

特殊講義C: 量子多体問題の計算科学

2日目

2018/8/7

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

1. Quantum mechanics by linear algebra
2. Quantum many-body problem by linear algebra
3. Eigenvalue problem of large and sparse matrix
4. Example of application of Lanczos method

Quantum Mechanics by Linear Algebra (One Body Problem)

Quantum Mechanics by Linear Algebra

Naïvely, linear partial differential equations are rewritten by Linear equations

Schrödinger equation represented by partial diff. eq.

$$i\hbar \frac{d}{dt} \psi(\vec{r}, t) = \left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] \psi(\vec{r}, t)$$

Stationary solution: $\psi(\vec{r}, t) = \phi(\vec{r}) e^{-iEt/\hbar}$

$$\left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] \phi(\vec{r}) = E\phi(\vec{r})$$

Quantum Mechanics by Linear Algebra

Schrödinger equation represented by linear eqs.

$$\left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] \phi(\vec{r}) = E\phi(\vec{r})$$

Expanded by orthonormal basis

$$\phi(\vec{r}) = \sum_m c_m u_m(\vec{r})$$

$$\int d^3r u_\ell^*(\vec{r}) u_m(\vec{r}) = \delta_{\ell,m}$$

$$\int d^3r \phi^*(\vec{r}) \phi(\vec{r}) = \sum_m |c_m|^2$$

Matrix representation

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

$$\sum_m H_{\ell m} c_m = E c_\ell$$

Quantum Mechanics by Linear Algebra

$$\sum_m H_{\ell m} c_m = E c_\ell$$

Hermitian matrix $H_{\ell m} = H_{m\ell}^*$

-Diagonalizable by unitary matrices

-Real eigenvalues

$$\sum_m H_{\ell m} U_{m\alpha} = U_{\ell\alpha} E_\alpha$$

$$\sum_m (U^\dagger)_{\beta m} U_{m\alpha} = \sum_m (U_{m\beta})^* U_{m\alpha} = \delta_{\beta,\alpha}$$

Quantum Mechanics by Linear Algebra

$$\sum_m H_{\ell m} c_m = E c_\ell$$

Vector representation of expectation value

$$\begin{aligned} \frac{\int d^3r \phi^*(\vec{r}) \hat{O} \phi(\vec{r})}{\int d^3r \phi^*(\vec{r}) \phi(\vec{r})} &= \frac{\sum_{\ell,m} c_\ell^* c_m \int d^3r u_\ell^*(\vec{r}) \hat{O} u_m(\vec{r})}{\sum_n |c_n|^2} \\ &= \frac{\sum_{\ell,m} c_\ell^* O_{\ell m} c_m}{\sum_n |c_n|^2} \end{aligned}$$

Linear Algebra by Computer

Linear Algebra by Computer

$$\sum_m H_{\ell m} U_{m\alpha} = U_{\ell\alpha} E_\alpha$$

Hermitian matrix $H_{\ell m} = H_{m\ell}^*$

[LAPACK](#) (Linear Algebra PACKage)

<http://www.netlib.org/lapack/explore-html/index.html>

zheev

z: double complex

he: hermitian

ev: eigenvalue & eigenvector

```
subroutine zheev ( character JOBZ,  
                   character UPLO,  
                   integer N,  
                   complex*16, dimension( lda, * ) A,  
                   integer LDA,  
                   double precision, dimension( * ) W,  
                   complex*16, dimension( * ) WORK,  
                   integer LWORK,  
                   double precision, dimension( * ) RWORK,  
                   integer INFO  
 )
```

Linear Algebra by Computer

[LAPACK](#) (Linear Algebra PACKage)

<http://www.netlib.org/lapack/explore-html/index.html>

-Language: Fortran
C & C++ can call LAPACK

-License:
Modified BSD license

-Parallelized version:
ScaLAPACK

-Transformation
-Eigenvalue
-Singular value

cf.) intel MKL
(commercial library)

Quantum Many-Body Problems by Linear Algebra

Quantum Many-Body Problem by Linear Algebra

Hamiltonian in 2nd quantization form

Many-body electrons confined in one-body potential
(No spin-orbit coupling)

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

Quantum Many-Body Problem by Linear Algebra

Field operator

$$\hat{\phi}_\sigma(\vec{r}) = \sum_\ell u_\ell(\vec{r}) \hat{a}_{\ell\sigma}$$

$$\int d^3r \ u_\ell^*(\vec{r}) u_m(\vec{r}) = \delta_{\ell,m}$$

Fermions

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

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

Bosons

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

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

Quantum Many-Body Problem by Linear Algebra

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

→ General Hamiltonian with two-body interactions

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

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

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

Quantum Many-Body Problem by Linear Algebra

Hilbert space of N -particle fermions expanded by

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

Orthonormalized many-body basis

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

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

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

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

Quantum Many-Body Problem by Linear Algebra

Common important formula
between Hilbert and Fock spaces

Closure by orthonormalized basis

$$1 = \sum_{\mu} |\mu\rangle\langle\mu|$$

$$\langle\mu|\nu\rangle = \delta_{\mu,\nu}$$

$$\begin{aligned} \left(\sum_{\mu} |\mu\rangle\langle\mu| \right) \times |\Phi\rangle &= \left(\sum_{\mu} |\mu\rangle\langle\mu| \right) \times \sum_{\nu} d_{\nu} |\nu\rangle \\ &= \sum_{\nu} d_{\nu} |\nu\rangle \\ &= |\Phi\rangle \end{aligned}$$

Quantum Many-Body Problem by Linear Algebra

Schrödinger equation $\hat{H}|\Phi\rangle = E|\Phi\rangle$

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

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

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

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

Rewritten Schrödinger equation

$$\sum_\nu H_{\mu\nu} d_\nu = E d_\mu$$

$$H_{\mu\nu} = \langle\mu|\hat{H}|\nu\rangle$$

$$|\Phi\rangle = \sum_\mu d_\mu |\mu\rangle$$

Eigenvalue Problems

Diagonalizing Hermitian matrices

Standard approach:

Call LAPACK (Linear Algebra PACKage)

subroutine zheev:

Householder reflection + QR algorithm

→ $O(N^3)$ numerical cost

Computational and Memory Costs

1. Vector-vector product

$$\sum_{j=0}^{N_H-1} u_j^* v_j$$

Computational: $\mathcal{O}(N_H)$

Memory: $\mathcal{O}(N_H)$

2. Matrix-vector product

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

Computational: $\mathcal{O}(N_H^2)$

Memory: $\mathcal{O}(N_H^2)$

3. Matrix-matrix product

$$C_{ij} = \sum_{k=0}^{N_H-1} A_{ik} B_{kj}$$

Computational: $\mathcal{O}(N_H^3)$

Memory: $\mathcal{O}(N_H^2)$

Eigenvalue Problems

1. Tridiagonalization

by Householder reflection

$$\hat{P}_j = \hat{1} - 2 \frac{\vec{v}_j \vec{v}_j^\dagger}{\|\vec{v}_j\|^2}$$

$$\hat{H}_{\text{td}} = \hat{P}_{N_{\text{H}}-3} \cdots \hat{P}_1 \hat{P}_0 \hat{H} \hat{P}_0 \hat{P}_1 \cdots \hat{P}_{N_{\text{H}}-3} \quad \mathcal{O}(N_{\text{H}}^3)$$

$$N_{\text{H}} = 8$$

$$\hat{H}_{\text{td}} = \begin{pmatrix} \alpha_0 & \beta_0 & & & & & & \\ \beta_0 & \alpha_1 & \beta_1 & & & & & \\ & \beta_1 & \alpha_1 & \beta_2 & & & & \\ & & \beta_2 & \alpha_3 & \beta_3 & & & \\ & & & \beta_3 & \alpha_4 & \beta_4 & & \\ & & & & \beta_4 & \alpha_5 & \beta_5 & \\ & & & & & \beta_5 & \alpha_6 & \beta_6 \\ & & & & & & \beta_6 & \alpha_7 \end{pmatrix}$$

Eigenvalue Problems

2. QR algorithm

$$\hat{A}_0 = \hat{H}_{\text{td}}$$

$$\hat{A}_k = \hat{Q}_k \hat{R}_k \quad \mathcal{O}(N_{\text{H}})$$

$$\hat{A}_{k+1} = \hat{R}_k \hat{Q}_k \quad \mathcal{O}(N_{\text{H}}^3)$$

$$\hat{U} = \lim_{k \rightarrow +\infty} \hat{A}_k$$

→ Diagonal elements
are eigenvalues of H

Upper triangle matrix

$$N_{\text{H}} = 8$$

$$\hat{R} = \begin{pmatrix} a_0 & b_0 & c_0 & d_0 & e_0 & f_0 & g_0 & h_0 \\ & a_1 & b_1 & c_1 & d_1 & e_1 & f_1 & g_1 \\ & & a_1 & b_2 & c_2 & d_2 & e_2 & f_2 \\ & & & a_3 & b_3 & c_3 & d_3 & e_3 \\ & & & & a_4 & b_4 & c_4 & d_4 \\ & & & & & a_5 & b_5 & c_5 \\ & & & & & & a_6 & b_6 \\ & & & & & & & a_7 \end{pmatrix}$$

Difficulties in Many-Body Problems

- Summation over exponentially large
of configurations

←Monte Carlo

- $O(N^3)$ numerical cost and $O(N^2)$ memory

←Krylov subspace method

Hamiltonian & Many-Body Wave Functions

Hamiltonian in 2nd quantization form

$$\hat{H} = \hat{H}_K + \hat{H}_I$$

$$\hat{H}_K = - \sum_{\ell_1, \ell_2} \sum_{\sigma_1, \sigma_2} t_{\ell_1 \ell_2}^{\sigma_1 \sigma_2} \hat{c}_{\ell_1 \sigma_1}^\dagger \hat{c}_{\ell_2 \sigma_2}$$

$$\hat{H}_I = \sum_{\ell_1, \ell_2, \ell_3, \ell_4} \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4} I_{\ell_1 \ell_2 \ell_3 \ell_4}^{\sigma_1 \sigma_2 \sigma_3 \sigma_4} \hat{c}_{\ell_1 \sigma_1}^\dagger \hat{c}_{\ell_2 \sigma_2}^\dagger \hat{c}_{\ell_3 \sigma_3}^\dagger \hat{c}_{\ell_4 \sigma_4}$$

Numerically exact eigenvalues and eigenvectors

$$\hat{H}|\phi\rangle = E|\phi\rangle$$

$$|\phi\rangle = \sum_{\{I_j, \bar{I}_j\}} C_{I_0 \bar{I}_0 I_1 \bar{I}_1 \dots I_{N-1} \bar{I}_{N-1}} \left[\prod_{j=0}^{N-1} (\hat{c}_{\ell_j \uparrow}^\dagger)^{I_j} (\hat{c}_{\ell_j \downarrow}^\dagger)^{\bar{I}_j} \right] |\text{vac}\rangle$$

Cl coefficients

Pauli principle: $I_j, \bar{I}_j \in \{0, 1\}$

Dimension of Fock Space

Fock space dimension can be stored in memory

- Hubbard-like hamiltonian
 $N (< 30\text{-}40)$ orbital systems
- Heisenberg-like hamiltonian
 $N (< 50)$ *spin* systems

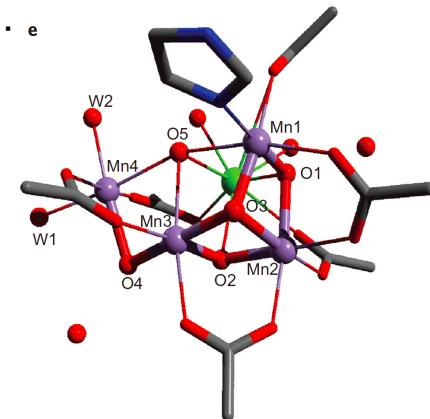
Examples of finite size systems from chemistry

-A H₂O molecule: 5 \uparrow & 5 \downarrow electrons in 41 orbitals
 $\rightarrow 5.6 \times 10^{11}$ dimensional ($\sim 2^{39}$)

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

-Manganese cluster in photosystem II:
44 electrons in 35 orbitals
 $\rightarrow 2 \times 10^{18}$ dimensional ($\sim 2^{61}$)

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



Dimension of Fock Space

Fock space dimension can be stored in memory

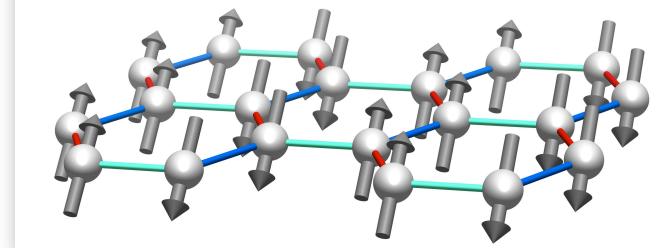
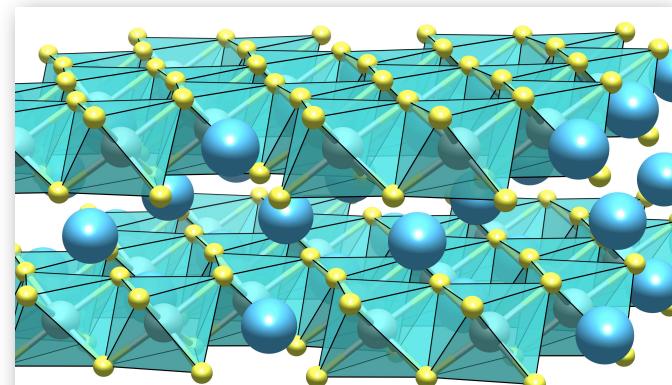
- Hubbard-like hamiltonian
 $N (< 30\text{-}40)$ orbital systems
- Heisenberg-like hamiltonian
 $N (< 50)$ *spin* systems

How about crystalline lattice ?
(with periodic boundary)

-Finite N calculations are useful?

Nearsightedness

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

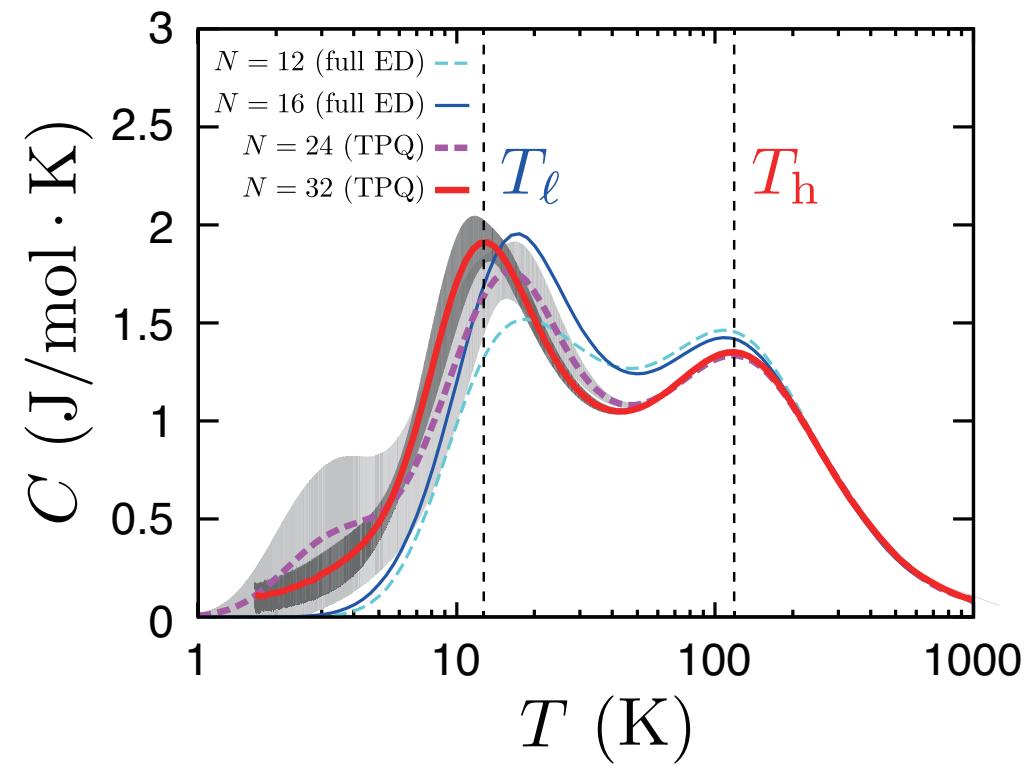
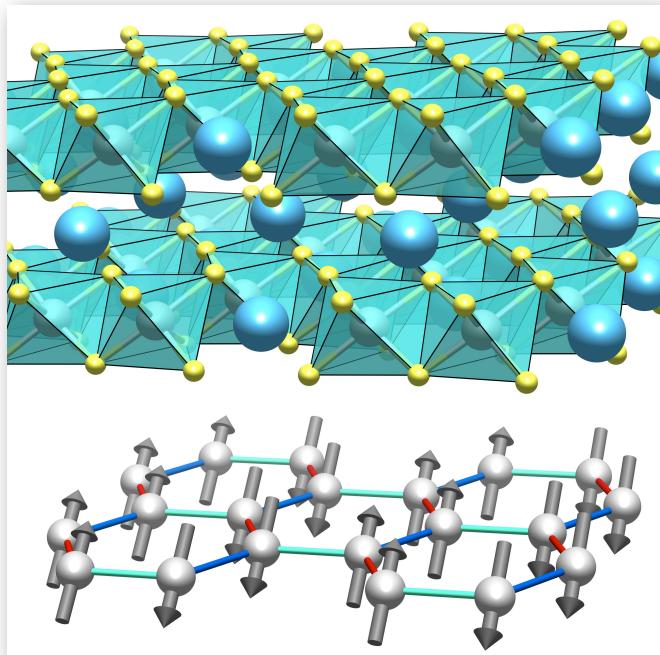


Nearsightedness

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



Numerical Approaches for Quantum Many-Body Systems

Numerical Methods for Quantum Many-Body Problems in CMP

- Numerical exact diagonalization: **Lanczos method** (Krylov subspace)
Ground state and low-lying excited states (equivalent to full CI)
- Quantum Monte Carlo:
Hirsch-Fye, World line, CTQMC, AFQMC, PQMC, DQMC, ...
Negative sign problem
- Matrix/Tensor Product State:
DMRG, NRG, MPS, TN, MERA, ...
- Negative-sign-free Quantum Monte Carlo:
Green's function Monte Carlo
Fixed node *DFT/LDA $E_{XC}[\rho]$ was derived by these techniques
Variational Monte Carlo
Biased by initial wave function
- Dynamical mean-field theory:
Lanczos method, Hirsch-Fye QMC, CTQMC, NRG, ...
No spatial fluctuations (Similar to MRCI?)
- One-body approximation or mean-field (Hartree-Fock, ...)

Eigenvalue Problems of Large and Sparse Matrices

Sparse Matrix

- Particle or orbital number: N
- Fock space dimension: $\exp[N \times \text{const.}]$
- # of terms in Hamiltonian: Polynomial of N
 - # of matrix elements of Hamiltonian matrix:
(Polynomial of N) $\times \exp[N \times \text{const.}]$

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

Then, the Hamiltonian matrix is **sparse**

Larger TFIM Revisit

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

-Non-commutative

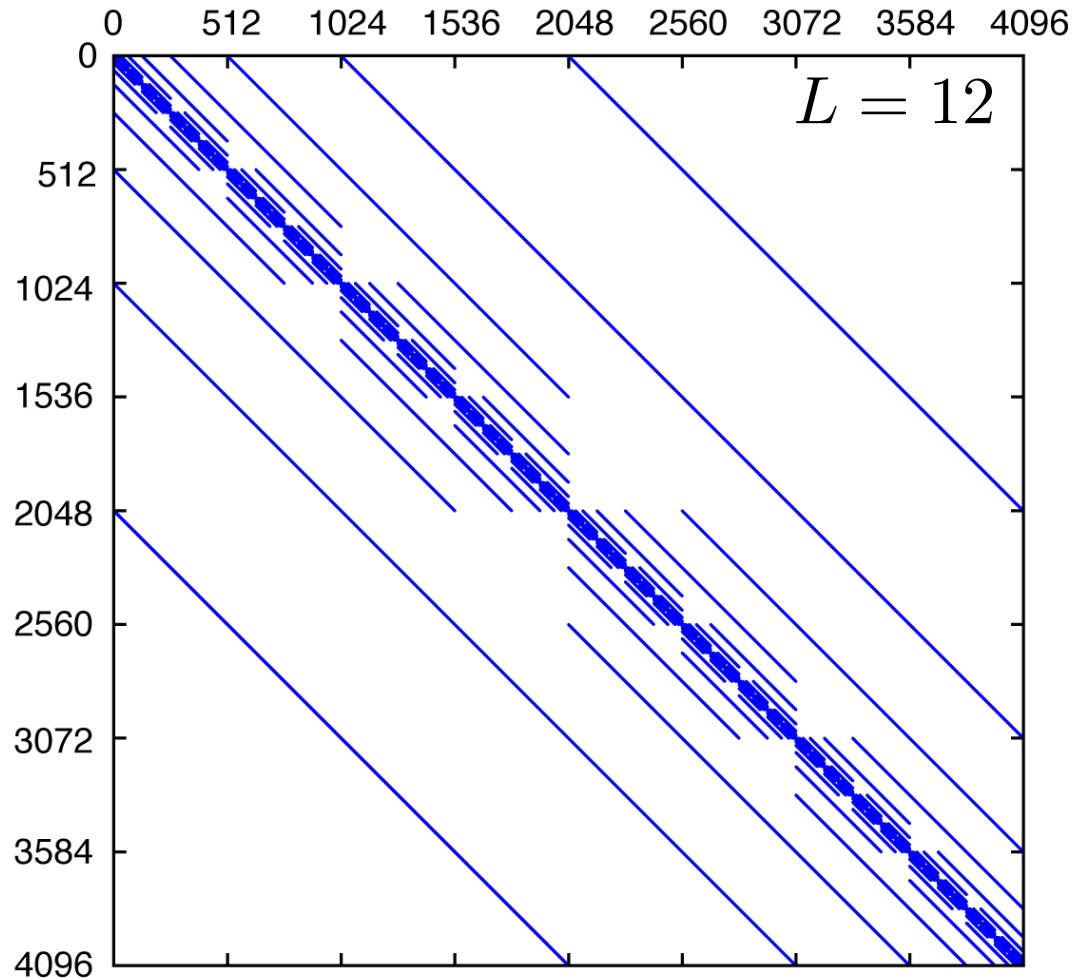
$$\left[\sum_{i=0}^{L-1} \hat{S}_i^z \hat{S}_{i+1}^z, \sum_{i=0}^{L-1} \hat{S}_i^x \right] \neq 0$$

→ Quantum fluctuations
or Zero point motion

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

-Solvable

-Hierarchical matrix?



Computational and Memory Costs

Matrix-vector product of dense matrix

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

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

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

Matrix-vector product of
large and sparse matrix

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

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

Hamiltonian is not stored in memory

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

Min. Eigenvalue of hermitian

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

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

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

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

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

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

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

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

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

Advanced Algorithm: Krylov Subspace Method

Krylov subspace

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

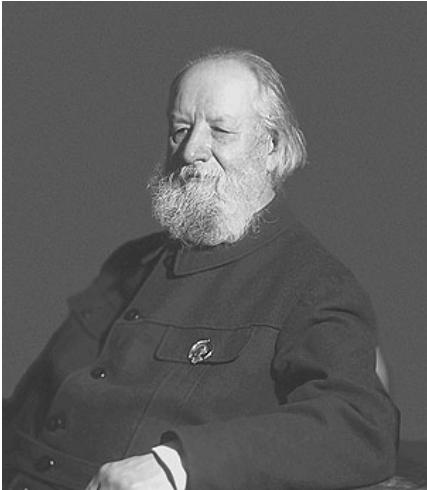
Shift invariance:

$$\mathcal{K}_m(\hat{H}, |v_1\rangle) = \mathcal{K}_m(\hat{H} + z\mathbf{1}, |v_1\rangle)$$

Krylov subspace method:

- Lanczos method (symmetric/hermitian),
- Arnoldi method (general matrix)
- Conjugate gradient method (CG method)
(many variation)

Krylov Subspace Method for Sparse and Huge Matrices



Alexey Krylov

Aleksey Nikolaevich Krylov

1863-1945

Russian naval engineer and applied mathematician

Krylov subspace

$$A \in \mathbb{C}^{L \times L}$$

$$\mathcal{K}_n(A, \vec{b}) = \text{span}\{\vec{b}, A\vec{b}, \dots, A^{n-1}\vec{b}\}$$

Numerical cost to construct K_n : $\mathcal{O}(\text{nnz}(A) \times n)$

Numerical cost to orthogonalize K_n : $\mathcal{O}(L \times n^2)$

Cornelius Lanczos 1950

Walter Edwin Arnoldi 1951

*nnz: Number of non-zero entries/elements

Krylov Subspace Method

from *SIAM News*, Volume 33, Number 4

The Best of the 20th Century: Editors Name Top 10 Algorithms

By Barry A. Cipra

1950: Magnus Hestenes, Eduard Stiefel, and Cornelius Lanczos, all from the Institute for Numerical Analysis at the National Bureau of Standards, initiate the development of **Krylov subspace iteration methods**.

These algorithms address the seemingly simple task of solving equations of the form $Ax = b$. The catch, of course, is that A is a huge $n \times n$ matrix, so that the algebraic answer $x = b/A$ is not so easy to compute. (Indeed, matrix “division” is not a particularly useful concept.) Iterative methods—such as solving equations of

the form $Kx_{i+1} = Kx_i + b - Ax_i$ with a simpler matrix K that’s ideally “close” to A —lead to the study of Krylov subspaces. Named for the Russian mathematician Nikolai Krylov, Krylov subspaces are spanned by powers of a matrix applied to an initial “remainder” vector $r_0 = b - Ax_0$. Lanczos found a nifty way to generate an orthogonal basis for such a subspace when the matrix is symmetric. Hestenes and Stiefel proposed an even niftier method, known as the conjugate gradient method, for systems that are both symmetric and positive definite. Over the last 50 years, numerous researchers have improved and extended these algorithms. The current suite includes techniques for non-symmetric systems, with acronyms like GMRES and Bi-CGSTAB. (GMRES and Bi-CGSTAB premiered in *SIAM Journal on Scientific and Statistical Computing*, in 1986 and 1992, respectively.)

Lanczos Method

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

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

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

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

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

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

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

Lanczos Method

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

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

Orthogonalization

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

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

Lanczos Method

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

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

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

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

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

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

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

Lanczos Method

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

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

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

Hamiltonian projected onto m D Krylov subspace

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

Eigenvalues of projected Hamiltonian

→ Approximate eigenvalues of original Hamiltonian

Lanczos Method: # of Vectors Required

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

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

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

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

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

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

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

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

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

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

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

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

Convergence of Lanczos Method

Yousef Saad,

Numerical Methods for Large Eigenvalue Problems (2nd ed)

The Society for Industrial and Applied Mathematics 2011

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

Convergence theorem for the largest eigenvalue

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

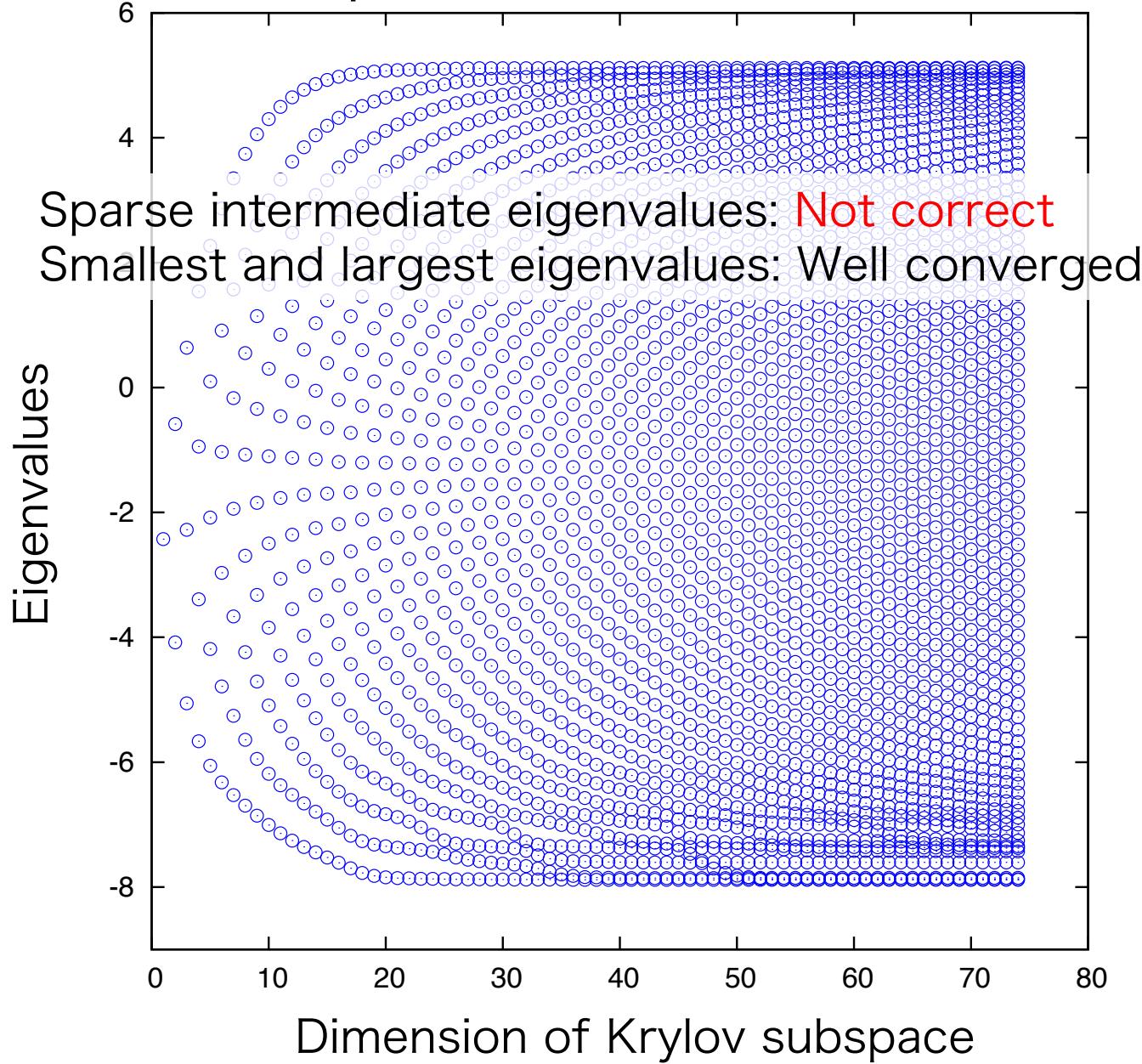
$$\gamma_1 = \frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_n}$$

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

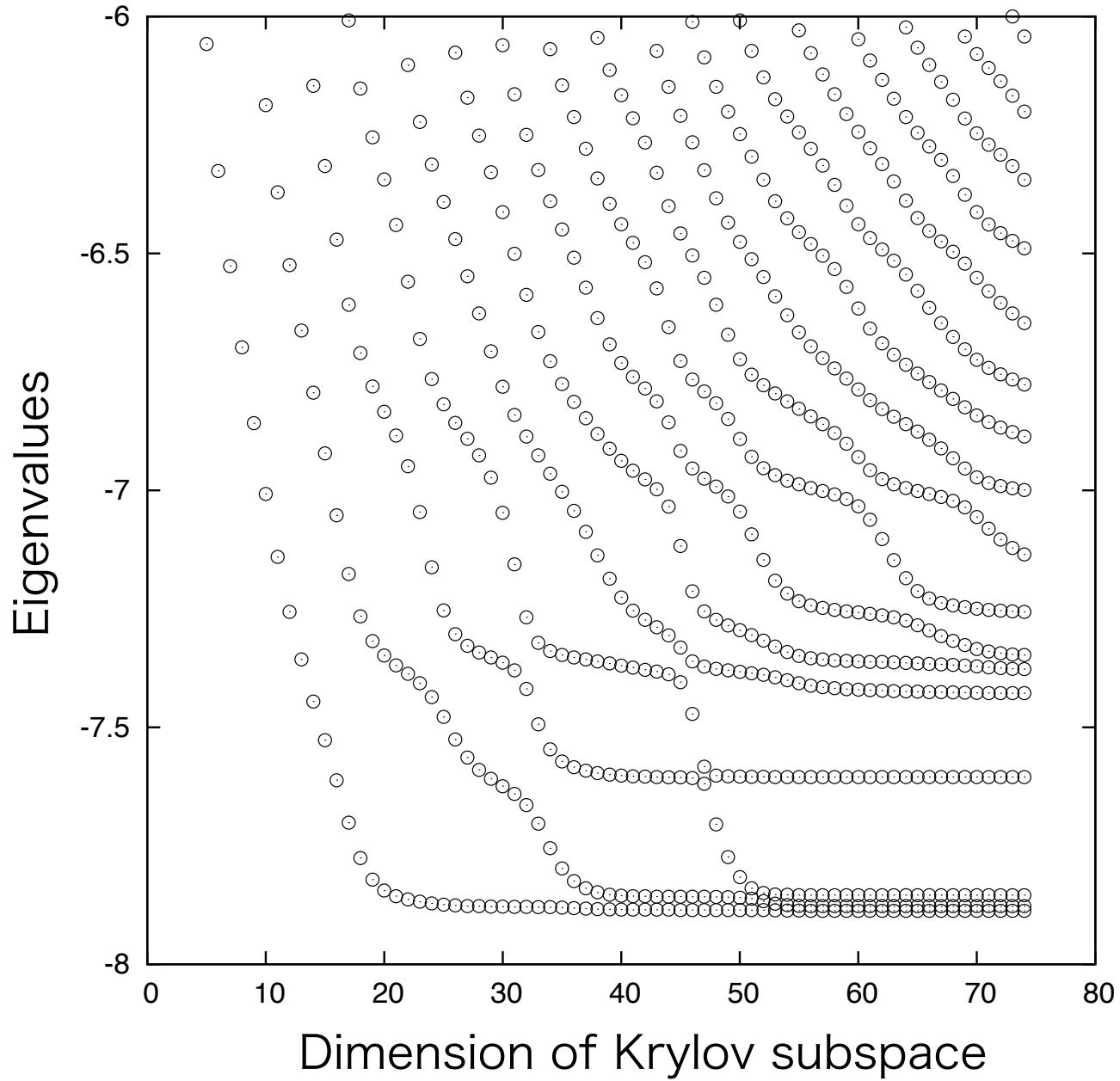
Approximate Eigenvalues by Lanczos Method

24 site cluster of Kitaev- Γ model (frustrated $S=1/2$ spins)

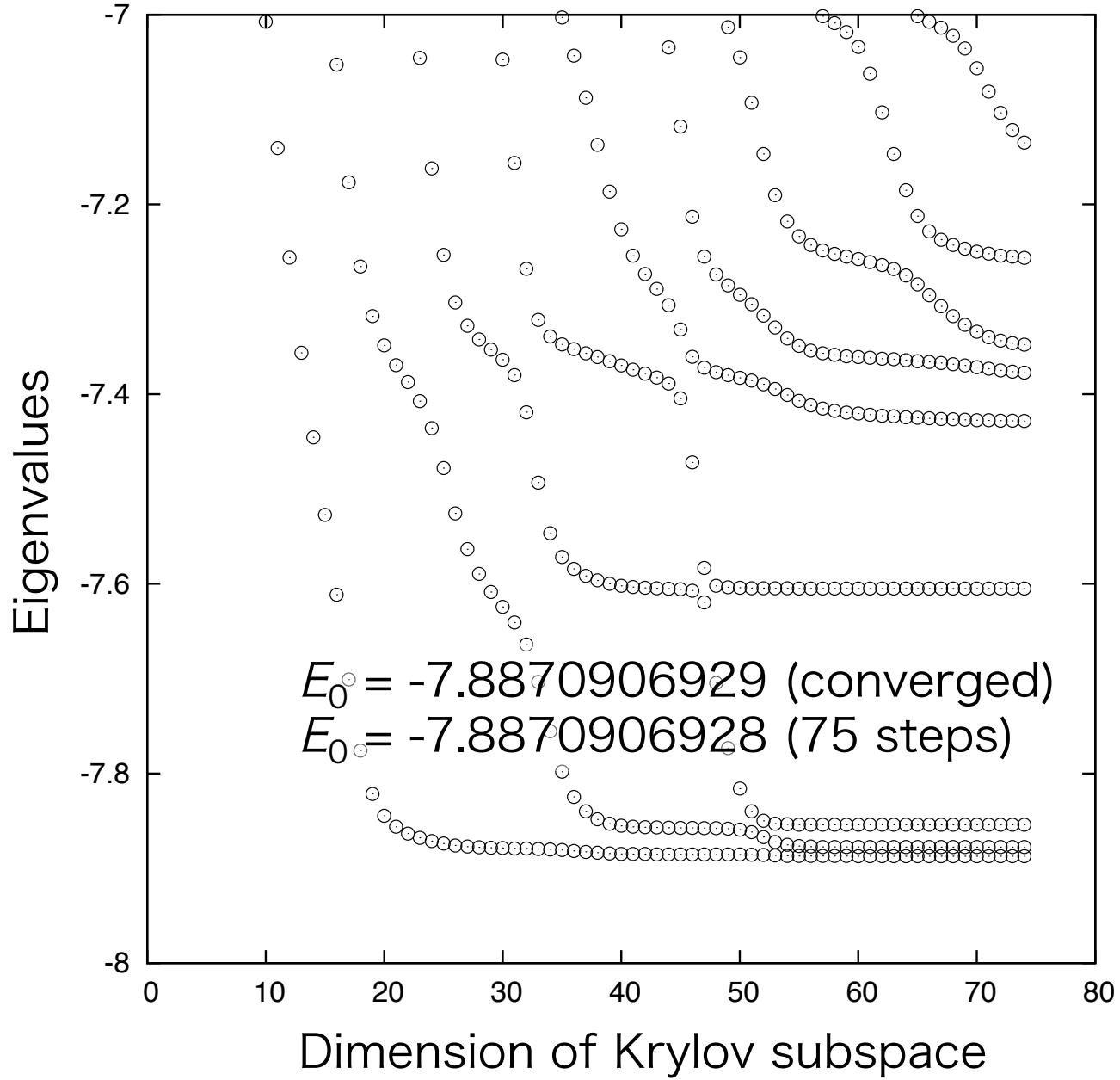
Dimension of Fock space: $2^{24}=16777216$



Lanczos法による近似固有値



Lanczos法による近似固有値



Example of Distribution of Eigenvalues: Random Symmetric Matrices

Eugene P. Wigner, Annals of Mathematics, 2nd Series, 67, 325 (1958)

Wigner's random matrix $(A)_{ij} = a_{ij}$

$$a_{ij} = a_{ji} \quad (\text{Not necessarily sparse})$$

$$\int p_{ij}(a)da = 1$$

$$p_{ij}(+a) = p_{ij}(-a)$$

$$\langle a_{ij}^n \rangle = \int p_{ij}(a)a^n da \leq B_n$$

$$\langle a_{ij}^2 \rangle = \int p_{ij}(a)a^2 da = 1$$

Example of Distribution of Eigenvalues: Random Symmetric Matrices

Eugene P. Wigner, Annals of Mathematics, 2nd Series, 67, 325 (1958)

Density of states of $N_{\text{H}} \times N_{\text{H}}$ symmetric random matirx

$$A\vec{v} = E\vec{v}$$

$$\sigma(E) = \begin{cases} \frac{\sqrt{4N_{\text{H}} - E^2}}{2\pi N_{\text{H}}} & (E^2 < 4N_{\text{H}}) \\ 0 & (E^2 > 4N_{\text{H}}) \end{cases}$$

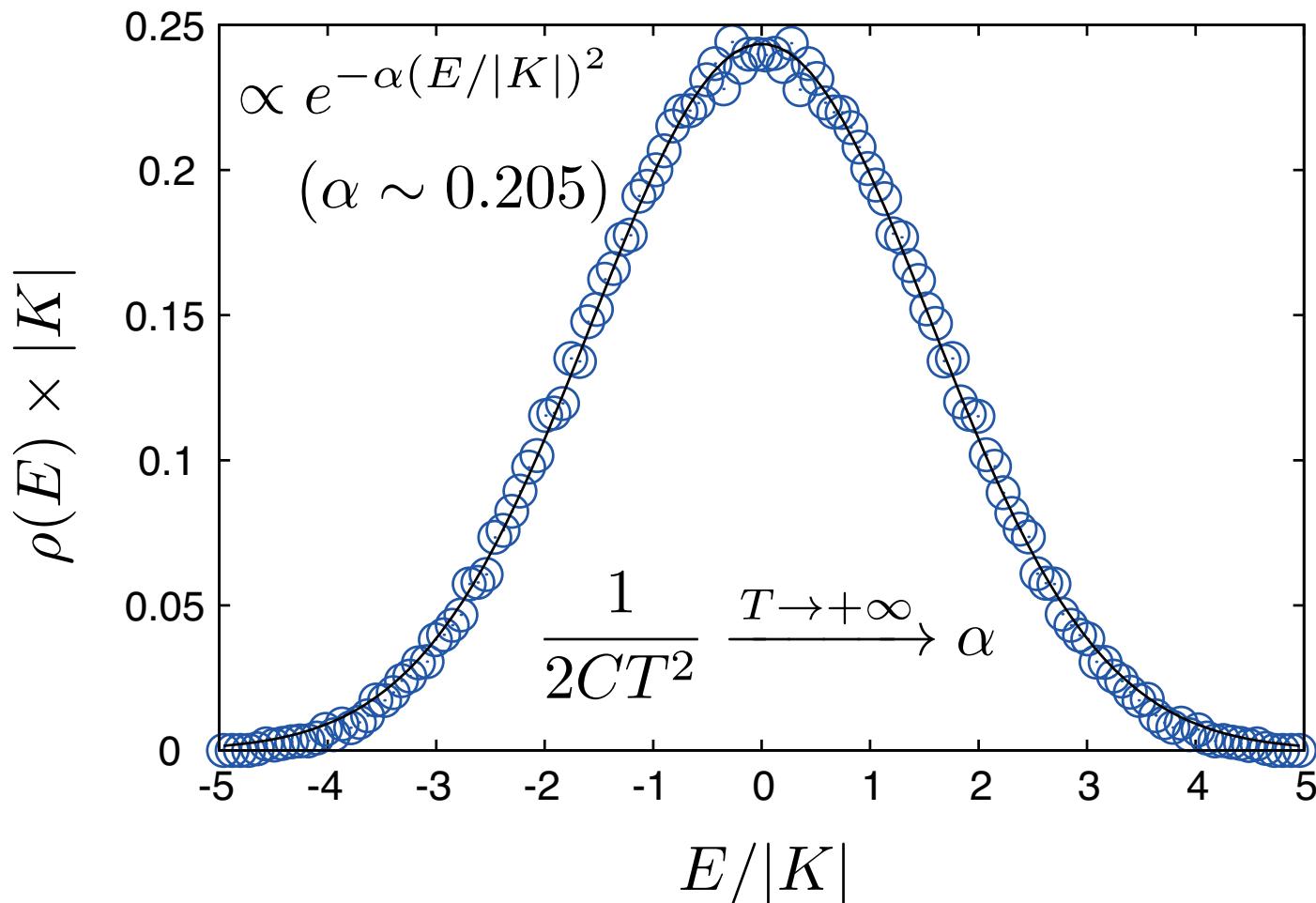
Comment:

Sparse matrices in quantum many-body problems show smaller density of states than random matrices
→ Sparse around maximum/minimum eigenvalues
→ Lanczos method may work well

An Example of Density of State by A Random Vector

24 site cluster of Kitaev model
(frustrated $S=1/2$ spins)

A. Kitaev, Annals Phys. 321, 2 (2006).
 $2^{24} = 16,777,216$



Numerical Methods Clarified Emergent Concepts in Many-Body Problems

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

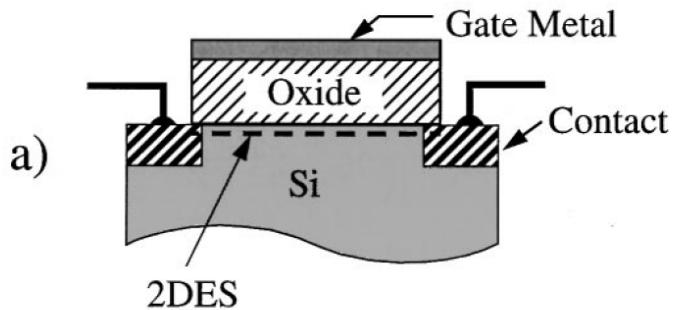
Thermalization of isolated quantum systems

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

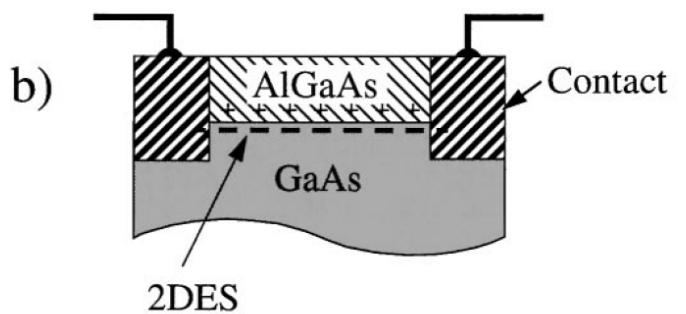
- Linear responses of strongly correlated electrons
- Frustrated magnetism
- **Haldane gap**

FQHE

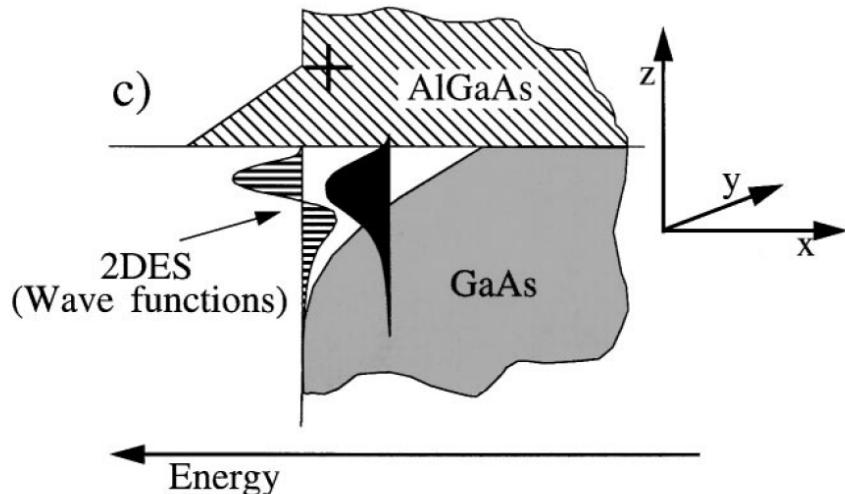
Two Dimensional Electron Gas



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).

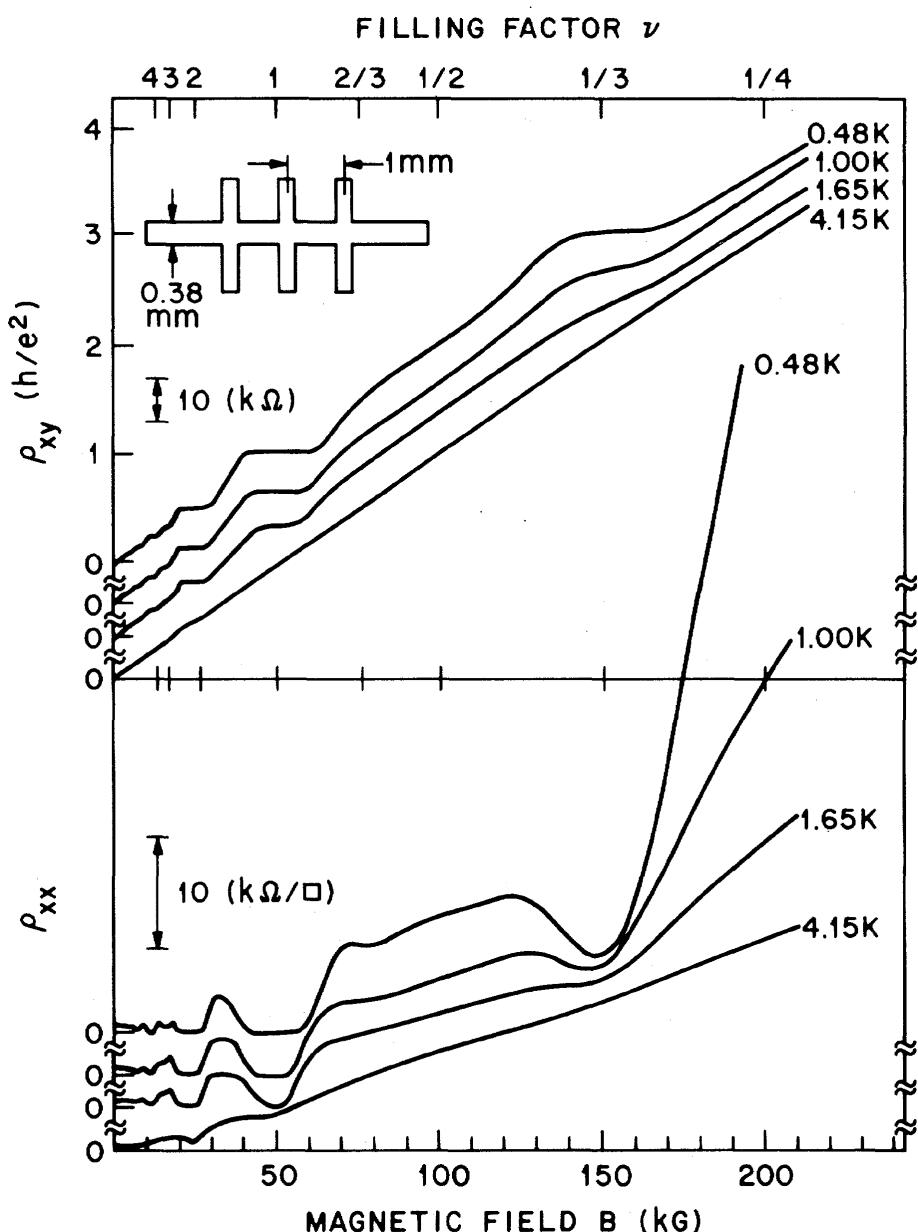
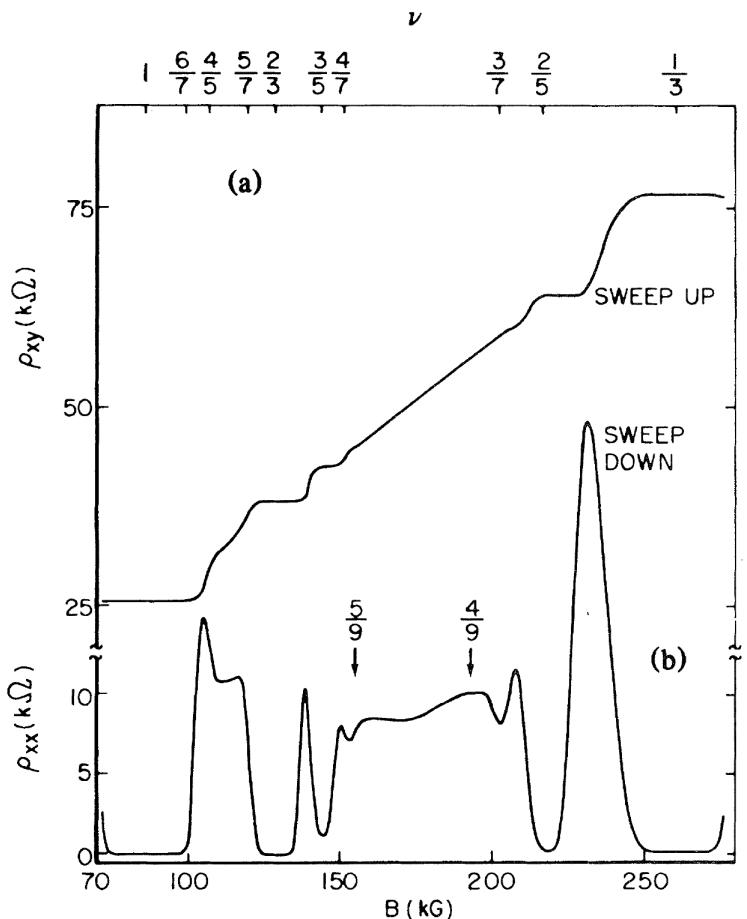


FIG. 1. ρ_{xy} and ρ_{xx} vs B , taken from a GaAs-Al_{0.3}-Ga_{0.7}As sample with $n = 1.23 \times 10^{11}/\text{cm}^2$, $\mu = 90\,000 \text{ cm}^2/\text{V sec}$, using $I = 1 \mu\text{A}$. The Landau level filling factor is defined by $\nu = nh/eB$.

Laughlin-Jastrow Trial Wave Function

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

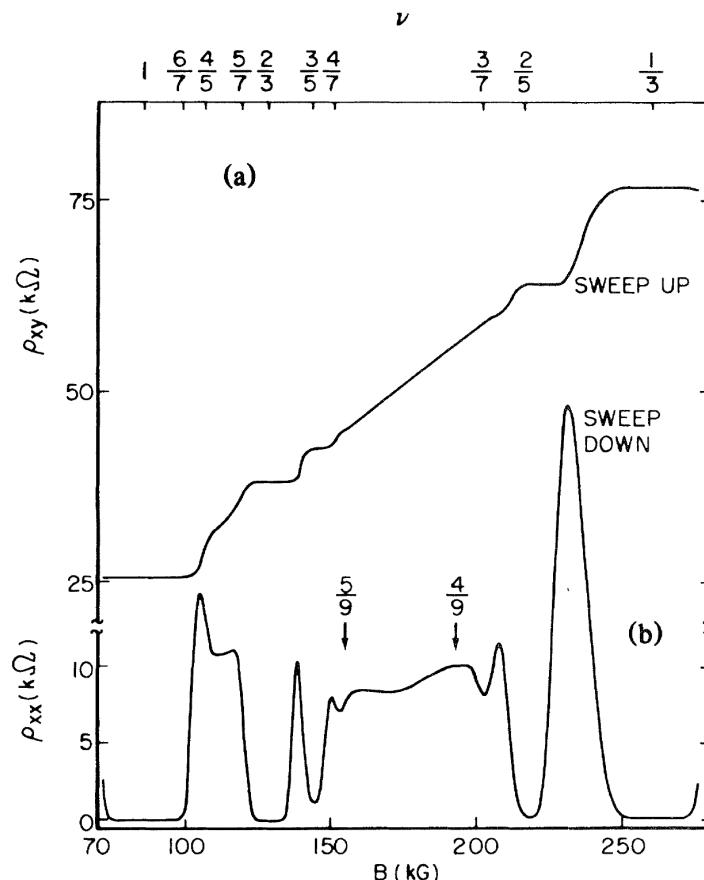
$$\psi_m(z_1, z_2, \dots, z_N) = \left[\prod_{i < j} (z_i - z_j)^m \right] \exp \left(-\frac{1}{4} \sum_k |z_k|^2 \right)$$

$$z_j = x_j - iy_j$$

$$m = 1/\nu$$

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

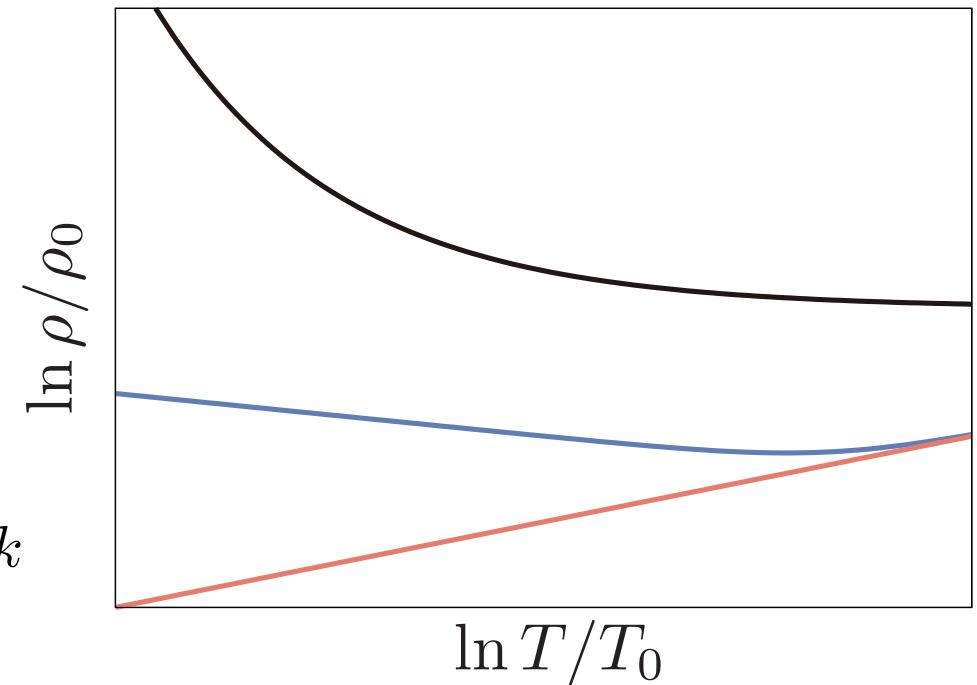
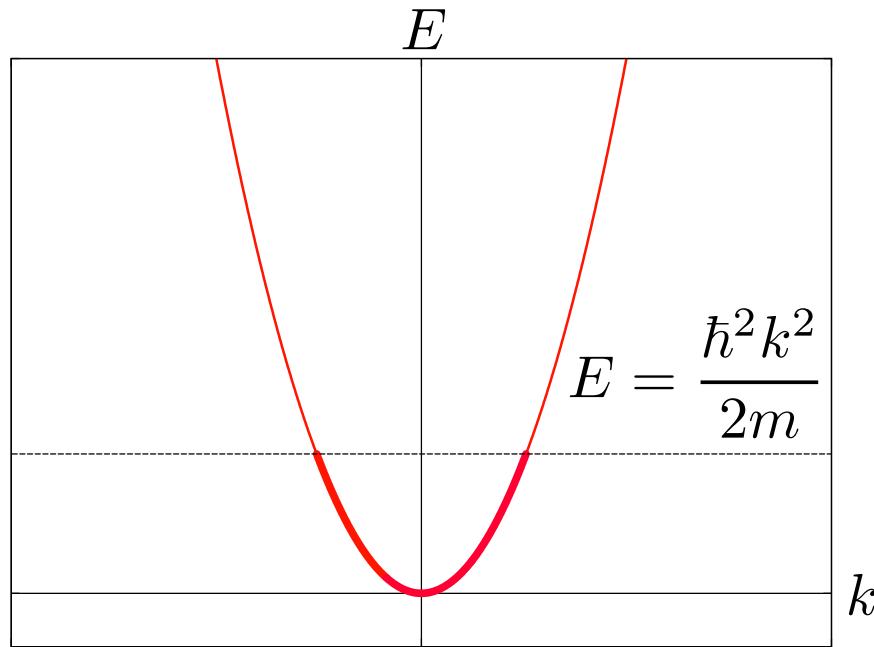
Background: Topological Phase

Classification of gapped quantum phases

Nobel Prize in 2016
“Topological phase transitions and
topological phases of matter”

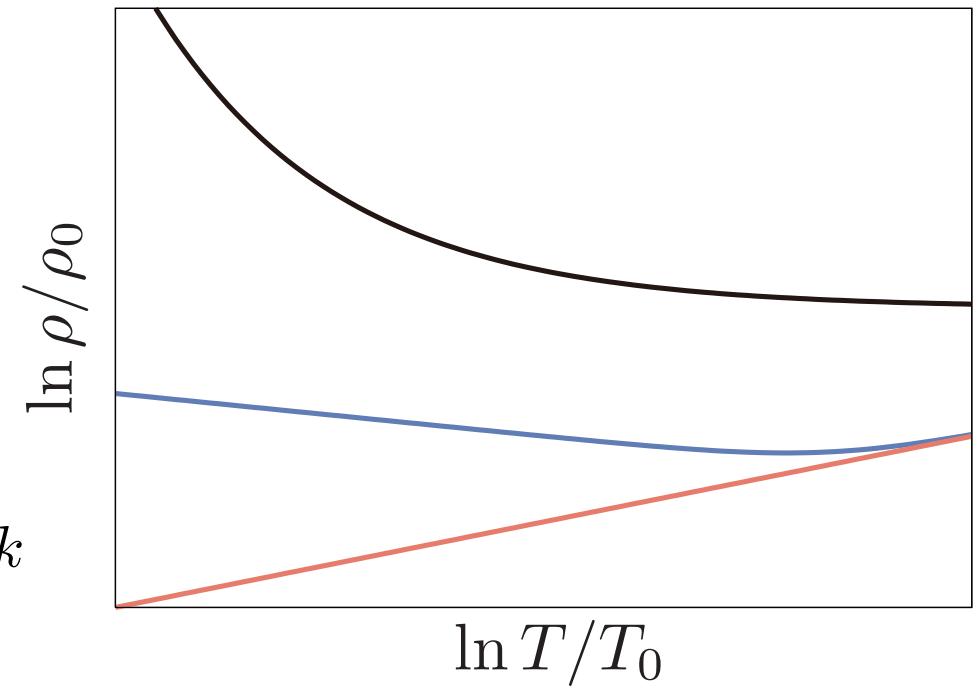
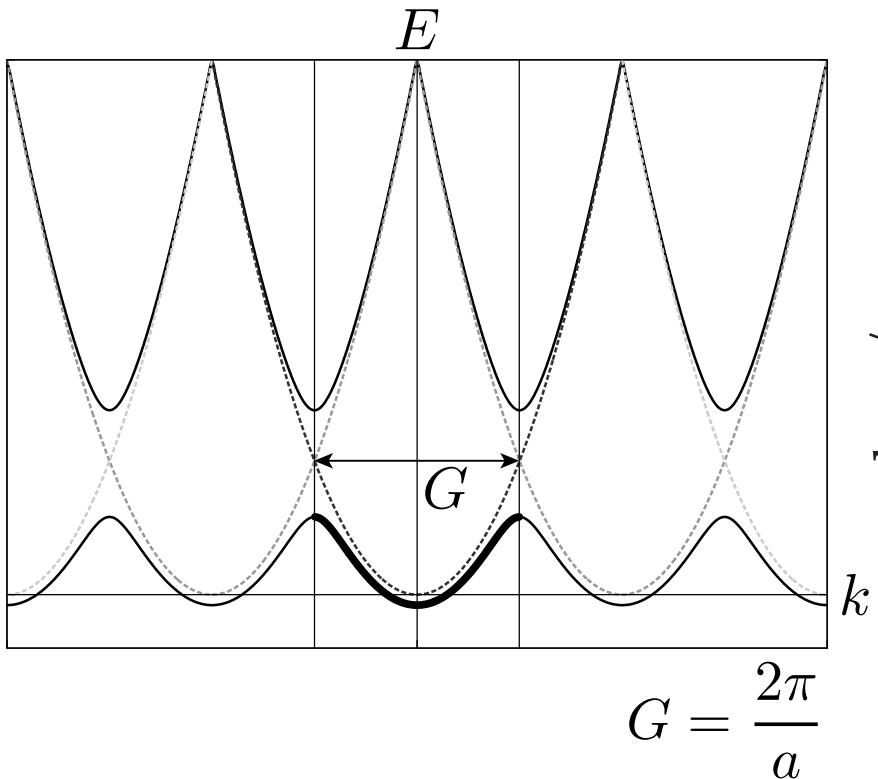
Classification of Crystalline Solids from Electric Transport

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



Classification of Crystalline Solids from Electric Transport

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

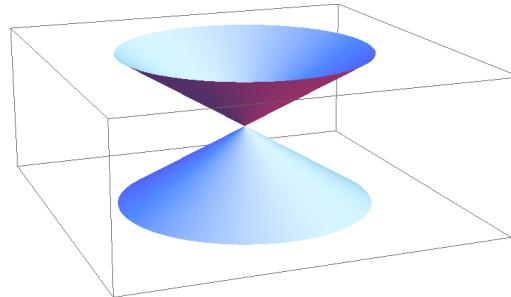
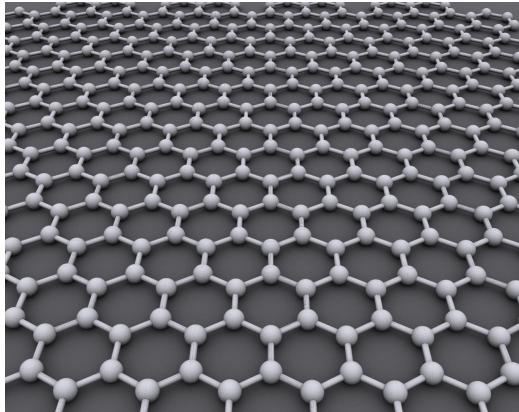


Classification of Crystalline Solids from Electric Transport

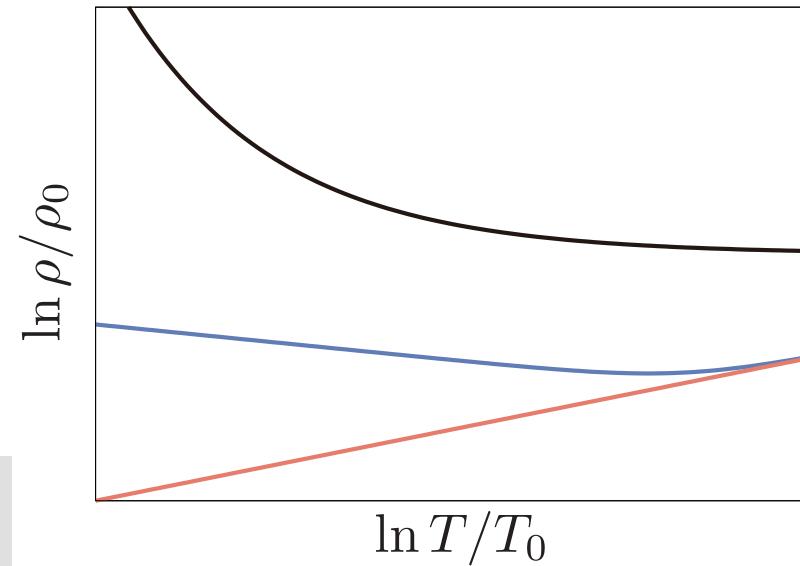
- Metal
- Zero gap semiconductor
- Band insulator
- Mott insulator

Example of zero gap semi.

2 D Dirac: Graphene

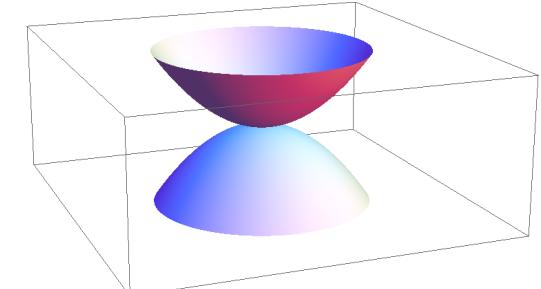


Castro Neto, Guinea, Peres, Novoselov, & Geim,
Rev. Mod. Phys. 81, 109 (2009)



3 D Dirac:
 Cd_3As_2 , Na_3Bi

HgTe, α -Sn (gray tin)



Classification of Crystalline Solids from Electric Transport

- Metal
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- Mott insulator

Trivial insulator

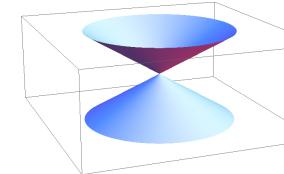
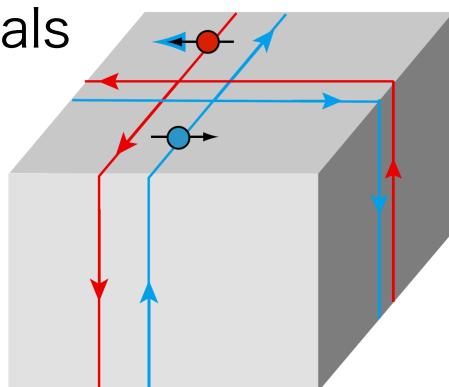
Si

Topological insulator

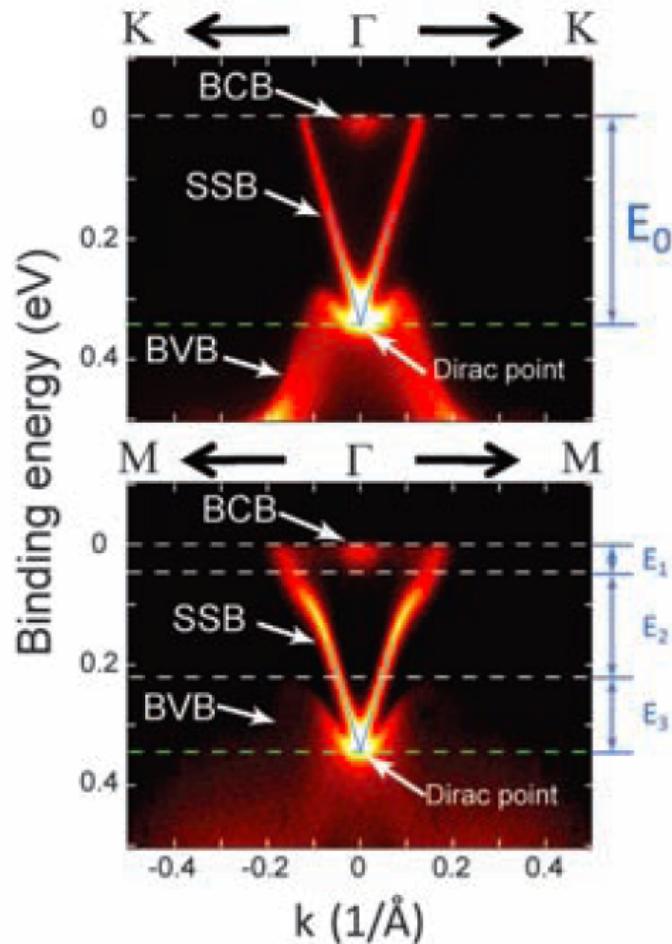
Bi_2Te_3

Thermoelectric

Surface metals

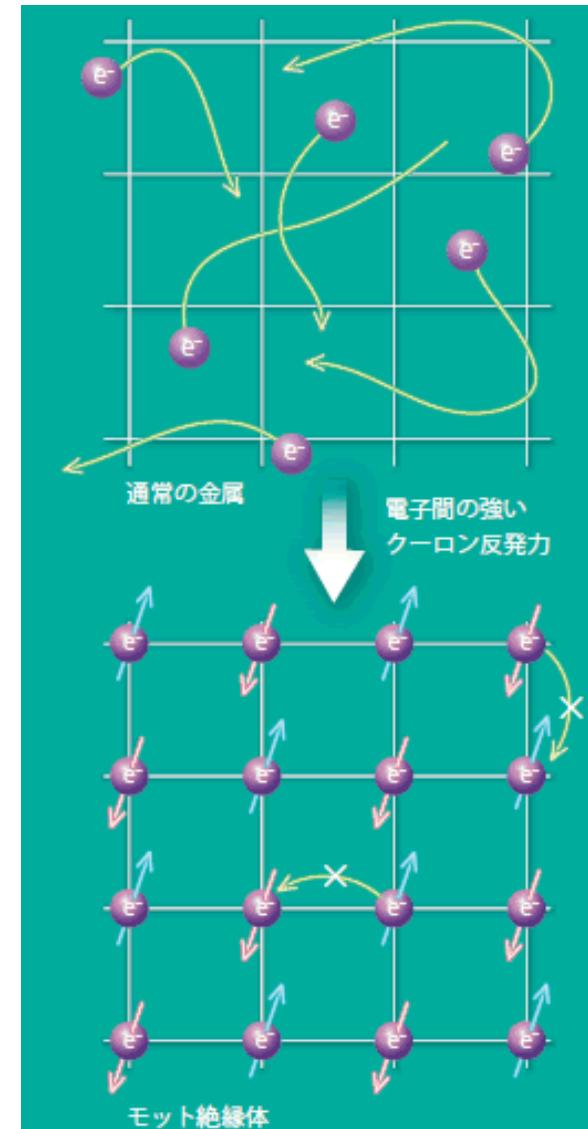


Y. L. Chen, *et al.*, Science 325, 178 (2009)



Classification of Crystalline Solids from Electric Transport

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



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CMSI広報誌
torrent No.5 より

Spin Angular Momentum Coupling

- An electron has $S = 1/2$ ((spin angular momentum) = $h/4\pi$)
- 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

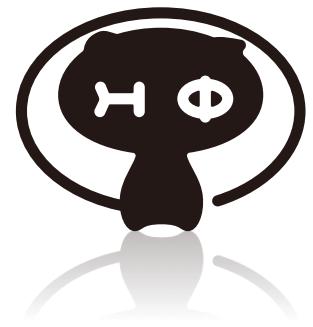
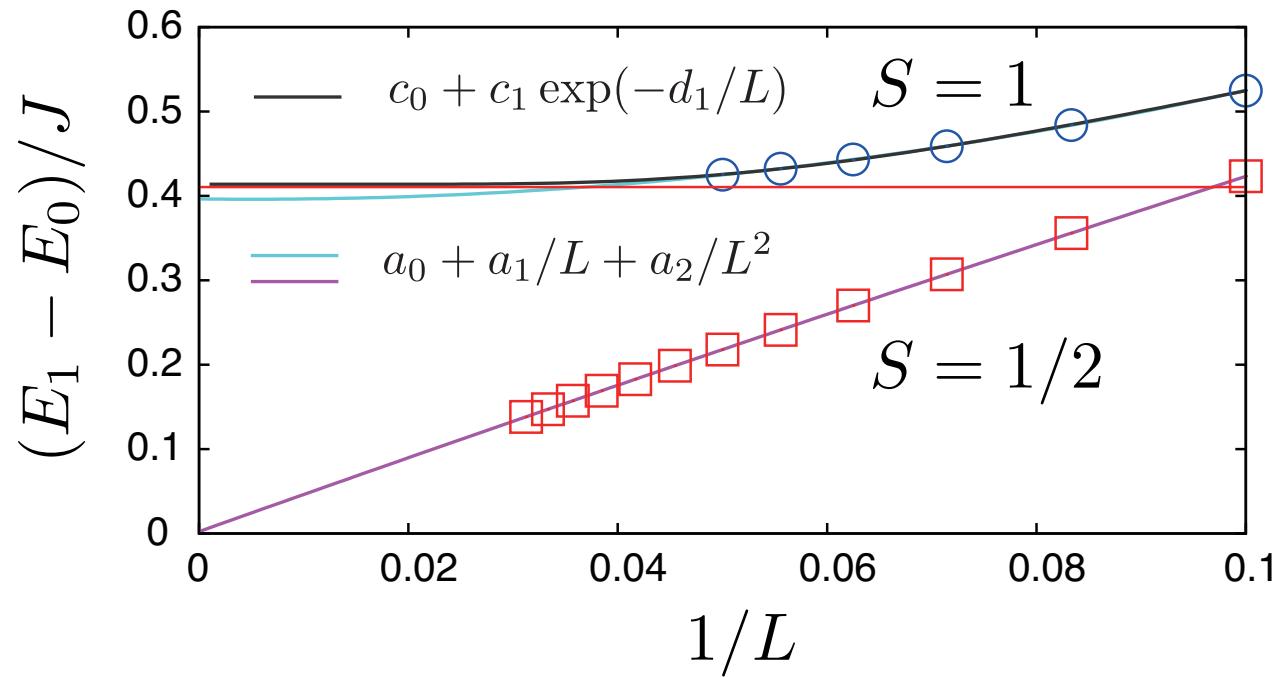
Edge states

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).

Typicality Approach

Finite Temperature: Heat Capacity

Spread of energy distribution

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

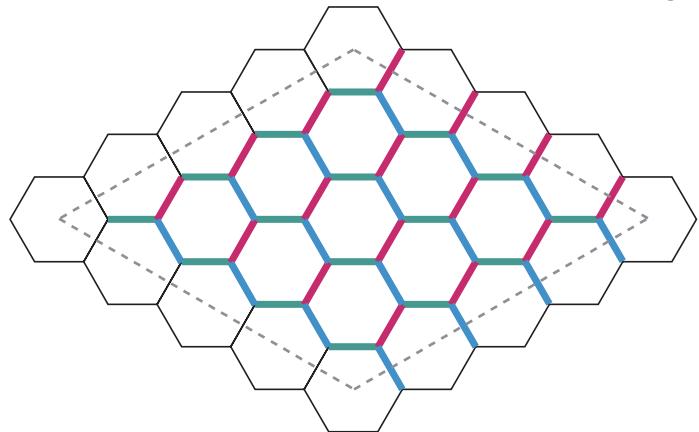
-Average with Boltzmann distribution

$$\langle \hat{O}_\beta^{\text{ens}} \rangle = \frac{\sum_n e^{-E_n/k_B T} \langle n | \hat{O} | n \rangle}{\sum_n e^{-E_n/k_B T}}$$

Complexity $\mathcal{O}(N_{\text{H}}^3)$

Memory $\mathcal{O}(N_{\text{H}}^2)$

32 site cluster of Na_2IrO_3



$$N_{\text{H}} = 2^{32}$$

Hamiltonian
 $\sim 3 \times 10^8 \text{ TB!}$

$|n\rangle \sim 69 \text{ GB}$

Typical Pure State Approach

Complexity

$$\mathcal{O}(N_H)$$

Memory

Imada-Takahashi (1986)
 Lloyd (1988)
 Jacklic-Prelovsek (1994)
 Hams-De Raedt (2000)
 Sugiura-Shimizu (2012, 2013)

M. Imada & M. Takahashi, J. Phys. Soc. Jpn. 55, 3354 (1986).

$\beta = 0$ ($T \rightarrow +\infty$) Typical state: Random vector

$$|\phi_0\rangle = \sum_x c_x |x\rangle \quad (\sum_x |c_x|^2 = 1)$$

$$\langle \hat{O} \rangle_{\beta=0}^{\text{ens}} = \mathbb{E}[\langle \phi_0 | \hat{O} | \phi_0 \rangle]$$

At finite temperature

$$|\phi_\beta\rangle = e^{-\beta \hat{H}/2} |\phi_0\rangle$$

N. Ullah, Nucl. Phys. 58, 65 (1964).
 -Uniform distribution on
 unit sphere in \mathbb{R}^{2N_H}

$$\mathbb{E}[|c_x|^{2n}] = \frac{\Gamma(N_H)\Gamma(n+1)}{\Gamma(N_H+n)}$$

Average over the distribution

How large is the standard deviation?

$$\sigma_O^2 = \mathbb{E} \left[\left(\frac{\langle \phi_\beta | \hat{O} | \phi_\beta \rangle}{\langle \phi_\beta | \phi_\beta \rangle} - \langle \hat{O} \rangle_{\beta}^{\text{ens}} \right)^2 \right]$$

Typical Pure State Approach

- Seth Lloyd, Ph.D. Thesis, Rockefeller University (1988); arXiv:1307.0378.
A. Hams & H. De Raedt, Phys. Rev. E 62, 4365 (2000).
A. Sugita, RIMS Kokyuroku (Kyoto) 1507, 147 (2006).
P. Reimann, Phys. Rev. Lett. 99, 160404 (2007).
S. Sugiura & A. Shimizu, Phys. Rev. Lett. 108, 240401 (2012).
S. Sugiura & A. Shimizu, Phys. Rev. Lett. 111, 010401 (2013).

$$\sigma_O^2 \leq \frac{\langle (\Delta O)^2 \rangle_{2\beta}^{\text{ens}} + (\langle O \rangle_{2\beta}^{\text{ens}} - \langle O \rangle_{\beta}^{\text{ens}})^2}{\exp[2\beta\{F(2\beta) - F(\beta)\}]}$$

$$\propto \exp[-S(\beta^*)/2] \quad (\beta < \beta^* < 2\beta)$$

Exponentially small when system size increases

Construction of Typical Pure State

Thermal Pure Quantum (TPQ) States $|\phi_\beta\rangle = |\Phi_k\rangle$

Sugiura & Shimizu, Phys. Rev. Lett. 108, 240401 (2012)

Initial state (at $T = +\infty$): $|\Phi_0\rangle = (\text{Random vector})$
do $k=1, N_{\text{step}}$ If possible, taking random average

$$|\Phi_k\rangle = (\ell - \hat{H}/N) |\Phi_{k-1}\rangle / \sqrt{\langle \Phi_{k-1} | (\ell - \hat{H}/N)^2 | \Phi_{k-1} \rangle}$$

$$u_k = \langle \Phi_k | \hat{H}/N | \Phi_k \rangle$$

$$\beta = 2(k/N)/(\ell - u_k) \quad (\beta = 1/k_B T)$$

$$\overline{O}(\beta) = \langle \Phi_k | \hat{O} | \Phi_k \rangle + \mathcal{O}(1/N)$$

enddo

Hamiltonian-wave function product is essential

Nature of Random Vector

M. Imada and M. Takahashi, J. Phys. Soc. Jpn. 55, 3354 (1986).

Random wave function

$$|\phi_0\rangle = \sum_x c_x |x\rangle \quad \sum_x |c_x|^2 = 1$$
$$|x\rangle = |\sigma_0 \sigma_1 \cdots \sigma_{N-1}\rangle$$

Infinite-temperature result

$$\mathbb{E}[\langle\phi_0|\hat{O}|\phi_0\rangle] = N_{\text{H}}^{-1} \sum_n \langle n|\hat{O}|n\rangle = \langle\hat{O}\rangle_{\beta=0}^{\text{ens}}$$

$$\mathbb{E}[|c_x|^2] = N_{\text{H}}^{-1}$$
$$|n\rangle = \sum_x U_{xn} |x\rangle$$

Every eigenstate contained
in a random vector with
equal probability

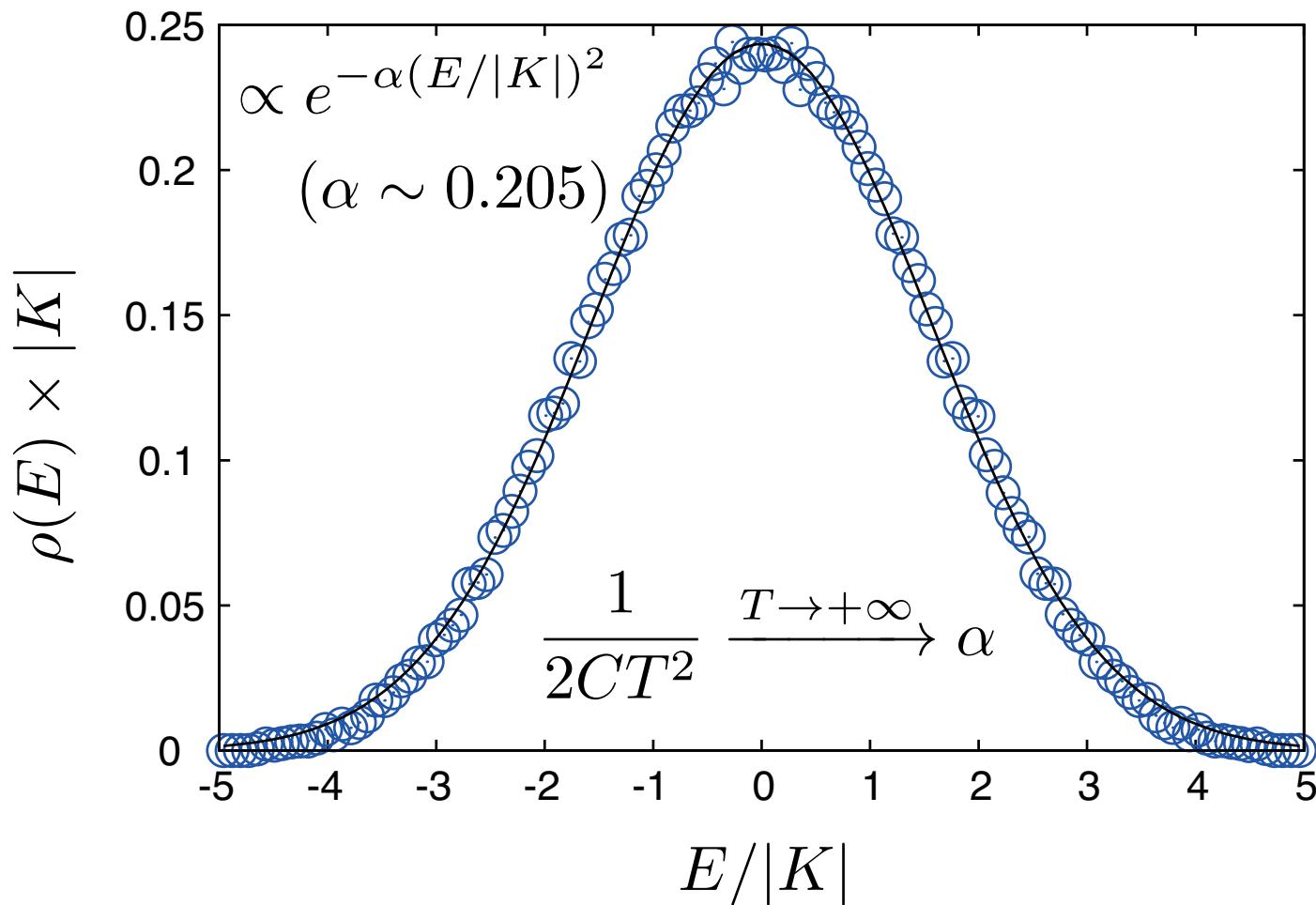
N. Ullah, Nucl. Phys. 58, 65 (1964).
-Uniform distribution on
unit sphere in $\mathbb{R}^{2N_{\text{H}}}$

$$\mathbb{E}[|c_x|^{2n}] = \frac{\Gamma(N_{\text{H}})\Gamma(n+1)}{\Gamma(N_{\text{H}}+n)}$$

An Example of Density of State by A Random Vector

24 site cluster of Kitaev model
(frustrated $S=1/2$ spins)

A. Kitaev, Annals Phys. 321, 2 (2006).
 $2^{24} = 16,777,216$



Preparation for Exercises

Appendix: Variational Monte Carlo

Variational Method Revisited

Variational principle: $E(\vec{\alpha}) = \frac{\langle \Psi(\vec{\alpha}) | \hat{H} | \Psi(\vec{\alpha}) \rangle}{\langle \Psi(\vec{\alpha}) | \Psi(\vec{\alpha}) \rangle} \geq E_0$

Variational wave function: $|\Psi(\vec{\alpha})\rangle$

Variational parameters: $\vec{\alpha} = (\alpha_1, \alpha_2, \dots, \alpha_M)$

Example: ${}^4\text{He}$ atom (see J. J. Sakurai)

One-body approximation: $\psi_{100}(\vec{r}_1)\psi_{100}(\vec{r}_2)\chi_0 = \frac{Z^3}{\pi a_B^3} e^{-Z(r_1+r_2)}\chi_0$

Variational wf: $\psi(\vec{r}_1, \vec{r}_2)\chi_0 = \frac{Z_{\text{eff}}^3}{\pi a_B^3} e^{-Z_{\text{eff}}(r_1+r_2)}\chi_0$

Variational parameter: $Z_{\text{eff}} = Z - \frac{5}{16} = 2 - \frac{5}{16}$

$E = -77.5 \text{ eV}$

Screening of ionic Coulomb force by the other electrons

1st order perturbation: $E_1 = -74.8 \text{ eV}$

Experiment: $E_{\text{exp}} = -78.8 \text{ eV}$

VMC

$$E(\vec{\alpha}) = \frac{\langle \Psi(\vec{\alpha}) | \hat{H} | \Psi(\vec{\alpha}) \rangle}{\langle \Psi(\vec{\alpha}) | \Psi(\vec{\alpha}) \rangle} \geq E_0$$

Variational wave function: $|\Psi(\vec{\alpha})\rangle$

Variational parameters: $\vec{\alpha} = (\alpha_1, \alpha_2, \dots, \alpha_M)$

When analytical methods are not available

→ Energy expectation values evaluated by MC

■ N -body wf: complex function with $3N$ variables

$$\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \quad \begin{aligned} &\cdot \text{Volume: } L^3 \\ &\cdot \text{Discretization: } L^{3N} \rightarrow M^{3N} \times (L/M)^{3N} \\ &\rightarrow O(M^{3N}) \text{ Riemann sum} \end{aligned}$$

MC for real space configuration instead of Riemann sum

$$\frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \simeq \frac{1}{N_{\text{MC}}} \sum_{\ell=1}^{N_{\text{MC}}} \frac{\langle \Psi | \hat{O} | \vec{r}_1^{(\ell)}, \vec{r}_2^{(\ell)}, \dots, \vec{r}_N^{(\ell)} \rangle}{\langle \Psi | \vec{r}_1^{(\ell)}, \vec{r}_2^{(\ell)}, \dots, \vec{r}_N^{(\ell)} \rangle}$$

Liquid Helium 4 (boson): LJ Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m_{^4\text{He}}} \sum_i \nabla_i^2 + \sum_{i < j; i,j=1}^N V(r_{ij})$$

$$r_{ij} \equiv |\vec{r}_i - \vec{r}_j|$$

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$$

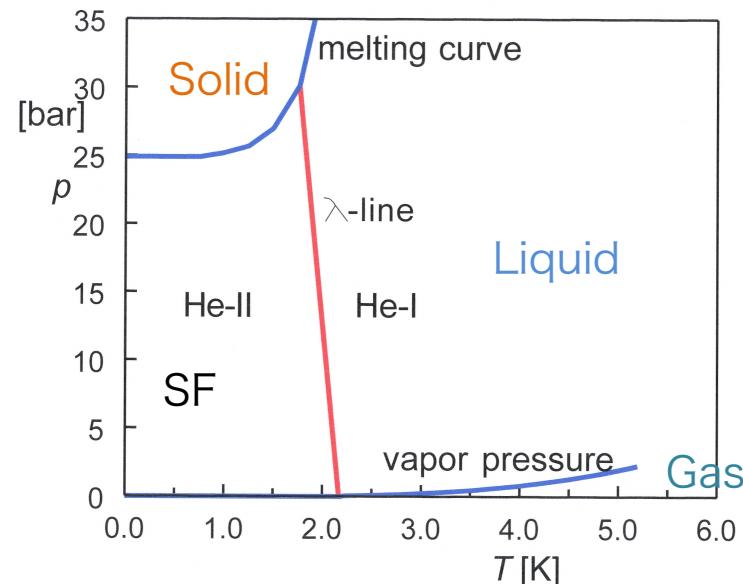
$$m_{^4\text{He}}/\hbar^2 = 0.597639 \times 10^{22} \text{ J}^{-1} \cdot \text{\AA}^{-2}$$

$$\sigma = 2.556 \text{ \AA}$$

$$\epsilon = 1.41102 \times 10^{-22} \text{ J}$$

Lennard-Jones (LJ) potential
← Determined by correction to
equation of state
(2nd virial coefficient)

Phase diagram



VWF of Liquid Helium 4

W. L. McMillan, Phys. Rev. 138, A442 (1965)

Trial wf symmetric under exchange of two particles

$$\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \prod_{i < j; i, j=1}^N f(r_{ij})$$

$$f(r) = \exp[-u(r)]$$

cf.) Partition function of classical gas & Boltzmann weight

$$Z = \frac{1}{V^N} \int \prod_{\ell=1}^N d^3 r_\ell \exp \left[- \sum_{i < j} \frac{U(r_{ij})}{k_B T} \right]$$

$$P_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = Z^{-1} V^{-N} \left[- \sum_{i < j} \frac{U(r_{ij})}{k_B T} \right]$$

VWF of Liquid Helium 4

How to choose vwf?

$$f(r) = \exp [-(a_1/r)^{a_2}] \quad a_1, a_2 : \text{variational parameters}$$

LJ interaction is repulsive at a short distance

Asymptotic form of two particle problem ($r \rightarrow 0$)

$$-\frac{\hbar^2}{4m_{^4\text{He}}} \frac{d^2 f(r)}{dr^2} + 4\epsilon \left(\frac{\sigma}{r}\right)^{12} f(r) \sim 0$$

$$a_1 = \left(\frac{16m_{^4\text{He}}\epsilon\sigma^{12}}{25\hbar^2} \right)^{1/10} \quad a_2 = 5$$

cf.) Gutzwiller vwf for Hubbard model (Exact for 2 sites)

M. C. Gutzwiller, Phys. Rev. Lett. 10, 159 (1963); Phys. Rev. 137, A1726 (1965).

In Japanese, 斯波弘行: 電子相関の物理 (岩波書店, 2001). §1.3

VWF in 2nd Quantization Form

2nd quantization VWF

$$|\Psi\rangle = \frac{1}{\sqrt{N}} \exp \left[-\frac{1}{2} \int d^3r d^3r' \textcolor{red}{u(|\vec{r} - \vec{r}'|)} \hat{\phi}^\dagger(\vec{r}) \hat{\phi}(\vec{r}) \hat{\phi}^\dagger(\vec{r}') \hat{\phi}(\vec{r}') \right] \left(\hat{a}_{\vec{k}=\vec{0}}^\dagger \right)^N |0\rangle$$

Jastrow factor

One-body part
(Mean field wf)

Field operator $\hat{\phi}(\vec{r}) = V^{-1/2} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \hat{a}_{\vec{k}}$

Commutation $[\hat{\phi}(\vec{r}), \hat{\phi}^\dagger(\vec{r}')] = \delta(\vec{r} - \vec{r}')$ $[\hat{a}_{\vec{k}}, \hat{a}_{\vec{k}'}^\dagger] = \delta_{\vec{k}, \vec{k}'}$

Relation to WF in 1st quantization form

$$\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \propto \langle 0 | \hat{\phi}(\vec{r}_N) \cdots \hat{\phi}(\vec{r}_2) \hat{\phi}(\vec{r}_1) | \Psi \rangle = \frac{\sqrt{N} e^{-\sum_{i < j} f(r_{ij})}}{V^{\frac{N}{2}}}$$

2nd Quantization Form

Hamiltonian

$$\hat{H} = - \int d^3r \frac{\hbar^2}{2m_{^4\text{He}}} \hat{\phi}^\dagger(\vec{r}) \nabla^2 \hat{\phi}(\vec{r}) + \frac{1}{2} \int d^3r \int d^3r' \hat{\phi}^\dagger(\vec{r}) \hat{\phi}(\vec{r}) V(|\vec{r} - \vec{r}'|) \hat{\phi}^\dagger(\vec{r}') \hat{\phi}(\vec{r}')$$

Real space bases $|\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N\rangle = \hat{\phi}^\dagger(\vec{r}_1) \hat{\phi}^\dagger(\vec{r}_2) \cdots \hat{\phi}^\dagger(\vec{r}_N) |0\rangle$

Inner product $\langle \Psi | \Psi \rangle = \frac{1}{V^N} \int \prod_{i=1}^N d^3r_i \langle \Psi | \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N \rangle \langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N | \Psi \rangle$

Expectation value

$$\frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{1}{V^N} \int \prod_{i=1}^N d^3r_i \frac{\langle \Psi | \hat{O} | \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N \rangle}{\langle \Psi | \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N \rangle} \frac{|\langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N | \Psi \rangle|^2}{\langle \Psi | \Psi \rangle}$$

Weight

$$P_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \frac{1}{V^N} \frac{|\langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N | \Psi \rangle|^2}{\langle \Psi | \Psi \rangle}$$

Sampling

$$\frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \simeq \frac{1}{N_{\text{MC}}} \sum_{\ell=1}^{N_{\text{MC}}} \frac{\langle \Psi | \hat{O} | \vec{r}_1^{(\ell)}, \vec{r}_2^{(\ell)}, \dots, \vec{r}_N^{(\ell)} \rangle}{\langle \Psi | \vec{r}_1^{(\ell)}, \vec{r}_2^{(\ell)}, \dots, \vec{r}_N^{(\ell)} \rangle}$$

Many-Body WF

Gutzwiller WF (Potentially exact for 2-site Hubbard model)

$$|\Psi_G\rangle = \exp \left[-g \sum_{i=1}^2 \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} \right] \frac{(\hat{c}_{1\uparrow}^\dagger + \hat{c}_{2\uparrow}^\dagger)}{\sqrt{2}} \frac{(\hat{c}_{1\downarrow}^\dagger + \hat{c}_{2\downarrow}^\dagger)}{\sqrt{2}} |0\rangle$$



Gutzwiller factorOne-body part
(Mean-field WF)

McMillan's VWF

$$|\Psi\rangle = \frac{1}{\sqrt{N}} \exp \left[-\frac{1}{2} \int d^3r d^3r' \color{red} u(|\vec{r} - \vec{r}'|) \hat{\phi}^\dagger(\vec{r}) \hat{\phi}(\vec{r}) \hat{\phi}^\dagger(\vec{r}') \hat{\phi}(\vec{r}') \right] \left(\hat{a}_{\vec{k}=\vec{0}}^\dagger \right)^N |0\rangle$$

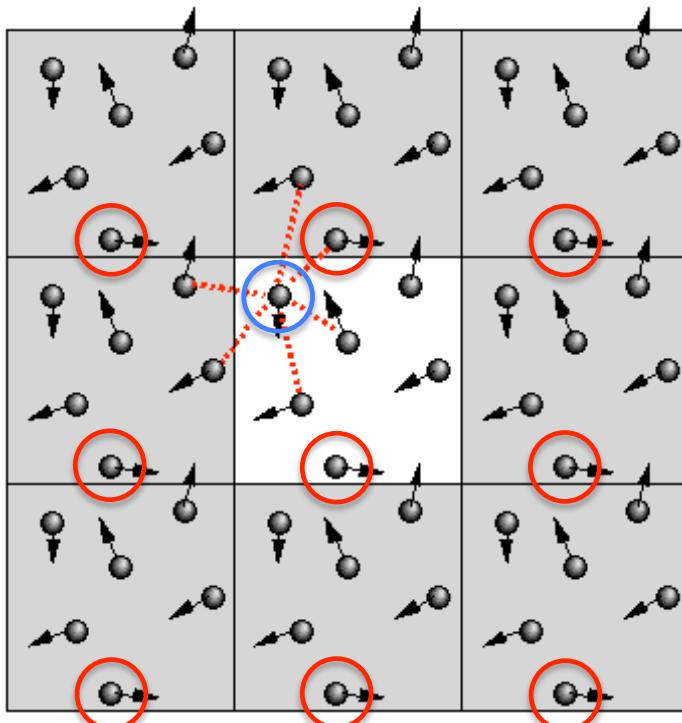


Jastrow factorOne-body part
(Mean-field WF)

Metropolis

Probability distribution, instead of Boltzmann weight

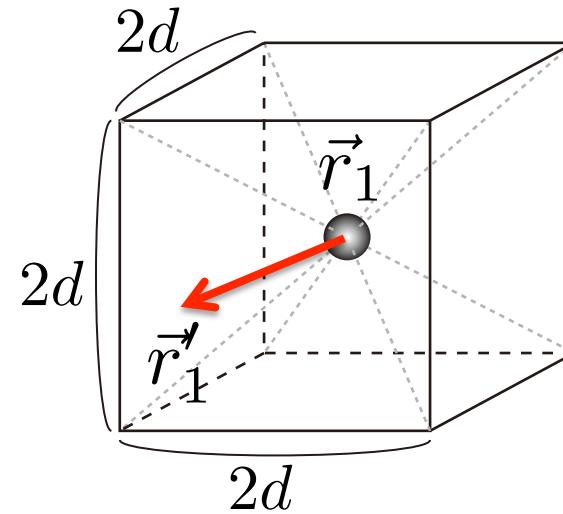
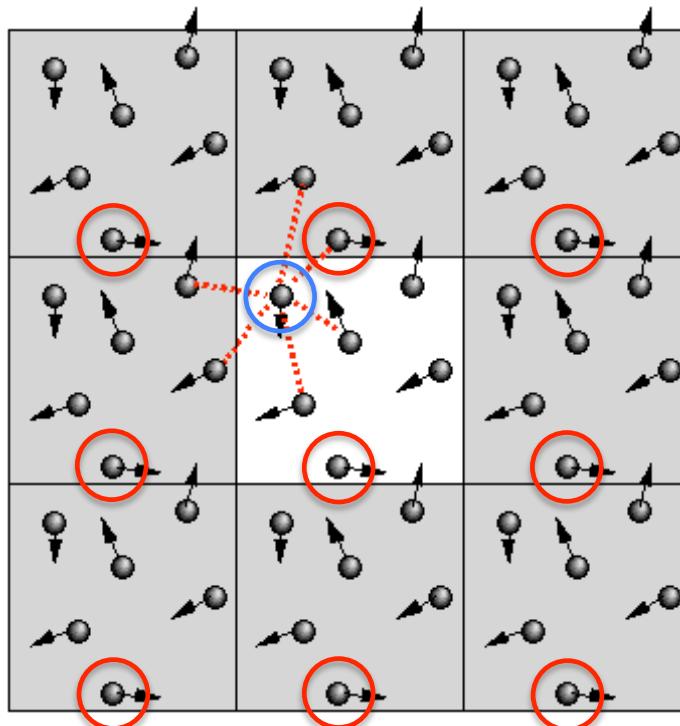
$$P_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \frac{|\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)|^2}{\int \prod_i d^3 r'_i |\psi(\vec{r}'_1, \vec{r}'_2, \dots, \vec{r}'_N)|^2}$$



Short-ranged interactions
→Nearest neighbor mirror image

cf.) For electron gas, Ewald summation

Trial Configuration



$$\vec{r}'_1 = \vec{r}_1 + d(\xi_1, \xi_2, \xi_3)^T \quad \xi_i \in [-1, 1]$$

$$\frac{P_N(\vec{r}'_1, \vec{r}_2, \dots, \vec{r}_N)}{P_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)} = \frac{|\psi(\vec{r}'_1, \vec{r}_2, \dots, \vec{r}_N)|^2}{|\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)|^2}$$

→ Metropolis algorithm

2 Point Distribution Function: $g(r)$

$$g(\vec{R}_1, \vec{R}_2) = \rho^{-2} \frac{\int \sum_{i \neq j} \delta(\vec{R}_1 - \vec{r}_i) \delta(\vec{R}_2 - \vec{r}_j) \psi(\vec{r}_1, \dots, \vec{r}_N)^2 \prod_{\ell=1}^N d^3 r_\ell}{\int \psi(\vec{r}_1, \dots, \vec{r}_N)^2 \prod_{\ell=1}^N d^3 r_\ell}, \quad (1)$$

where $\rho = N/\Omega$.

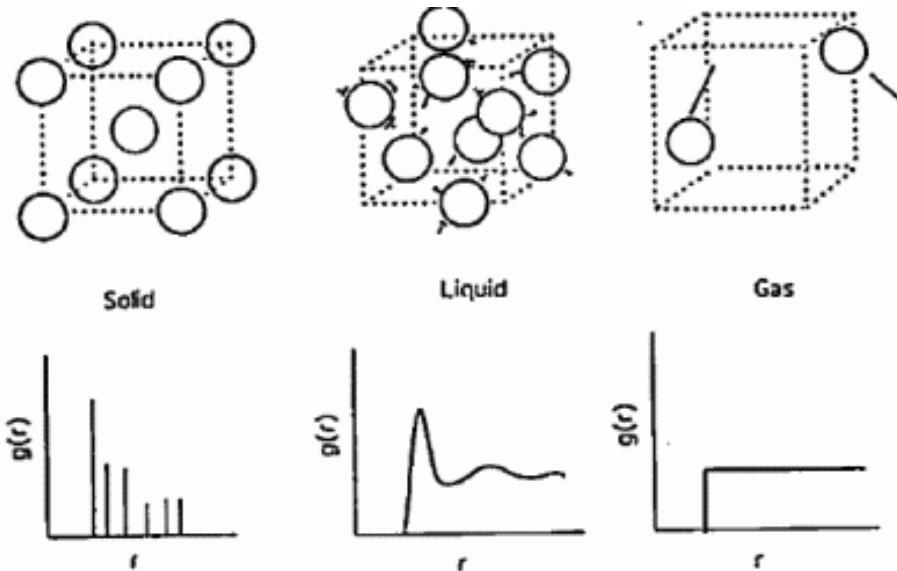
$$\begin{aligned} & \frac{1}{\Omega} \int d^3 R \int d(-\cos \theta) d\varphi \int_r^{r+\Delta r} dr' g(\vec{R} + \vec{r}', \vec{R}) \\ = & \rho^{-2} \frac{\frac{1}{\Omega} \int d^3 R \int d(-\cos \theta) d\varphi \int_r^{r+\Delta r} dr' \int \sum_{i \neq j} \psi(\vec{r}_1, \dots, \vec{r}_N)^2 |_{\vec{r}_i = \vec{R} + \vec{r}'}, \vec{r}_j = \vec{R}}{\int \psi(\vec{r}_1, \dots, \vec{r}_N)^2 \prod_{\ell=1}^N d^3 r_\ell} \\ \simeq & 4\pi r^2 \Delta r g(r) \end{aligned} \quad (2)$$

$$\simeq \rho^{-2} \frac{2}{\Omega} \frac{1}{M} \sum_{i=1}^M N_{[r, r+\Delta)}^{(i)}, \quad (3)$$

where we suppose translational invariance of the system. Here $N_{[r, r+\Delta)}^{(i)}$ is the number of particle pairs whose distances r' satisfy $r' \in [r, r + \Delta)$, in a particle configuration $R^{(i)}$.

2 Point Distribution Function: $g(r)$

Phase and $g(r)$



$g(r)$ of liquid ${}^4\text{He}$

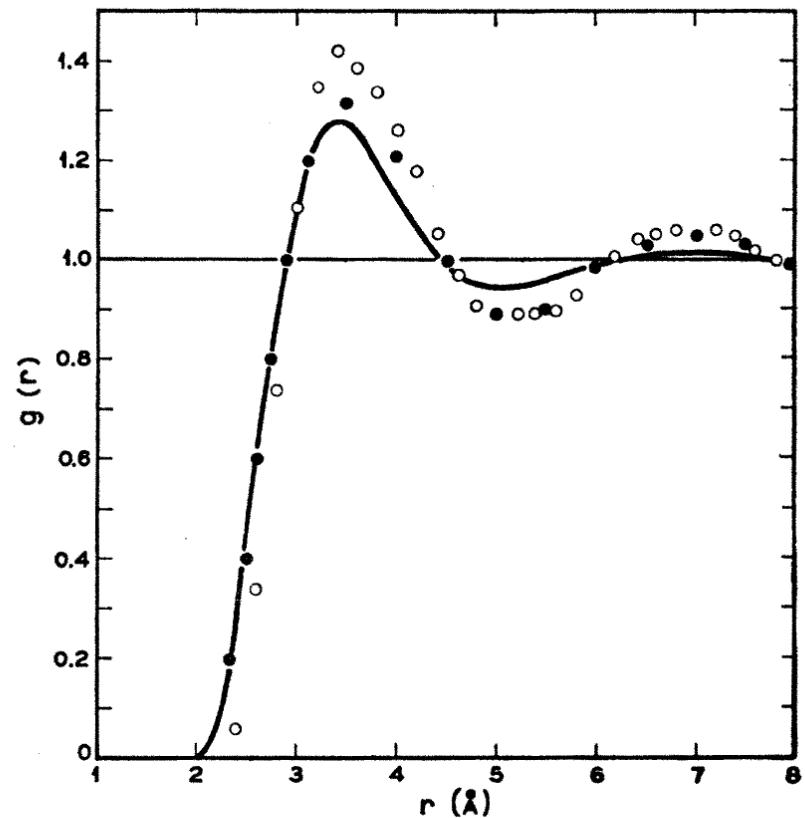
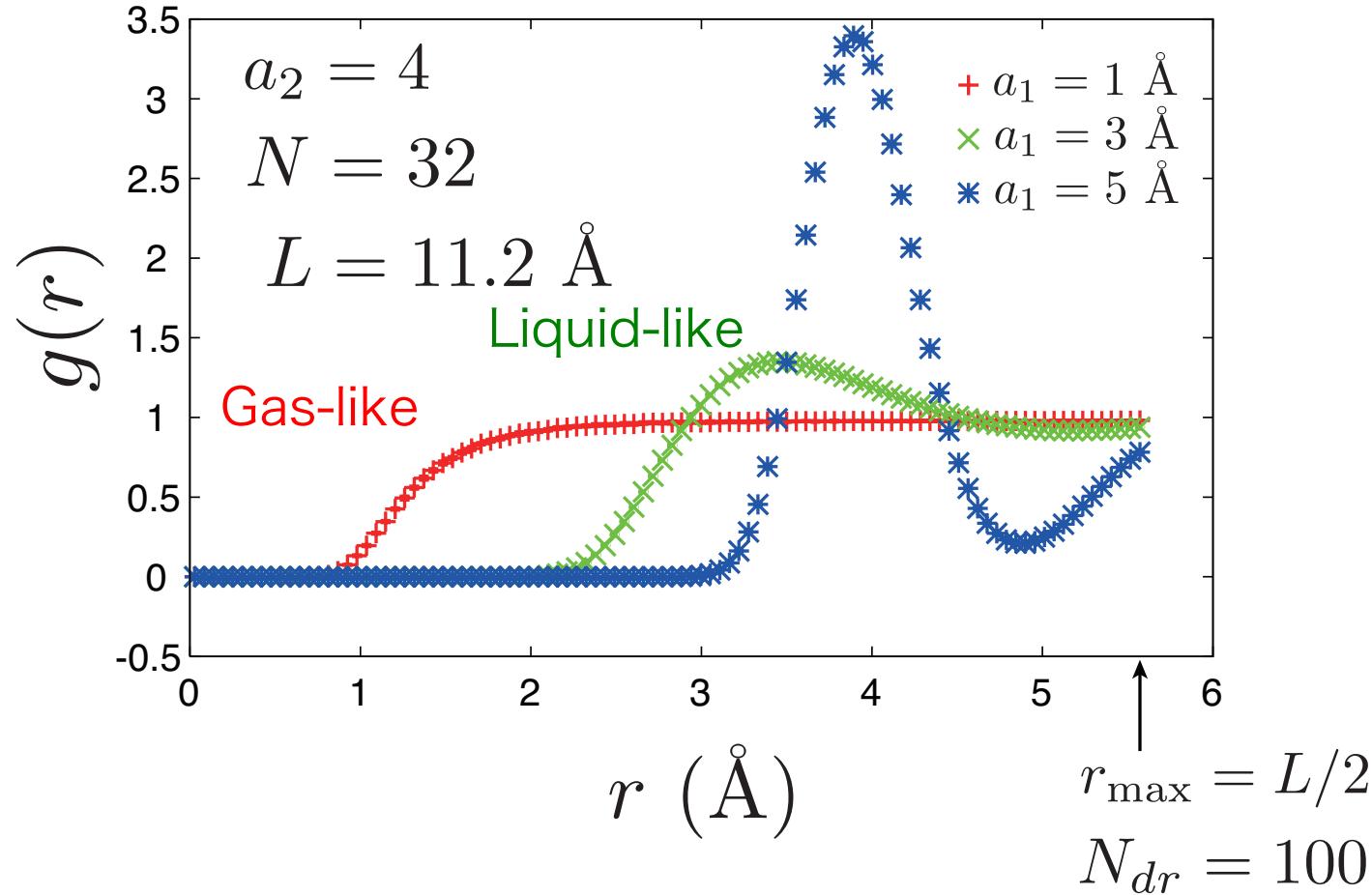


FIG. 5. Comparison of the two-body correlation function with experiment. The solid line is the theoretical curve, the solid circles are computed from the x-ray data of Gordon *et al.* (Ref. 26) and the open circles are computed from the neutron data of Henshaw (Ref. 27).

2 Point Distribution Function: $g(r)$



Comparison with Experiments

1. Energy

-Measure of accuracy

2. Two-point distribution function $g(r)$

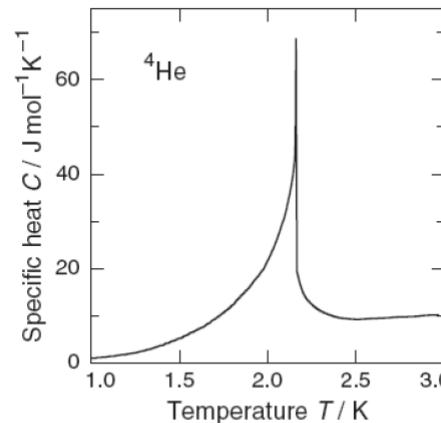
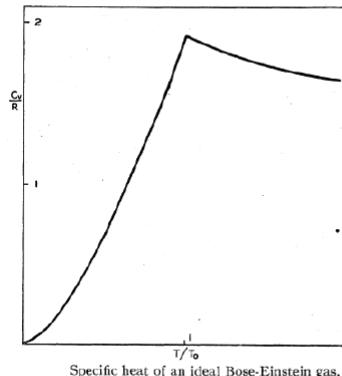
3. Structure factor (Fourier transformation of $g(r)$)

-*Structure* of liquid, observed by X ray/neutron diff.

4. Condensation fraction

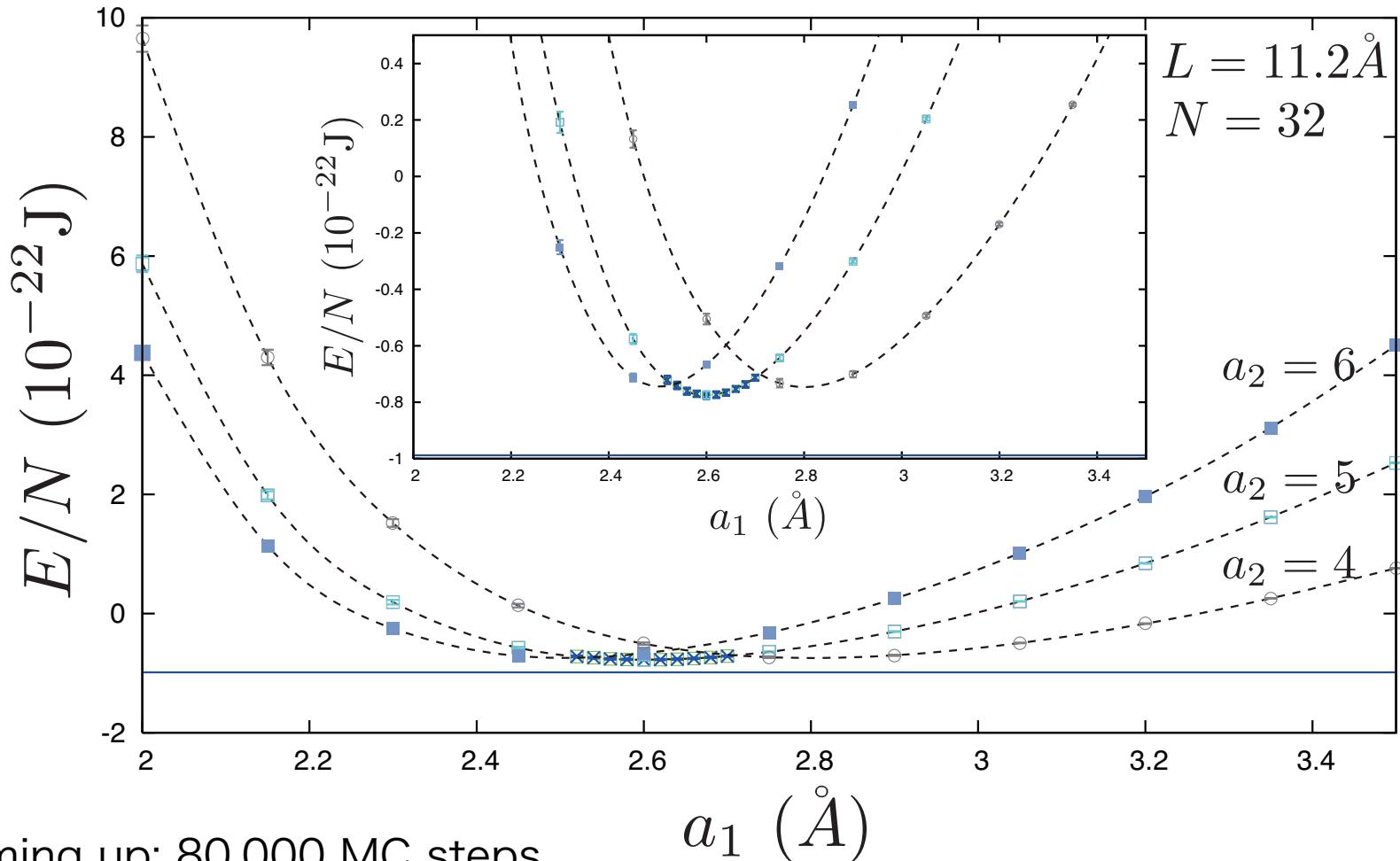
-Relation between Bose-Einstein condensation and He-II (superfluid phase)

Heat capacity: Ideal Bose gas and Liquid ^4He



Energy

$$\frac{E}{N} = \frac{1}{N} \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\rho}{2} \int \left[-\frac{\hbar^2}{2m_{^4\text{He}}} \nabla^2 \ln f(r) + V(r) \right] g(r) d^3r$$



Warming up: 80,000 MC steps
Sampling: 1,920,000 MC steps

How Is VWF Accurate?

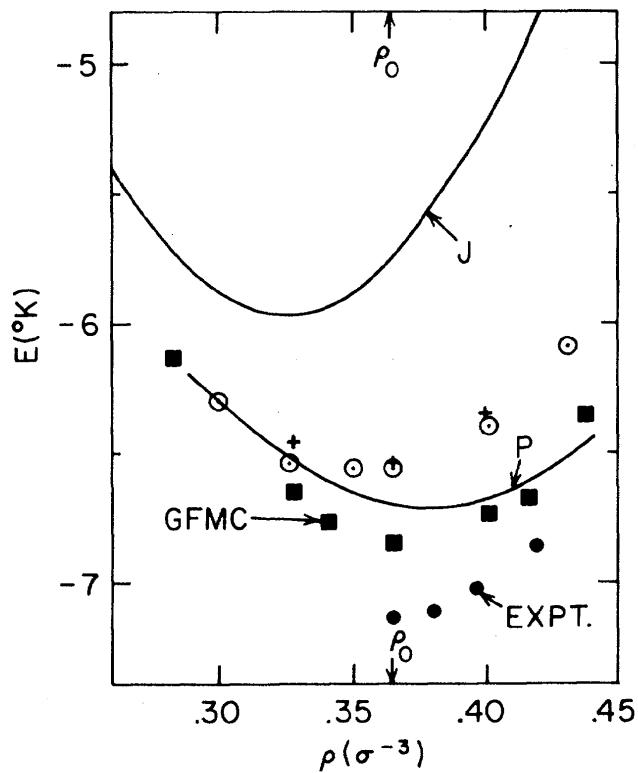


FIG. 1. Comparison of energy vs density. *J* indicates pure Jastrow results of Ref. 10; *P* indicates triplet calculations of Ref. 5; experimental results from Ref. 11; exact Lennard-Jones from Ref. 3; cross indicates present calculation; dot in circle indicates results from Ref. 4.

Origin of error:
-Choice of vwf
-LJ interaction

$$10^{-22} J = 7.246 \text{ K}$$

$$\rho_0 \sigma^3 = 0.3648$$

(Stable volume in experiment at zero pressure)

Density in the previous slide:
 $\rho \sigma^3 = 32 \times 2.556^3 / 11.2^3 = 0.380$

Liquid Helium 3 (fermion): LJ Hamiltonian

$$\hat{H} = \frac{\hbar^2}{2m_{^3\text{He}}} \sum_i \nabla_i^2 + \sum_{i < j; i,j=1}^N V(r_{ij})$$

$$r_{ij} \equiv |\vec{r}_i - \vec{r}_j|$$

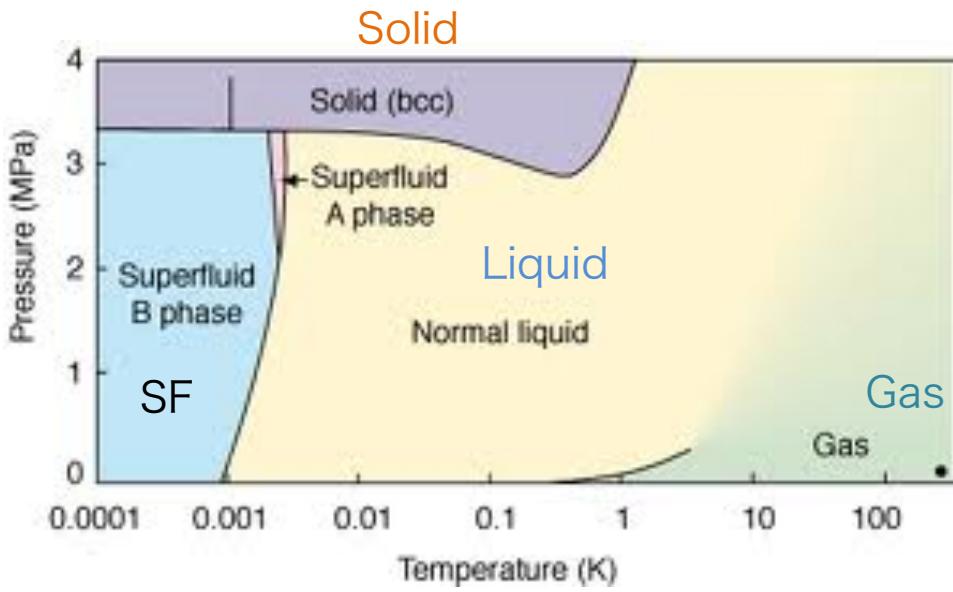
$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$$

$$m_{^3\text{He}}/\hbar^2 = \frac{3.01603}{4.00260} \times 0.597639 \times 10^{-42} \text{ J}^{-1} \cdot \text{m}^{-2}$$

$$\sigma = 2.556 \text{ \AA}$$

$$\epsilon = 1.41102 \times 10^{-22} \text{ J}$$

Phase diagram



VWF of Liquid Helium 3 ($S=1/2$ Fermion)

D. Ceperley, G. V. Chester, & M. H. Kalos, Phys. Rev. B 16, 3081 (1977)

Slater-Jastrow WF in 2nd quantization form (${}^3\text{He}$, electron gas)

$$|\Psi\rangle = \exp \left[-\frac{1}{2} \sum_{\sigma, \sigma'} \int d^3r d^3r' \color{red} u(|\vec{r} - \vec{r}'|) \right] \hat{\phi}_\sigma^\dagger(\vec{r}) \hat{\phi}_\sigma(\vec{r}) \hat{\phi}_{\sigma'}^\dagger(\vec{r}') \hat{\phi}_{\sigma'}(\vec{r}') \prod_{\vec{k} \in \text{FS}_\uparrow} \hat{c}_{\vec{k}\uparrow}^\dagger \prod_{\vec{k} \in \text{FS}_\downarrow} \hat{c}_{\vec{k}\downarrow}^\dagger |0\rangle$$

Jastrow factor

Slater determinant
(Mean-field WF)

Field operator $\hat{\phi}_\sigma(\vec{r}) = V^{-1/2} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \hat{c}_{\vec{k}\sigma}$

Commutation $\left\{ \hat{\phi}_\sigma(\vec{r}), \hat{\phi}_{\sigma'}^\dagger(\vec{r}') \right\} = \delta(\vec{r} - \vec{r}') \delta_{\sigma, \sigma'} \quad \left\{ \hat{c}_{\vec{k}\sigma}, \hat{c}_{\vec{k}'\sigma'}^\dagger \right\} = \delta_{\vec{k}, \vec{k}'} \delta_{\sigma, \sigma'}$

Relation to WF in 1st quantization form

$$\begin{aligned} & \psi(\vec{r}_1 \uparrow, \vec{r}_2 \uparrow, \dots, \vec{r}_{N_\uparrow} \uparrow; \vec{r}_{N_\uparrow+1} \downarrow, \vec{r}_{N_\uparrow+2} \downarrow, \dots, \vec{r}_{N_\uparrow+N_\downarrow} \downarrow) \\ &= \langle 0 | \hat{\phi}_\downarrow(\vec{r}_{N_\uparrow+N_\downarrow}) \cdots \hat{\phi}_\downarrow(\vec{r}_{N_\uparrow+2}) \hat{\phi}_\downarrow(\vec{r}_{N_\uparrow+1}) \hat{\phi}_\downarrow(\vec{r}_{N_\uparrow}) \cdots \hat{\phi}_\uparrow(\vec{r}_2) \hat{\phi}_\uparrow(\vec{r}_1) | \Psi \rangle \\ &= V^{-(N_\uparrow+N_\downarrow)/2} e^{-\sum_{i < j} f(r_{ij})} D_\uparrow D_\downarrow \end{aligned}$$

VWF of Liquid Helium 3 ($S=1/2$ Fermion)

1 st quantiztion VWF

$$\begin{aligned} \psi(\vec{r}_1 \uparrow, \vec{r}_2 \uparrow, \dots, \vec{r}_{N_\uparrow} \uparrow; \vec{r}_{N_\uparrow+1} \downarrow, \vec{r}_{N_\uparrow+2} \downarrow, \dots, \vec{r}_{N_\uparrow+N_\downarrow} \downarrow) \\ = V^{-(N_\uparrow+N_\downarrow)/2} e^{-\sum_{i < j} f(r_{ij})} D_\uparrow D_\downarrow \end{aligned}$$

Slater determinant originating from Fermi statistics

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

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

Jastrow VWF for Liquid Helium 3

Replace mean-field WF in Jastrow vwf for ${}^4\text{He}$:
Bose condensate \rightarrow Fermi sea (Slater determinant)

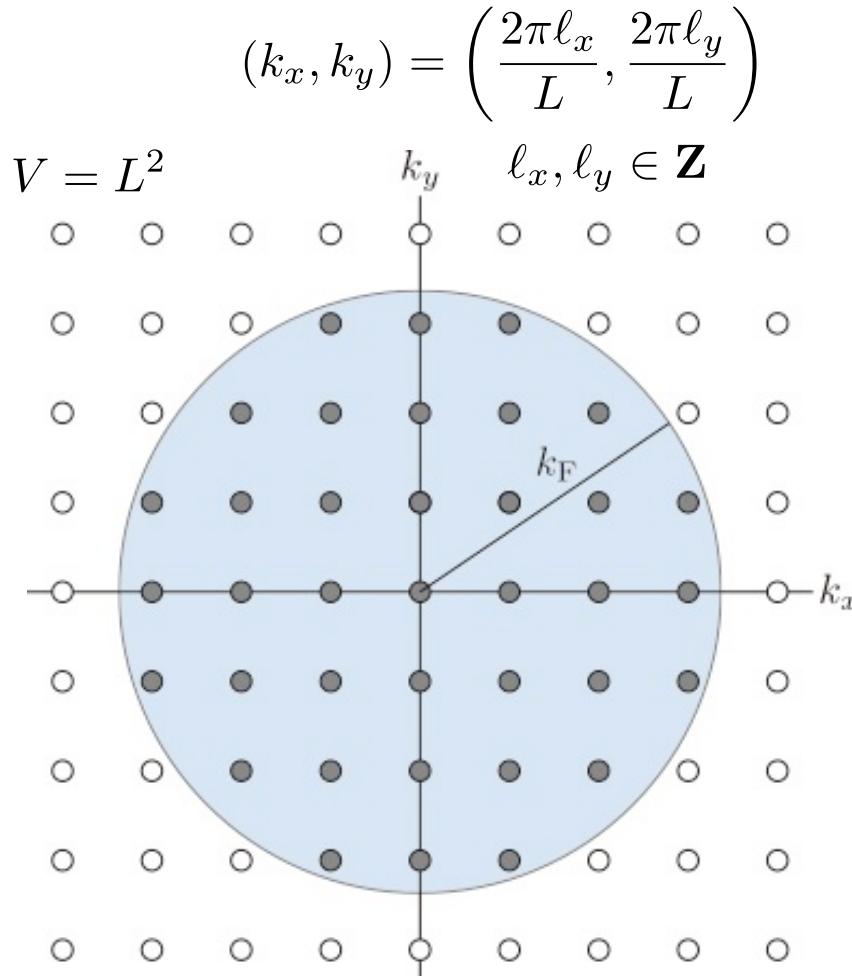
$$\begin{aligned}\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_\uparrow+N_\downarrow}) = & \psi_B(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_\uparrow+N_\downarrow}) \\ & \times D_\uparrow(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_\uparrow}) D_\downarrow(\vec{r}_{N_\uparrow+1}, \dots, \vec{r}_{N_\uparrow+N_\downarrow})\end{aligned}$$

Bosonic wf:

$$\psi_B(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_\uparrow+N_\downarrow}) = \exp \left[- \sum_{i < j; i, j=1}^{N_\uparrow+N_\downarrow} (a_1 / |\vec{r}_i - \vec{r}_j|)^{a_2} \right]$$

Fermi Sea

Fermi sea: WF for free fermions



37 k points
74 electrons

k_F : Fermi wave number

$$V = L^3$$

$$(k_x, k_y, k_z) = \left(\frac{2\pi\ell_x}{L}, \frac{2\pi\ell_y}{L}, \frac{2\pi\ell_z}{L} \right)$$
$$\ell_x, \ell_y, \ell_z \in \mathbf{Z}$$

2 dimensional case for simplicity

Updating Particle Configuration in Slater Determinant

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

Update location of particle: $\vec{r}_1 \rightarrow \vec{r}'_1$

Cost of calc. determinant: $O(N_{\uparrow} !)$ or $O(N_{\uparrow}^3)$

cf.) Update of $f(r_{ij}) : O(N_{\uparrow})$

$\leftarrow O(N_{\uparrow}^2)$ method: Sherman-Morrison formula

Sherman-Morrison

$$(A + \vec{u}\vec{v}^T)^{-1} = A^{-1} - \frac{A^{-1}\vec{u}\vec{v}^T A^{-1}}{1 + \vec{v}^T A^{-1} \vec{u}}$$
$$\det(A + \vec{u}\vec{v}^T) = (1 + \vec{v}^T A^{-1} \vec{u})\det A$$

Update location of particle: $\vec{r}_1 \rightarrow \vec{r}'_1$

$$A = D_{\uparrow}$$
$$\vec{u}^T = (1, 0, \dots, 0)$$
$$\vec{v}^T = (e^{i\vec{k}_1 \cdot \vec{r}'_1}, e^{i\vec{k}_2 \cdot \vec{r}'_1}, \dots, e^{i\vec{k}_{N_{\uparrow}} \cdot \vec{r}'_1}) - (e^{i\vec{k}_1 \cdot \vec{r}_1}, e^{i\vec{k}_2 \cdot \vec{r}_1}, \dots, e^{i\vec{k}_{N_{\uparrow}} \cdot \vec{r}_1})$$
$$D_{\uparrow} = \det \begin{bmatrix} e^{i\vec{k}_1 \cdot \vec{r}_1} & e^{i\vec{k}_2 \cdot \vec{r}_1} & \dots & e^{i\vec{k}_{N_{\uparrow}} \cdot \vec{r}_1} \\ e^{i\vec{k}_1 \cdot \vec{r}_2} & e^{i\vec{k}_2 \cdot \vec{r}_2} & \dots & e^{i\vec{k}_{N_{\uparrow}} \cdot \vec{r}_2} \\ \vdots & \vdots & & \vdots \\ e^{i\vec{k}_1 \cdot \vec{r}_{N_{\uparrow}}} & e^{i\vec{k}_2 \cdot \vec{r}_{N_{\uparrow}}} & \dots & e^{i\vec{k}_{N_{\uparrow}} \cdot \vec{r}_{N_{\uparrow}}} \end{bmatrix}$$

Keep and update determinant and inverse, simultaneously
by $O(N_{\uparrow}^2)$ matrix-vecotr

Essential Parameters for Simulations

```
integer :: Nup,Ndn ! # of particle with ↑ -spin, ↓ -spin
real(8) :: L ! linear scale of cubic cell (Å)
real(8) :: a1, a2 ! variational parameters
integer :: M ! # of MC steps
integer :: Nwup ! # of warming-up steps
```

Sample space

$$\vec{R} = (\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_\uparrow + N_\downarrow})$$

```
real(8) :: config_new(1:3,1:Nup+Ndn)
```

```
real(8) :: config_old(1:3,1:Nup+Ndn)
```

Information to calc. Jastrow factor

$$|\vec{r}_i - \vec{r}_j|$$

```
real(8) :: list_dist_new(1:Nup+Ndn,1:Nup+Ndn)
```

```
real(8) :: list_dist_old(1:Nup+Ndn,1:Nup+Ndn)
```

Occupied momenta

```
real(8) :: arrayk(1:3,1:Ne=Nup+Ndn)
```

Slater determinant

```
complex(8) :: Phiup(:, :, :), Phidn(:, :, :)
```

```
complex(8) :: Dup=det(Phiup), Ddn=det(Phidn)
```

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

Iteration Steps

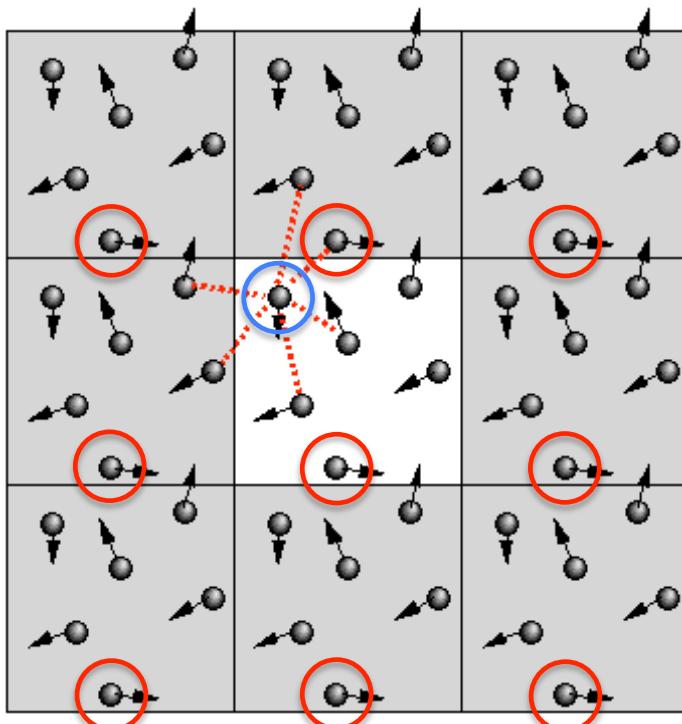
1. Generate initial config. `config_old` and `Dup` & `Ddn`
2. Generate `list_dist_old` from `config_old`
3. Generate `config_new` from `config_old` by Metropolis and Update `list_dist_new` from `list_dist_old` (`Nup +Ndn` times)
4. Update `Dup` & `Ddn` by Sherman-Morrison
5. Calc. physical quantities from `config_new`, `list_dist_new`, `Dup` & `Ddn`
6. Go back to 3. until M MC steps

* Warming up: Skipping 5.

Metropolis

Probability distribution, instead of Boltzmann weight

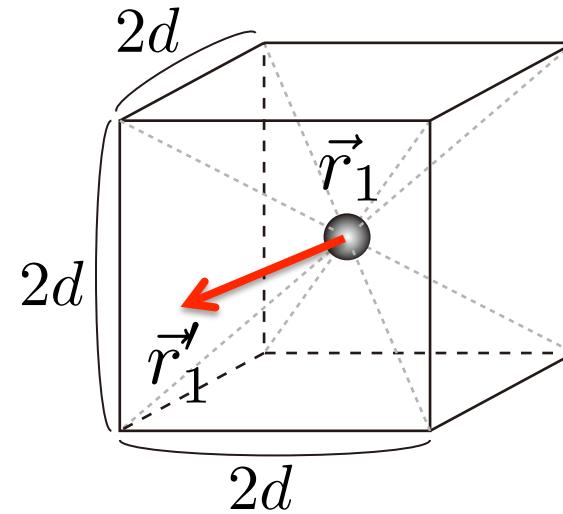
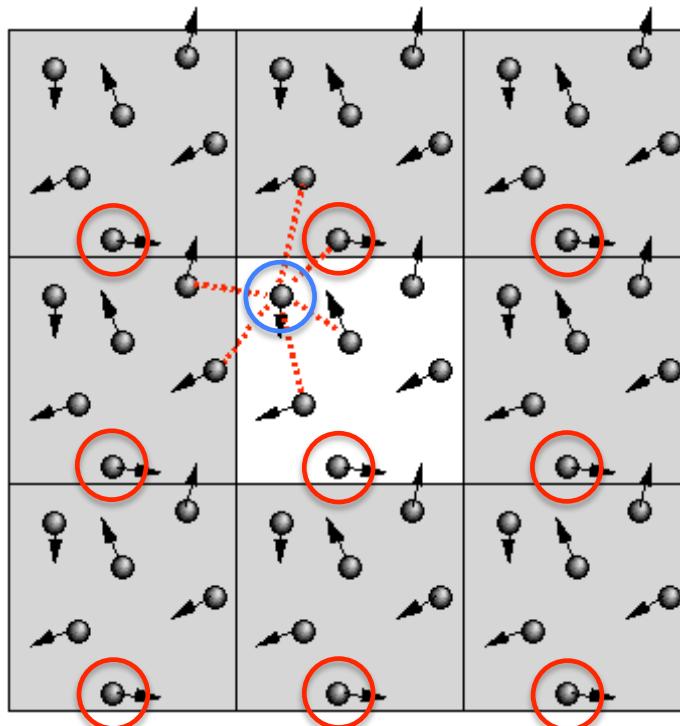
$$P_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \frac{|\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)|^2}{\int \prod_i d^3 r'_i |\psi(\vec{r}'_1, \vec{r}'_2, \dots, \vec{r}'_N)|^2}$$



Short-ranged interactions
→Nearest neighbor mirror image

cf.) For electron gas, Ewald summation

Trial Configuration



$$\vec{r}'_1 = \vec{r}_1 + d(\xi_1, \xi_2, \xi_3)^T \quad \xi_i \in [-1, 1]$$

$$\frac{P_N(\vec{r}'_1, \vec{r}_2, \dots, \vec{r}_N)}{P_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)} = \frac{|\psi(\vec{r}'_1, \vec{r}_2, \dots, \vec{r}_N)|^2}{|\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)|^2}$$

→ Metropolis algorithm

Spin Resolved $g(r)$: $g_{\text{L}}(r)$ & $g_{\text{U}}(r)$

Parallel spins $\uparrow \uparrow$

$$g_{\text{L}}(\vec{x}_1, \vec{x}_2) = 2\rho^{-2} \left\langle \sum_{i \neq j < N_{\uparrow}+1} \delta(\vec{x}_1 - \vec{r}_i) \delta(\vec{x}_2 - \vec{r}_j) \right\rangle$$

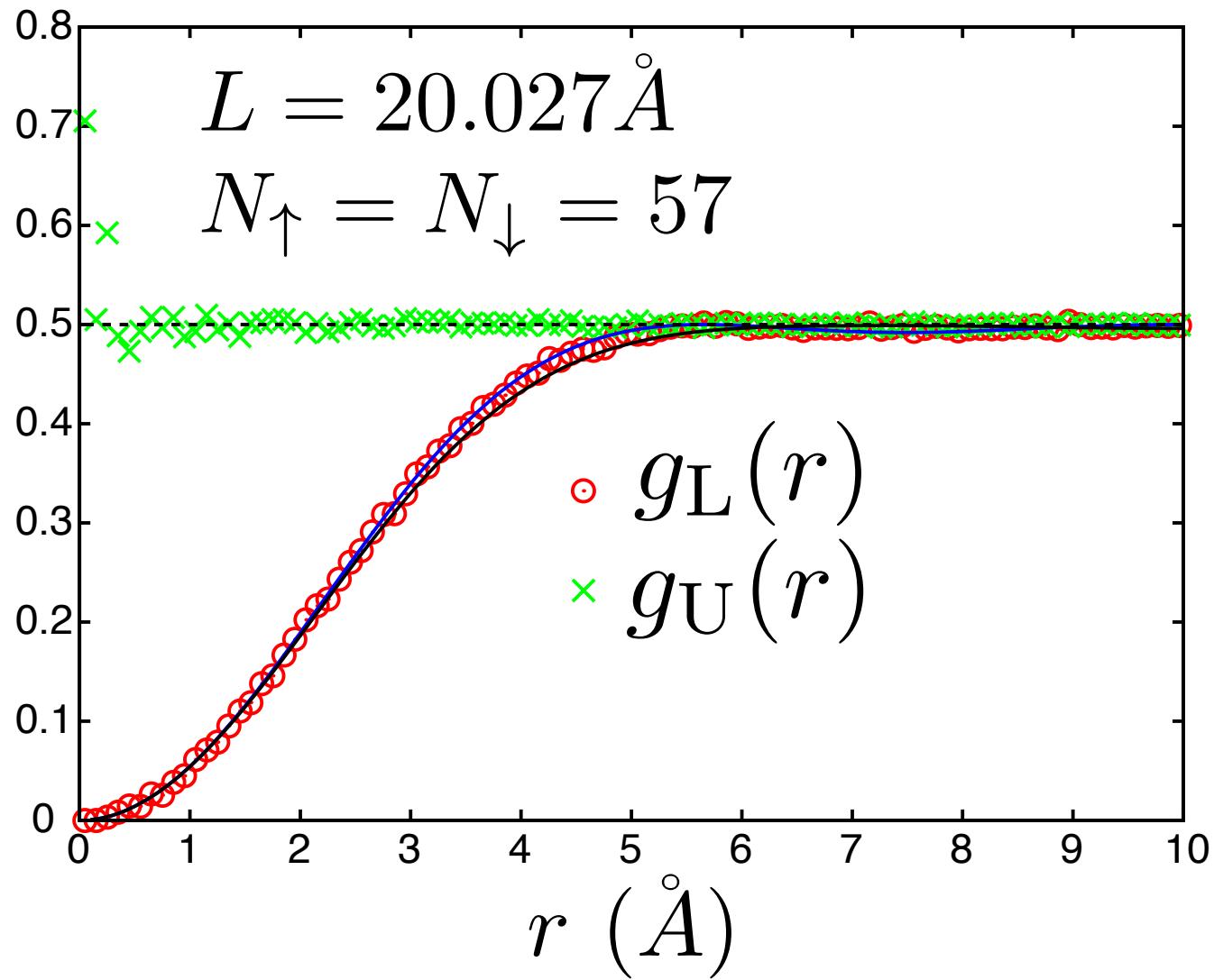
Antiparallel spins $\uparrow \downarrow$

$$g_{\text{U}}(\vec{x}_1, \vec{x}_2) = \rho^{-2} \left\langle \sum_{i=1}^{N_{\uparrow}} \sum_{j=N_{\uparrow}+1}^{N_{\uparrow}+N_{\downarrow}} \delta(\vec{x}_1 - \vec{r}_i) \delta(\vec{x}_2 - \vec{r}_j) \right\rangle$$

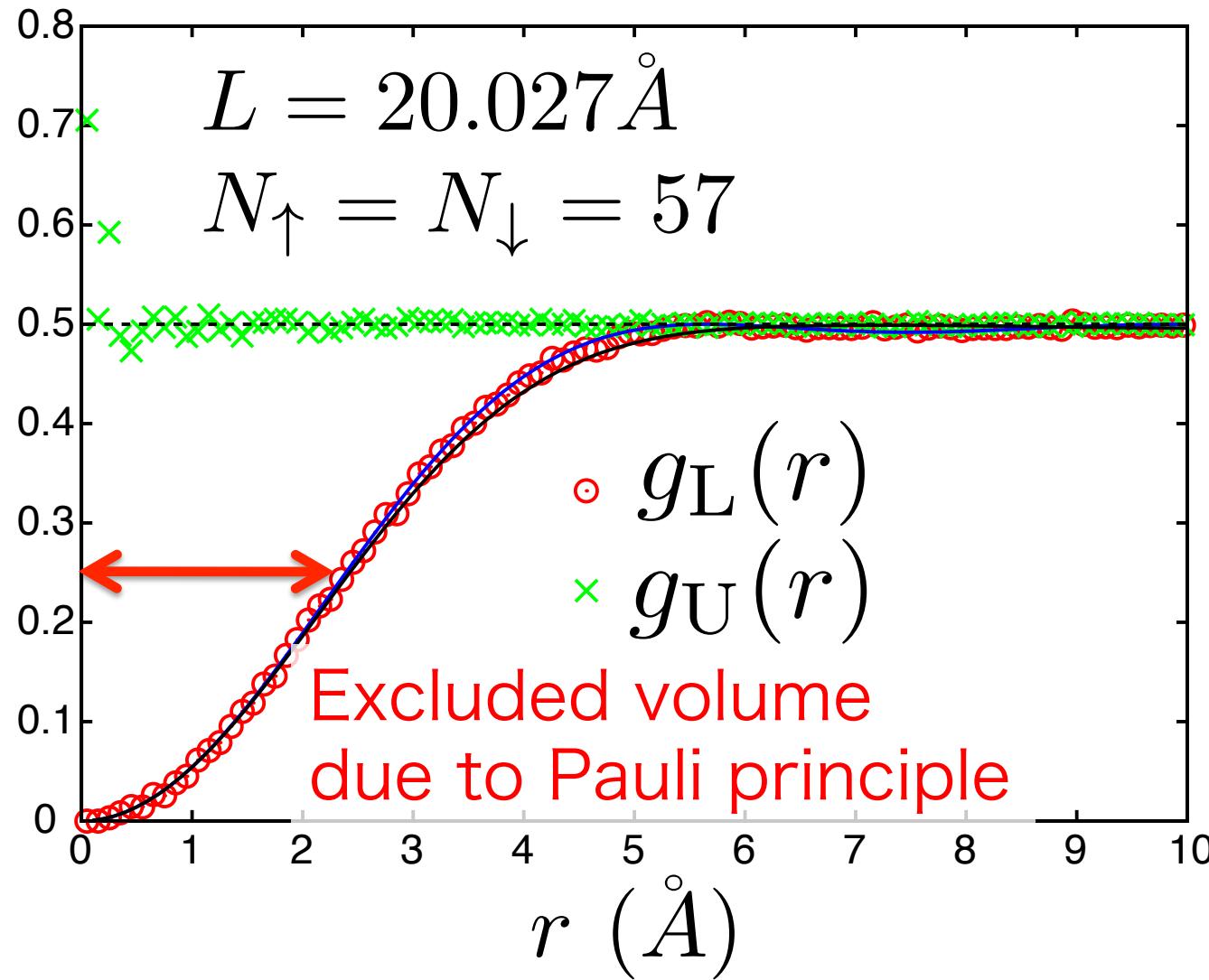
Expectation value

$$\langle F \rangle = \frac{\int \psi(\vec{R})^* F \psi(\vec{R}) \prod_{i=1}^{N_{\uparrow}+N_{\downarrow}} d^3 r_i}{\int |\psi(\vec{R})| \prod_{i=1}^{N_{\uparrow}+N_{\downarrow}} d^3 r_i} \simeq \frac{1}{M} \sum_{I=1}^M F_{\vec{R}_I}$$

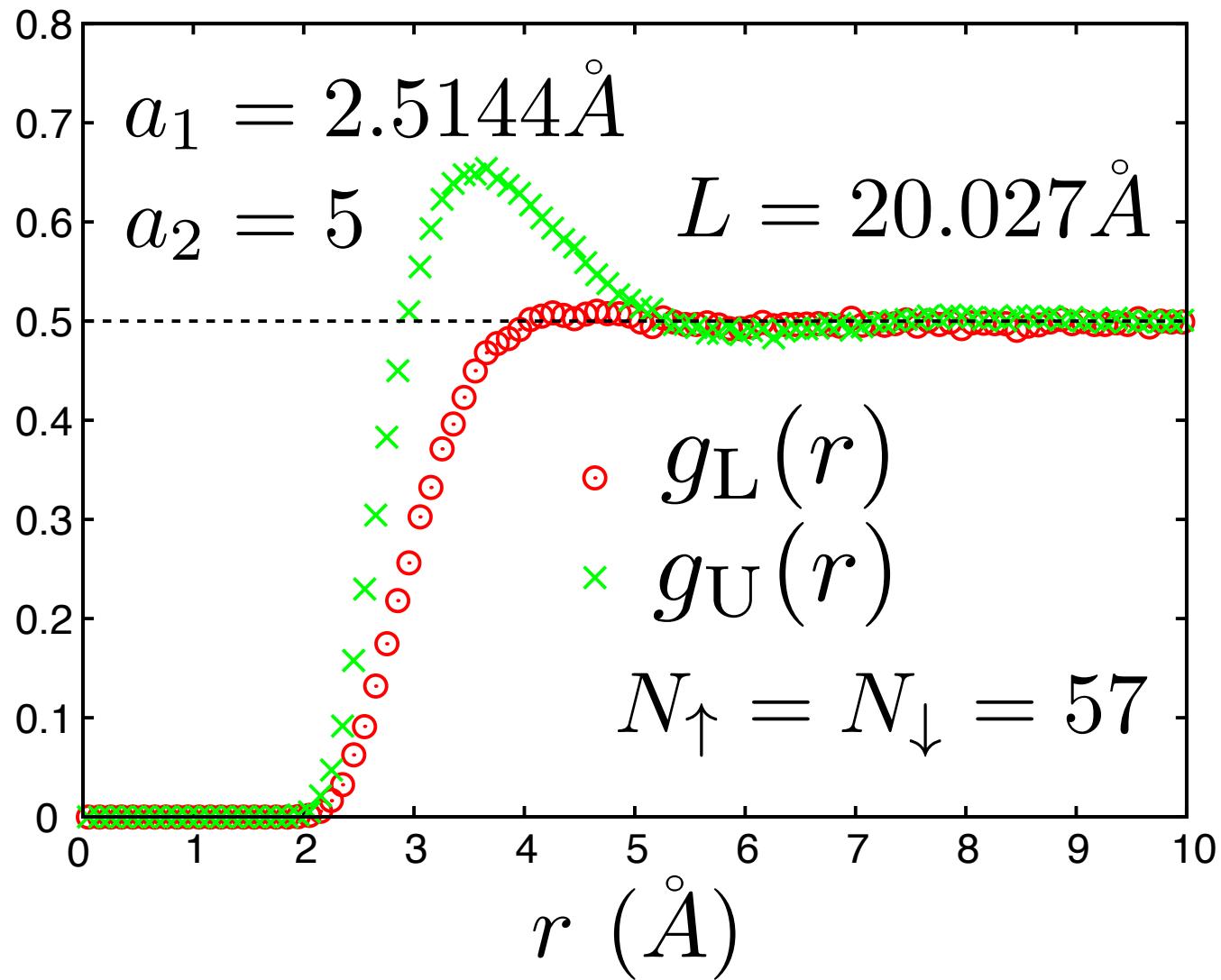
Free Fermions



Exchange Hole Due to Pauli Principle



Liquid Helium 3



Many-Body Effect: Correlation Hole

