際にソフトウェアを用いて大規模計算科学
シミュレーションを実行する

Many-Body Problems

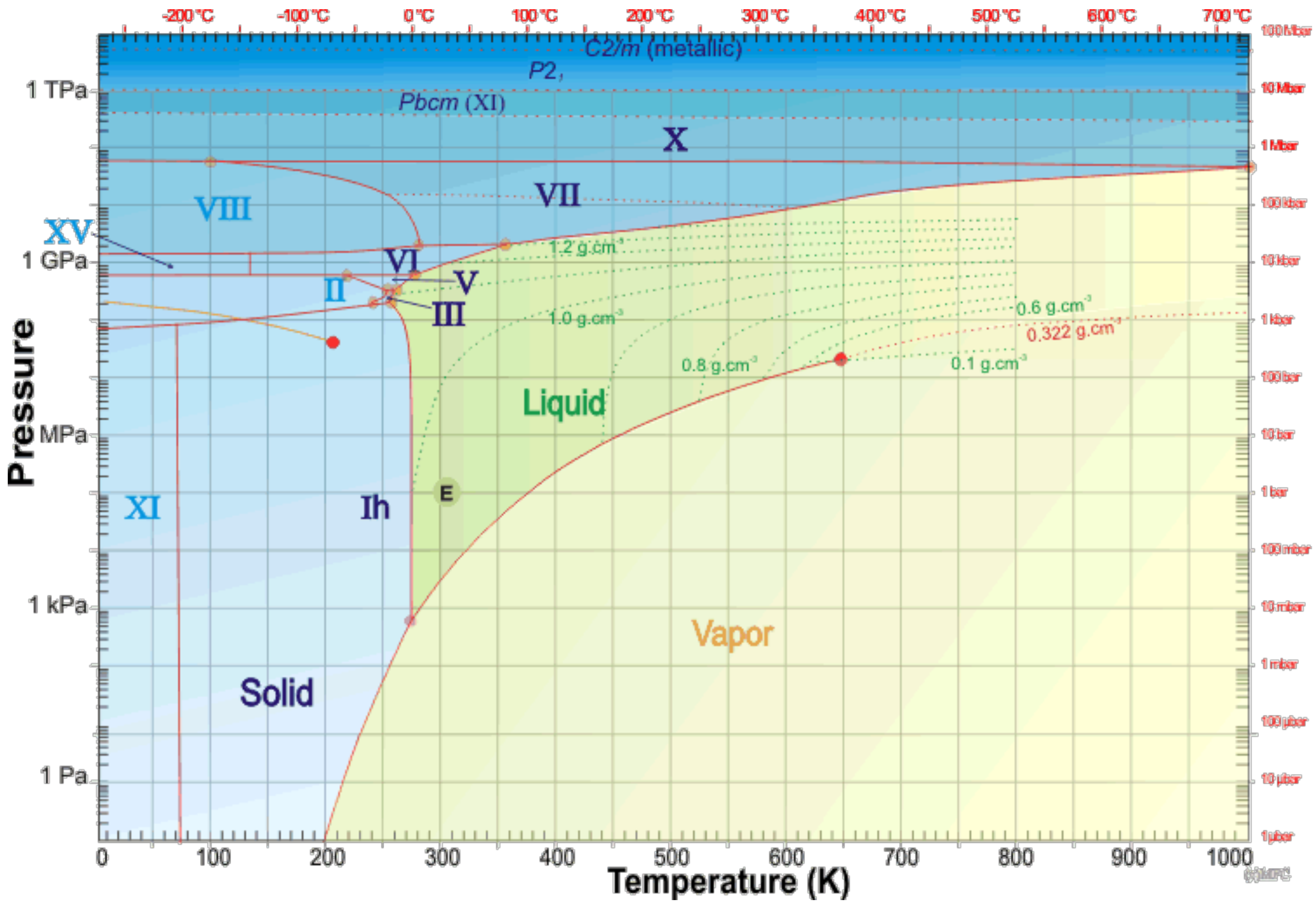
Many-body problems in Physics

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/

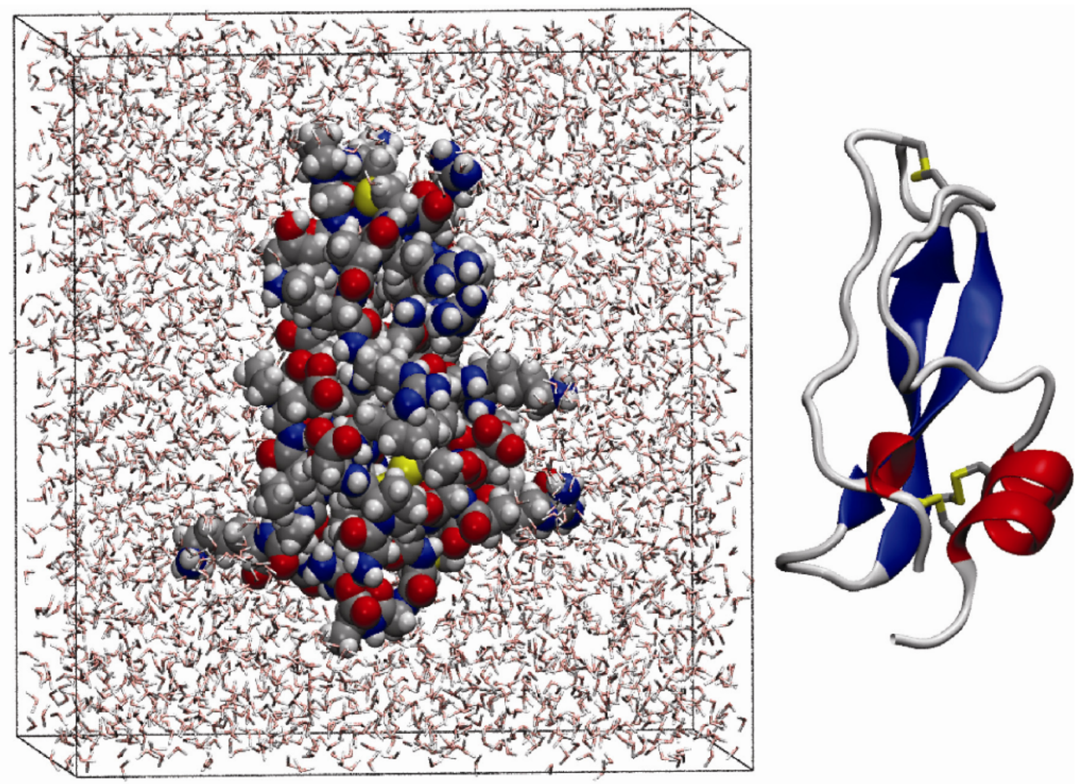
An Example of Many-Body Problems: Proteins

Proteins in water

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

The state of the system is determined by position and velocity of each particle

$$(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; \vec{v}_1, \vec{v}_2, \ldots, \vec{v}_N)$$



(a) (b)

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).

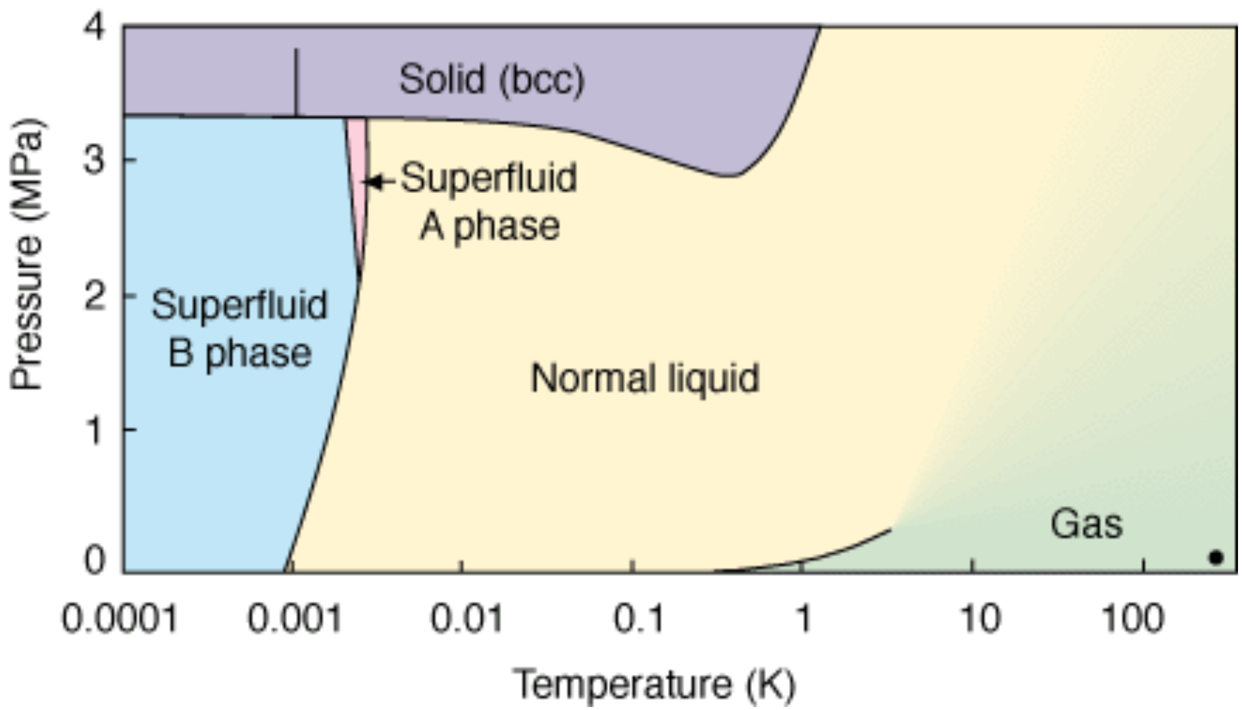
An Example of Many-Body Problems: Quantum Liquids

Phase diagram of ^3He

The system at zero temperature is represented by the wave function (complex function of particles' position)

$$\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; t)$$

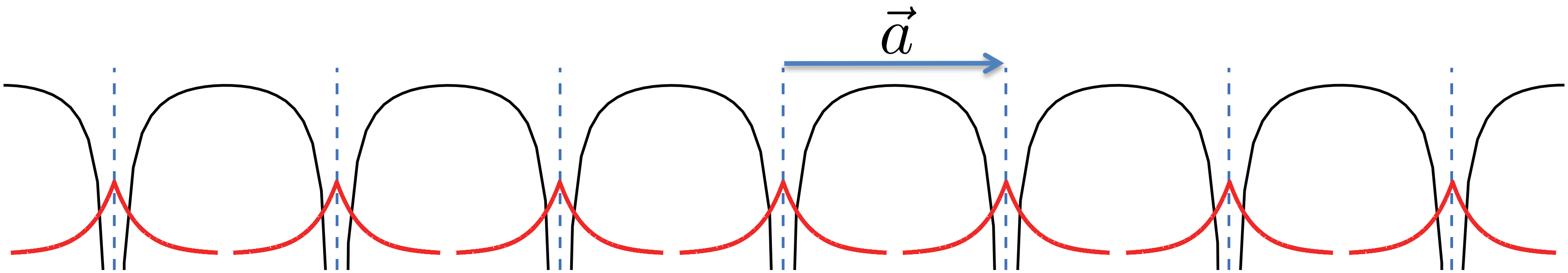
D. D. Osheroff, R. C. Richardson, and D. M. Lee, Phys. Rev. Lett. 28, 885 (1972).



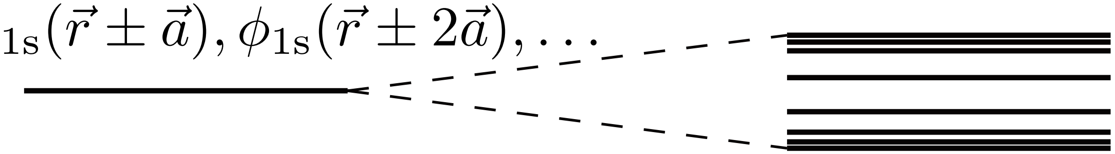
Erkki Thuneberg
http://ltl.tkk.fi/research/theory/helium.html

A Minimal Model of Many-Body Problems

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



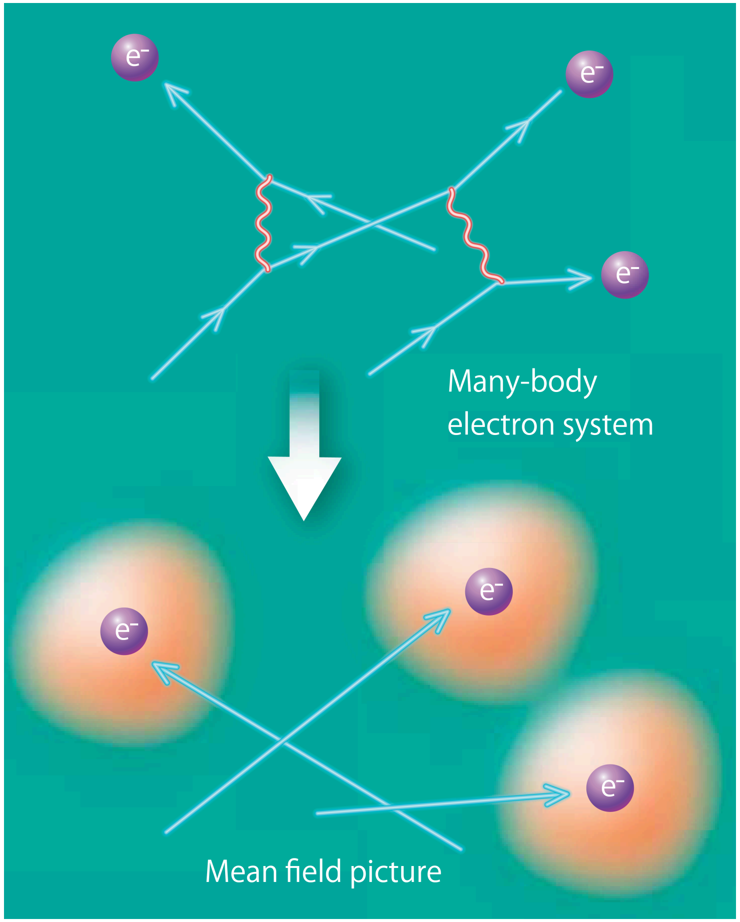
$$\phi_{1\mathrm{s}}(\vec{r}), \phi_{1\mathrm{s}}(\vec{r} \pm \vec{a}), \phi_{1\mathrm{s}}(\vec{r} \pm 2\vec{a}), \ldots$$



Gedankenexperiment of F. N. Mott

Starting from isolated one-body wave functions and constructing entangled $\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; t)$

Many-Body Problem & One-Body Picture in Solid State Physics



"One-body picture"

Basis of quantum many-body problem

Derive effective one-body picture

-Hartree-Fock (Mean-field)
-Landau's Fermi liquid (1956)
-Hohenberg-Kohn
& Kohn-Sham theory (1965)

Trend after Landau & Kohn

Ab initio
LDA, GGA, HF

Model calculations (direct approaches)
Hubbard model, Heisenberg model,…
ED,QMC,DMFT,…

cf.) Solvable model

Recent trends

GW, post HF, LDA+DMFT, GW+DMFT…

Finite Size and Discretization

- *Theory* handles infinite number of and continuous degrees of freedom

Naïvely, computers can not handle them

→ Reformulate the problems with finite number of and discrete degrees of freedom

Size of Quantum Many-Body Problems

Hilbert space dimension can be stored in memory

∼50 qubits or 50 spins

(Heisenberg-like hamiltonian with N (< 50) *spins*)

<u>Examples of finite size systems from chemistry</u>

-A H_2O molecule: 5↑ & 5↓electrons in 41 orbitals

→ 5.6×10^{11} dimensional (∼2^{39})

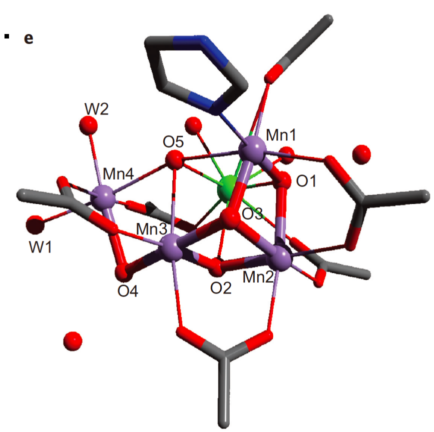
G. K.-L. Chan & M. Head-Gordon, J. Chem. Phys. 118, 8551 (2003).

-Manganese cluster in photosystem II:

44 electrons in 35 orbitals

→ 2×10^{18} dimensional (∼2^{61})

Y. Kurashige, G. K.-L. Ghan, & T. Yanai, Nat. Chem. 5, 660 (2013).



Size of Quantum Many-Body Problems

Hilbert space dimension can be stored in memory

～50 qubits or 50 spins
(Heisenberg-like hamiltonian with N (< 50) *spins*)

How about crystalline lattice ?
(with periodic boundary)

-Finite N calculations are useful?

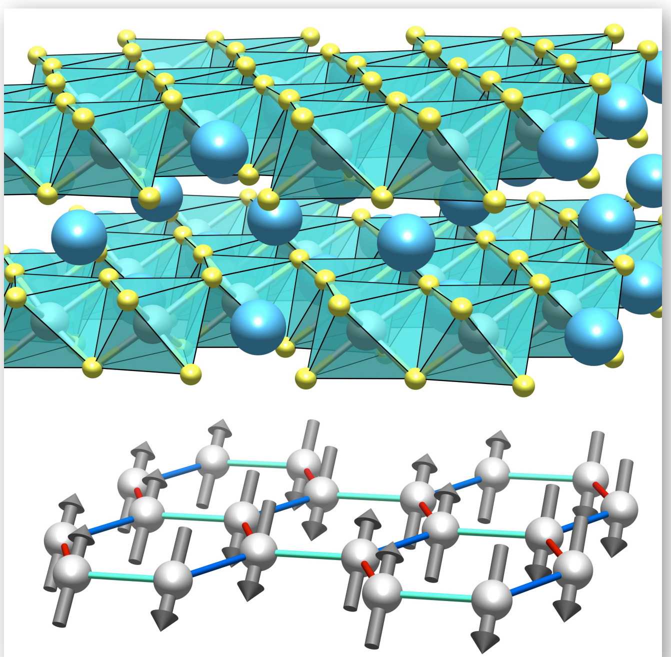
Finite size scaling (2nd & 3rd lectures):
Extracting information of infinite systems from finite ones
Nearsightedness
W. Kohn, Phys. Rev. Lett. 76, 3168 (1996).

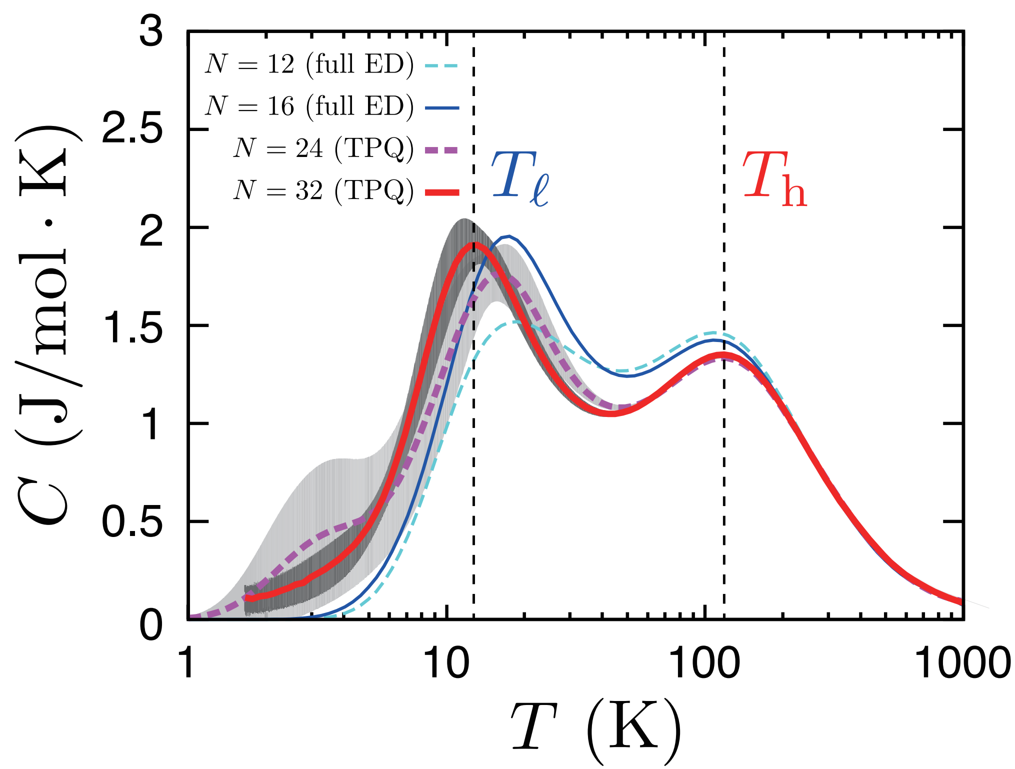
Nearsightness

For example, W. Kohn, Phys. Rev. Lett. 76, 3168 (1996).

-Excitation gap, temperature, frustration make correlation length shorter and, thus, finite-size effect smaller

An example: Frustrated magnet Na_2IrO_3 (12th)





From Continuous to Discrete

We need to rewrite *first principles* equations to calculate them in suitable and efficient way with (super)computers

A typical example: Discretization

Differential equation

$$\frac{\partial}{\partial t}u(t,r) = D\frac{\partial^2}{\partial r^2}u(t,r)$$

Difference equation

$$u(n+1,x) = \frac{1}{2}\left[u(n,x+1) + u(n,x-1)\right]$$

Other examples: Symplectic integral, variational methods, ⋯

Difference and Differential: Diffusion Eq.

Difference eq. $$u(n+1,x) = \frac{1}{2}\left[u(n,x+1) + u(n,x-1)\right]$$

Differential eq. $$\frac{\partial}{\partial t}u(t,r) = D\frac{\partial^2}{\partial r^2}u(t,r)$$

$$\boxed{D = \lim_{\delta t\to 0,\delta r\to 0}\frac{(\delta r)^2}{\delta t}}$$

$$u(t+\delta t,r) = \frac{1}{2}\left[u(t,r+\delta r) + u(t,r-\delta r)\right]$$

$$\begin{cases} u(t+\delta t,r) = u(t,r) + \delta t\frac{\partial}{\partial t}u(t,r) + \frac{\delta t^2}{2}\frac{\partial^2}{\partial t^2}u(t,r) + \mathcal{O}(\delta t^3) \\ u(t,r+\delta r) = u(t,r) + \delta r\frac{\partial}{\partial r}u(t,r) + \frac{\delta r^2}{2}\frac{\partial^2}{\partial r^2}u(t,r) + \mathcal{O}(\delta r^3) \end{cases}$$

$$\Longrightarrow \frac{\partial}{\partial t}u(t,r) = D\frac{\partial^2}{\partial r^2}u(t,r)$$

Classical vs Quantum Mechanics

classical point particles $(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; \vec{v}_1, \vec{v}_2, \ldots, \vec{v}_N)$

Every set of locations/positions and velocities of particles gives you an *eigenstate* of the hamiltonian:
The hamiltonian is already *diagonal*

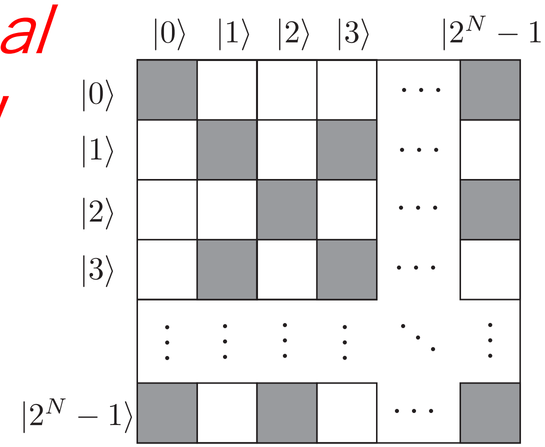
$$E = \sum_{j=1}^{N} \frac{m_j}{2} |\vec{v}_j|^2 + V(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$$

Example of potentila: gravitational or Coulomb force

$$V(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = g \sum_{i<j} \frac{1}{|\vec{r}_i - \vec{r}_j|}$$

quantum The hamiltonian is not *diagonal* when the basis set is given by positions of particles

$$|\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N\rangle$$



cf.) Uncertainty principle,
zero point motion, or quantum fluctuation

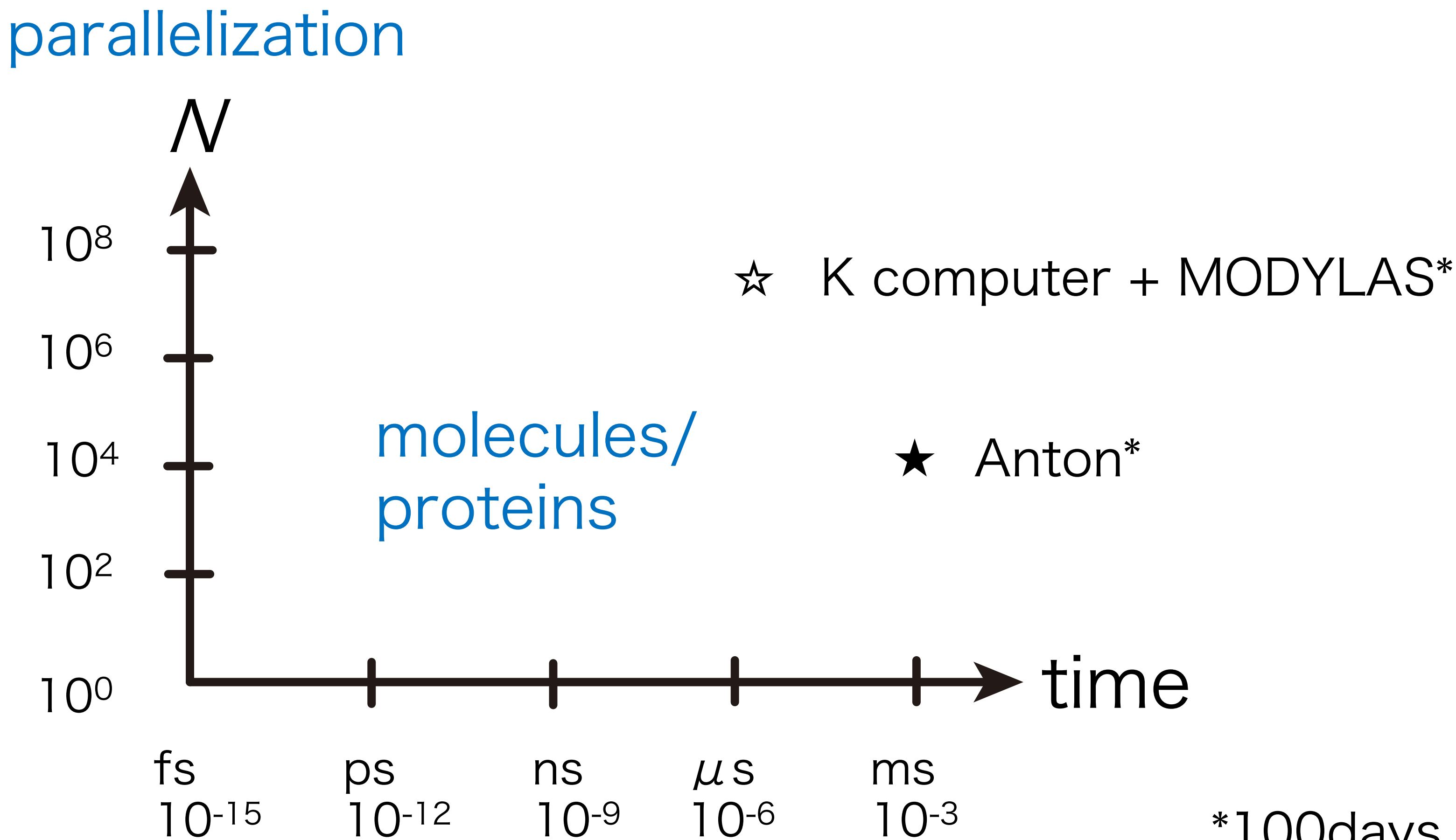
Why Many-Body Problem Is Hard to Solve

Target of this lecture:

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

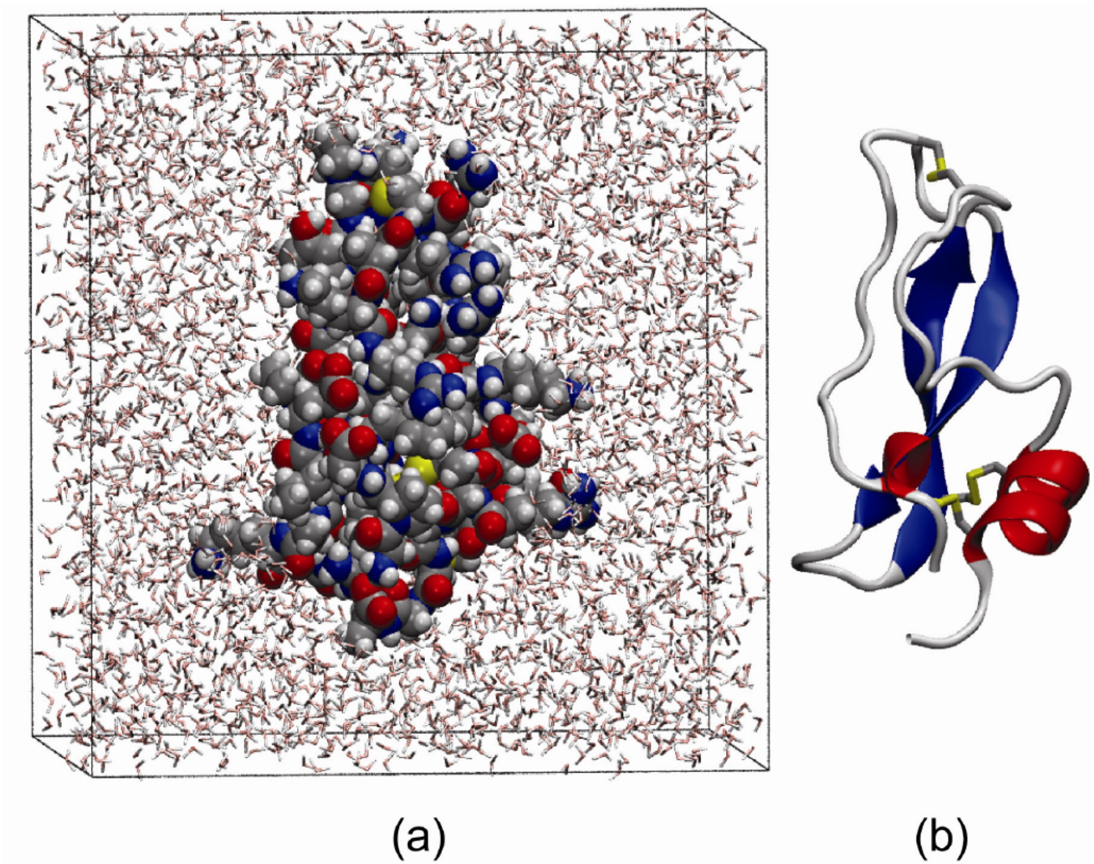


*100days

An Example of Many-Body Problems: Proteins

Proteins in water

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



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Why Many-Body Problem Is Hard to Solve

1. N-body Newtonian equation of motion

-Time evolution of 6N degrees of freedom:

*Larger Δt is desirable

Δt=1–2 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

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

* 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)

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

Forward difference

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

Do not use Euler!

Difference Equation for Hamiltonian Mechanics

Another formulation of forward difference

Hamiltonian split into kinetic energy T and potential V

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

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

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

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

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

Why Many-Body Problem Is Hard to Solve

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

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

Quantum Spin S=1/2 or Qubit

Operators acting on a single qubit

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

A two dimensional representation of Lie algebra SU(2)

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

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

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