

多体問題の計算科学

Computational Science for Many-Body Problems

#8 Quantum Monte Carlo methods

15:10-16:40 June 8, 2022

Quantum Monte Carlo Methods

0. Lattice model of solids

1. QMC

-Variational MC

Quantum Monte Carlo

Quantum Monte Carlo Methods

Monte Carlo Integration for Quantum Systems

-Inner product/expectation value of operators

- Variational MC+diffusion MC/Green's function MC

-Action/partition function

- Imaginary-time path integral

Quantum Monte Carlo Methods

Typical examples of QMC

■ Variational MC+diffusion MC/Green's function MC

No sign problems, but depend on variational wave functions

McMillan (^4He , 1965)

Ceperley-Chester-Kalos (^3He , 1977)

cf.) CASINO <https://vallico.net/casinoqmc/>

■ Imaginary-time path integral by Suzuki-Trotter decomposition

- D -dimensional Transverse field Ising model:

Mapped on $(D+1)$ -dimensional classical Mote Carlo

- Variation: Continuous-time MC, World line MC…
(implemented in ALPS)

- Power Lanczos by QMC (projective Monte Carlo)

Serious limitation: Sign *problems*

Bosons and fermions:

Blankenbecler-Scalapino-Sugar (1981)

Hirsch (1985)

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

$$\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$$

• Volume: L^3

• Discretization: $L^{3N} \rightarrow M^{3N} \times (L/M)^{3N}$
→ $O(M^{3N})$ Riemann sum

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

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

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

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

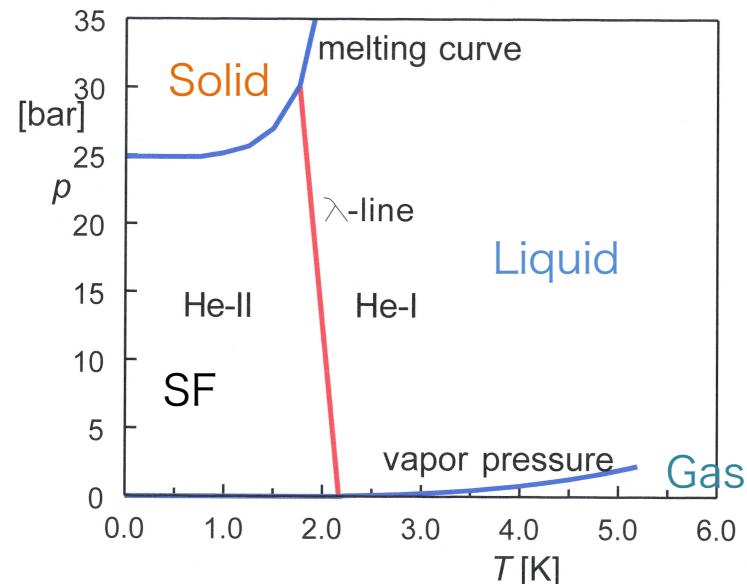
$$m_{^4}\text{He}/\hbar^2 = 0.597639 \times 10^{22} \text{ J}^{-1} \cdot \text{\AA}^{-2}$$

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

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

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

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

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

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

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

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

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

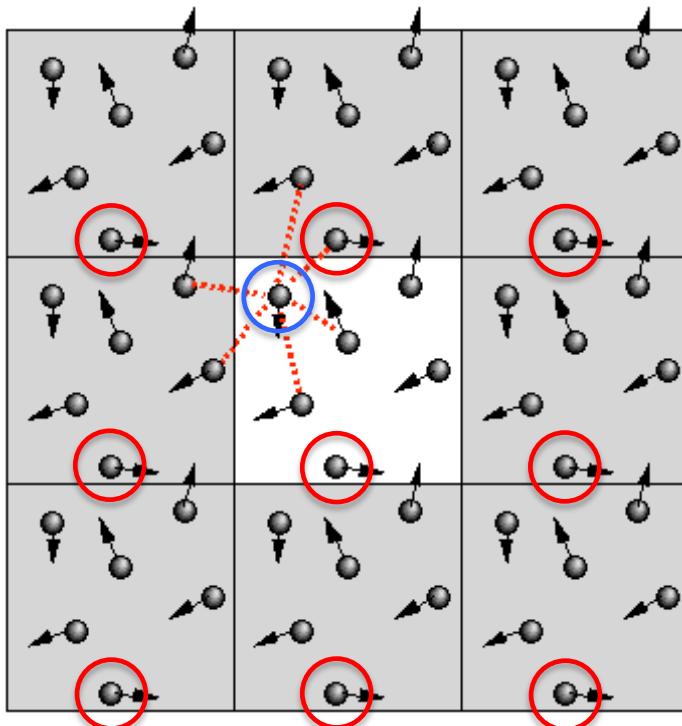
Weight/probability $P_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \frac{1}{V^N} \frac{|\langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N | \Psi \rangle|^2}{\langle \Psi | \Psi \rangle}$

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

Metropolis

Probability distribution, instead of Boltzmann weight

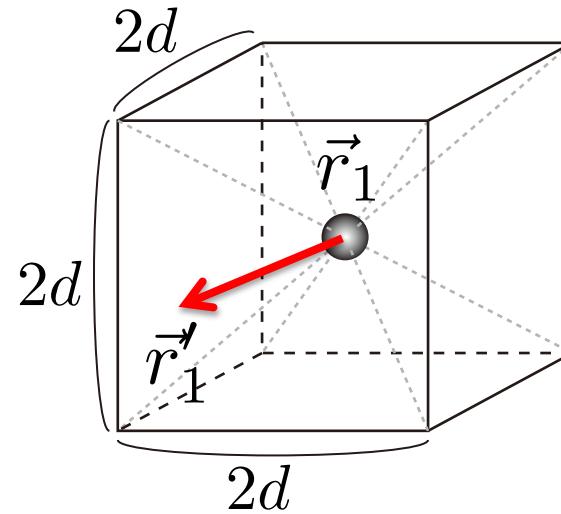
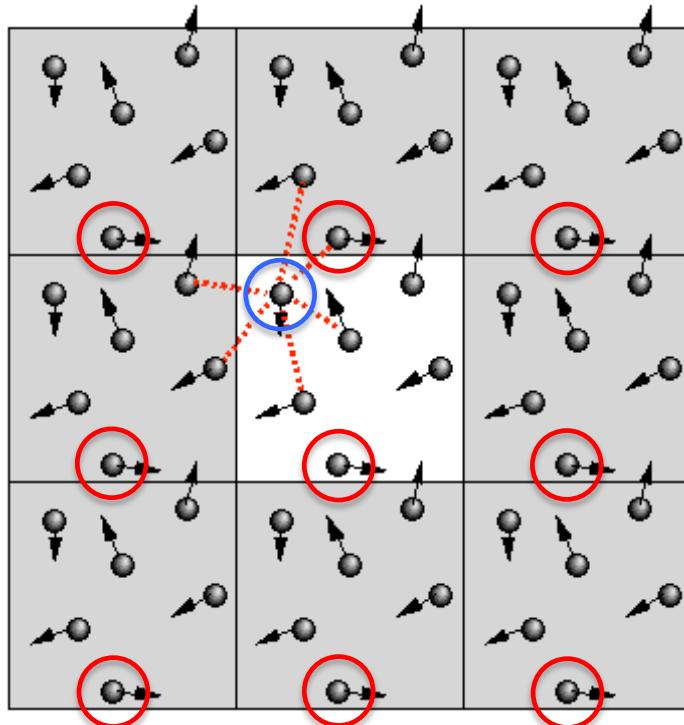
$$P_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \frac{|\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)|^2}{\int \prod_i d^3 r'_i |\psi(\vec{r}'_1, \vec{r}'_2, \dots, \vec{r}'_N)|^2}$$



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 $\rho = N/\Omega$.

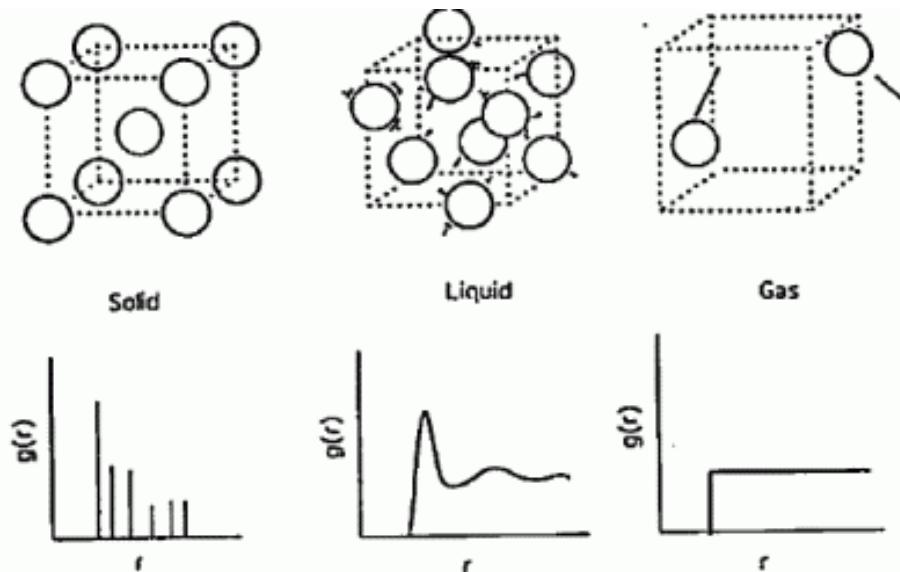
$$\begin{aligned} & \frac{1}{\Omega} \int d^3 R \int d(-\cos \theta) d\varphi \int_r^{r+\Delta r} dr' g(\vec{R} + \vec{r}', \vec{R}) \\ &= \rho^{-2} \frac{\frac{1}{\Omega} \int d^3 R \int d(-\cos \theta) d\varphi \int_r^{r+\Delta r} dr' \int \sum_{i \neq j} \psi(\vec{r}_1, \dots, \vec{r}_N)^2 |_{\vec{r}_i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

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

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 ${}^4\text{He}$

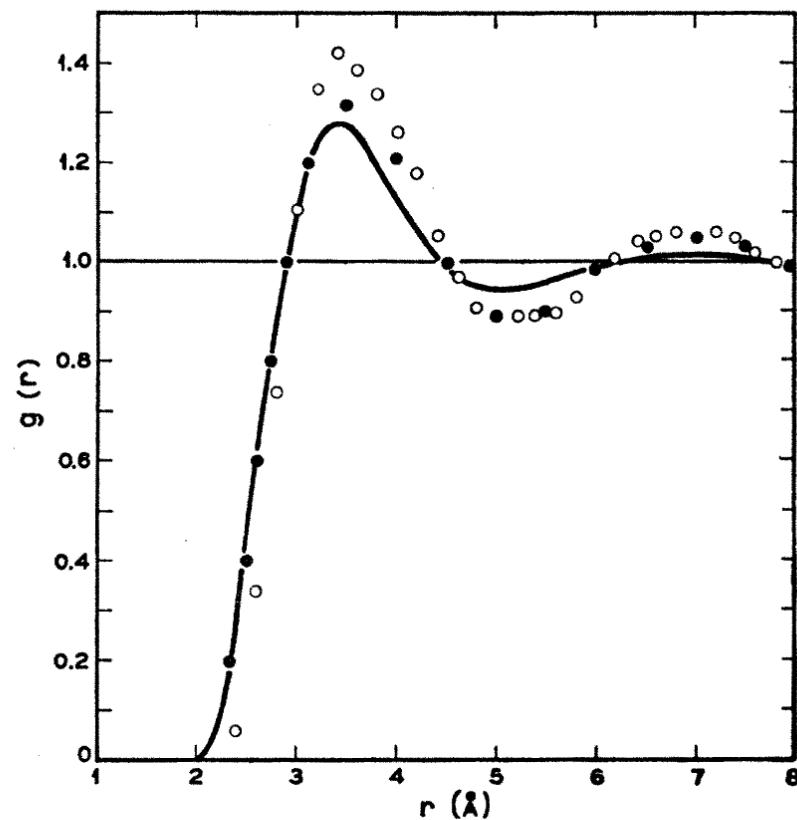
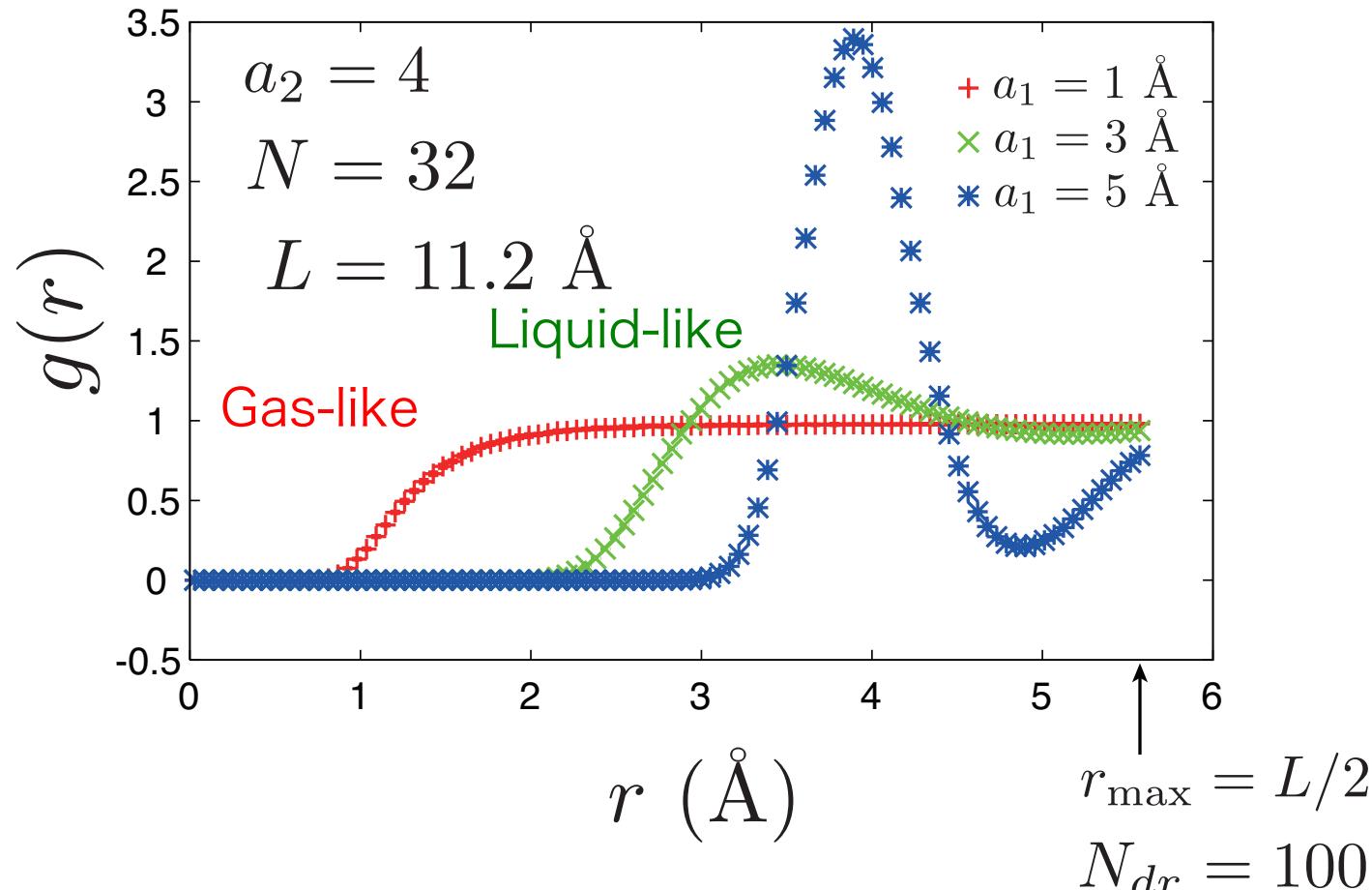


FIG. 5. Comparison of the two-body correlation function with experiment. The solid line is the theoretical curve, the solid circles are computed from the x-ray data of Gordon *et al.* (Ref. 26) and the open circles are computed from the neutron data of Henshaw (Ref. 27).

2 Point Distribution Function: $g(r)$



Volume per particle: 43.904 \AA^3

$$\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \prod_{i < j; i,j=1}^N f(r_{ij})$$
$$f(r) = \exp [-(a_1/r)^{a_2}]$$

Comparison with Experiments

1. Energy

-Measure of accuracy

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

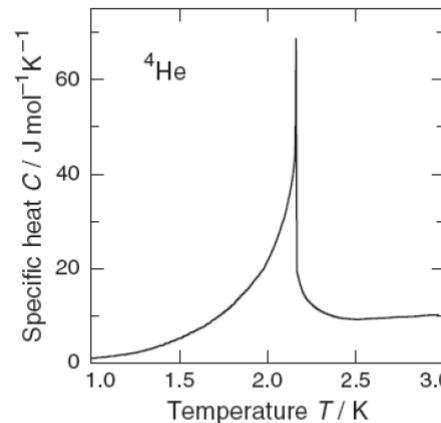
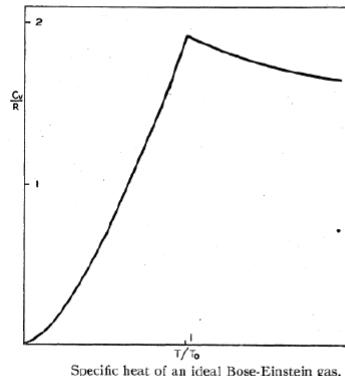
3. Structure factor (Fourier transformation of $g(r)$)

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

4. Condensation fraction

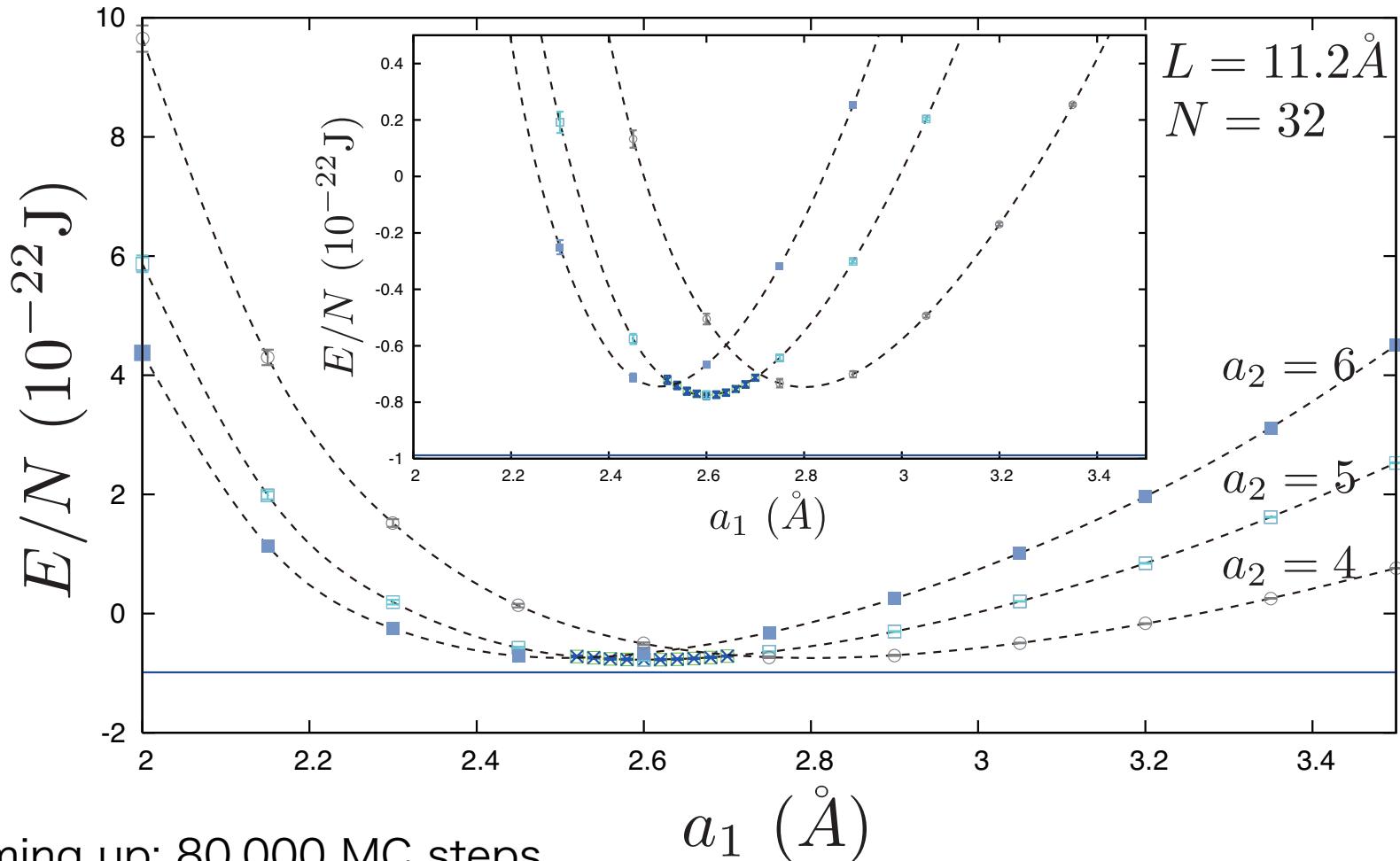
-Relation between Bose-Einstein condensation and He-II (superfluid phase)

Heat capacity: Ideal Bose gas and Liquid ^4He



Energy

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



How Is VWF Accurate?

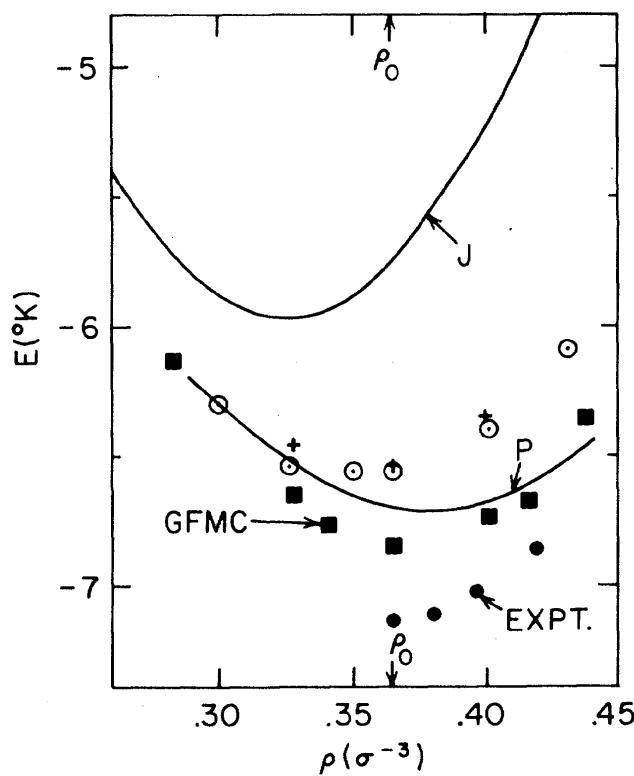


FIG. 1. Comparison of energy vs density. *J* indicates pure Jastrow results of Ref. 10; *P* indicates triplet calculations of Ref. 5; experimental results from Ref. 11; exact Lennard-Jones from Ref. 3; cross indicates present calculation; dot in circle indicates results from Ref. 4.

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:
 $\rho \sigma^3 = 32 \times 2.556^3 / 11.2^3 = 0.380$

Sample Code for ${}^4\text{He}$

vmc_helium4_2021.ipynb

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

- Simple implementation of McMillan's VMC
- You can run it on Google colaboratory

Output: $g(r)$

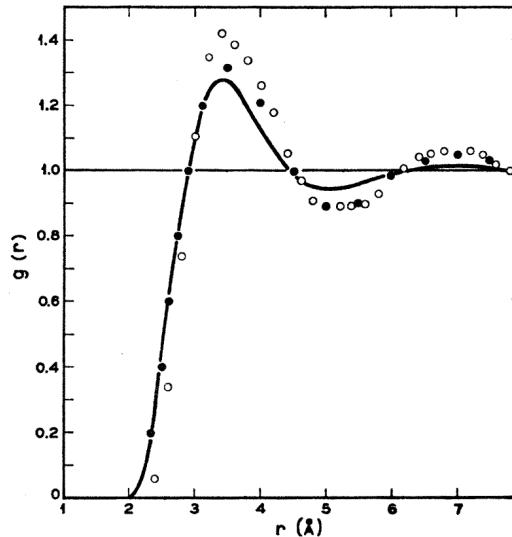


FIG. 5. Comparison of the two-body correlation function with experiment. The solid line is the theoretical curve, the solid circles are computed from the x-ray data of Gordon *et al.* (Ref. 26) and the open circles are computed from the neutron data of Henshaw (Ref. 27).

Liquid Helium 3 (fermion): LJ Hamiltonian

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

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

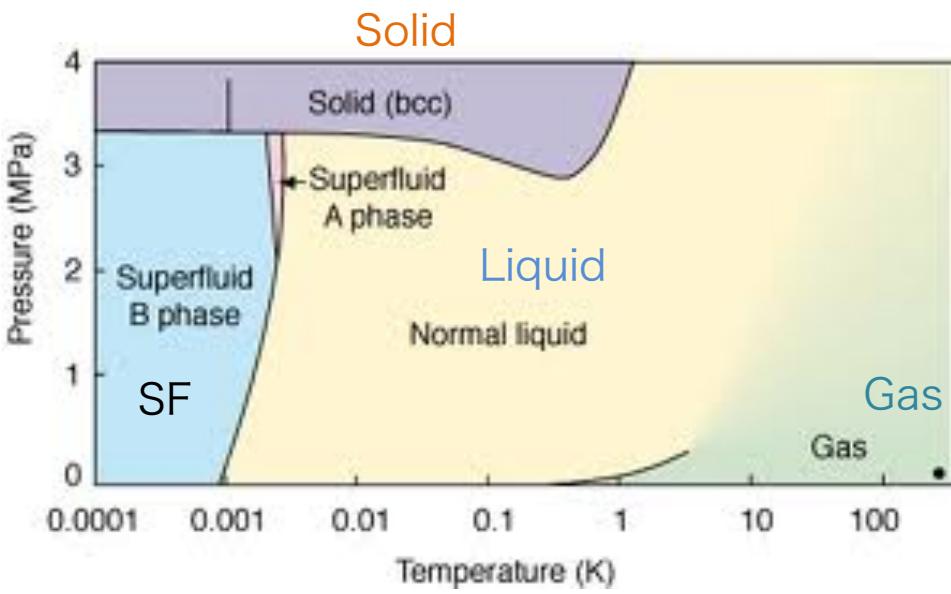
$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$$

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

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

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

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

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

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

1 st quantiztion VWF

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

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)

.

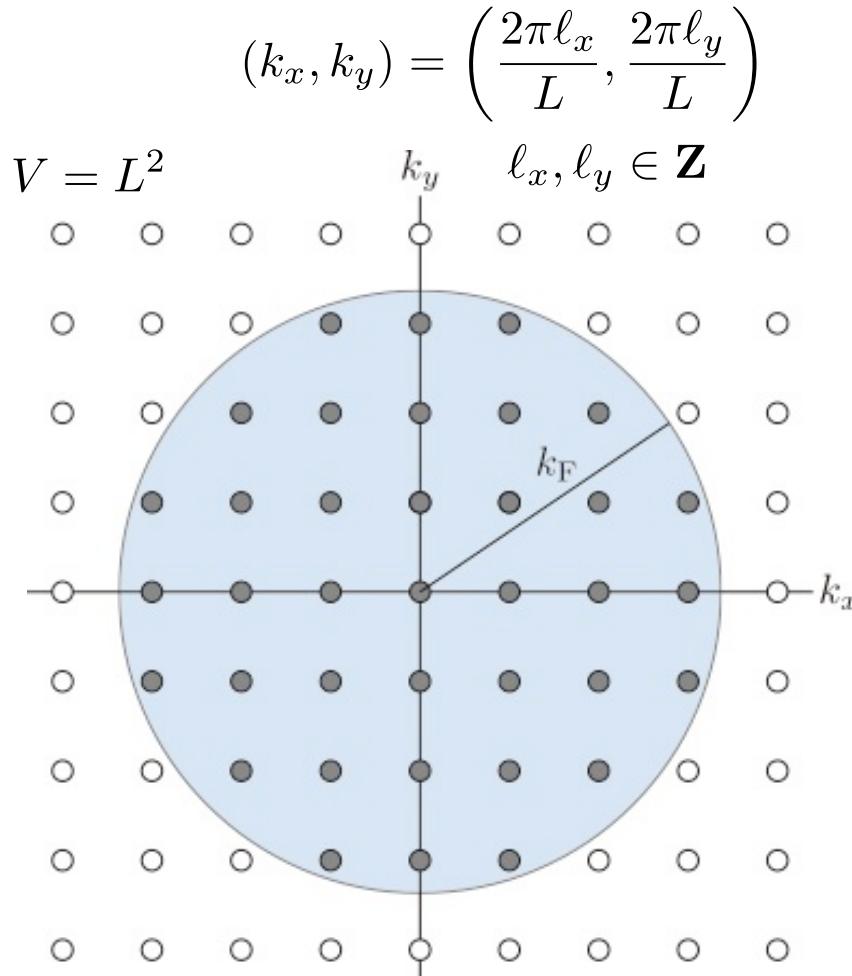
$$\begin{aligned}\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_\uparrow+N_\downarrow}) = & \psi_B(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_\uparrow+N_\downarrow}) \\ & \times D_\uparrow(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_\uparrow}) D_\downarrow(\vec{r}_{N_\uparrow+1}, \dots, \vec{r}_{N_\uparrow+N_\downarrow})\end{aligned}$$

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 $f(r_{jj}) : O(N_{\uparrow})$

$\leftarrow O(N_{\uparrow}^2)$ 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 $\mathcal{O}(N_{\uparrow}^2)$ matrix-vecotr

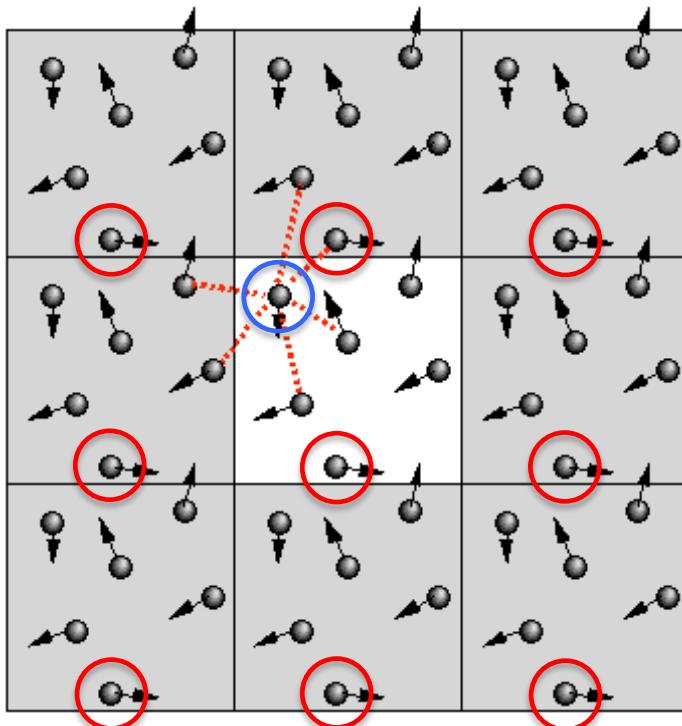
Iteration Steps

1. Generate an initial configuration and D_{\uparrow} & D_{\downarrow}
2. do loop $1 \leq i \leq (N_{\uparrow} + N_{\downarrow}) * M_{\text{warmup}}$.
Generate a new config. from old one by Metropolis
 - Update D_{\uparrow} & D_{\downarrow} by Sherman-Morrison
3. do loop $1 \leq i \leq N_{\uparrow} + N_{\downarrow}$
Generate a new config. from old one by Metropolis
 - Update D_{\uparrow} & D_{\downarrow} by Sherman-Morrison
4. Calc. physical quantities from the updated config. and D_{\uparrow} & D_{\downarrow} for average
5. Go back to 3. until M MC steps

Metropolis

Probability distribution, instead of Boltzmann weight

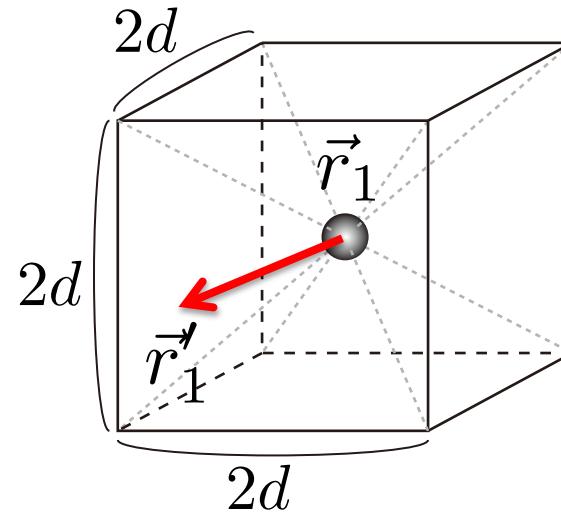
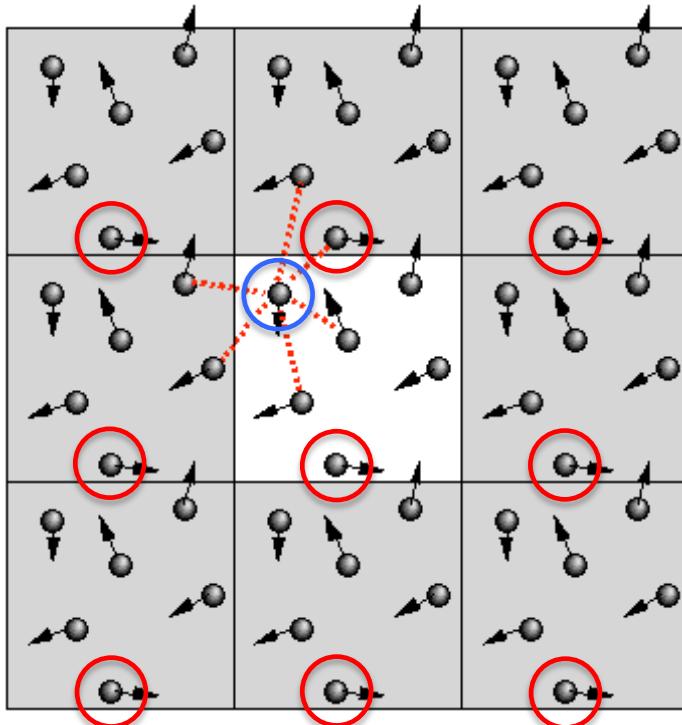
$$P_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \frac{|\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)|^2}{\int \prod_i d^3 r'_i |\psi(\vec{r}'_1, \vec{r}'_2, \dots, \vec{r}'_N)|^2}$$



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 $g(\vec{r})$: $g_L(\vec{r})$ & $g_U(\vec{r})$

Parallel spins $\uparrow \uparrow$

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

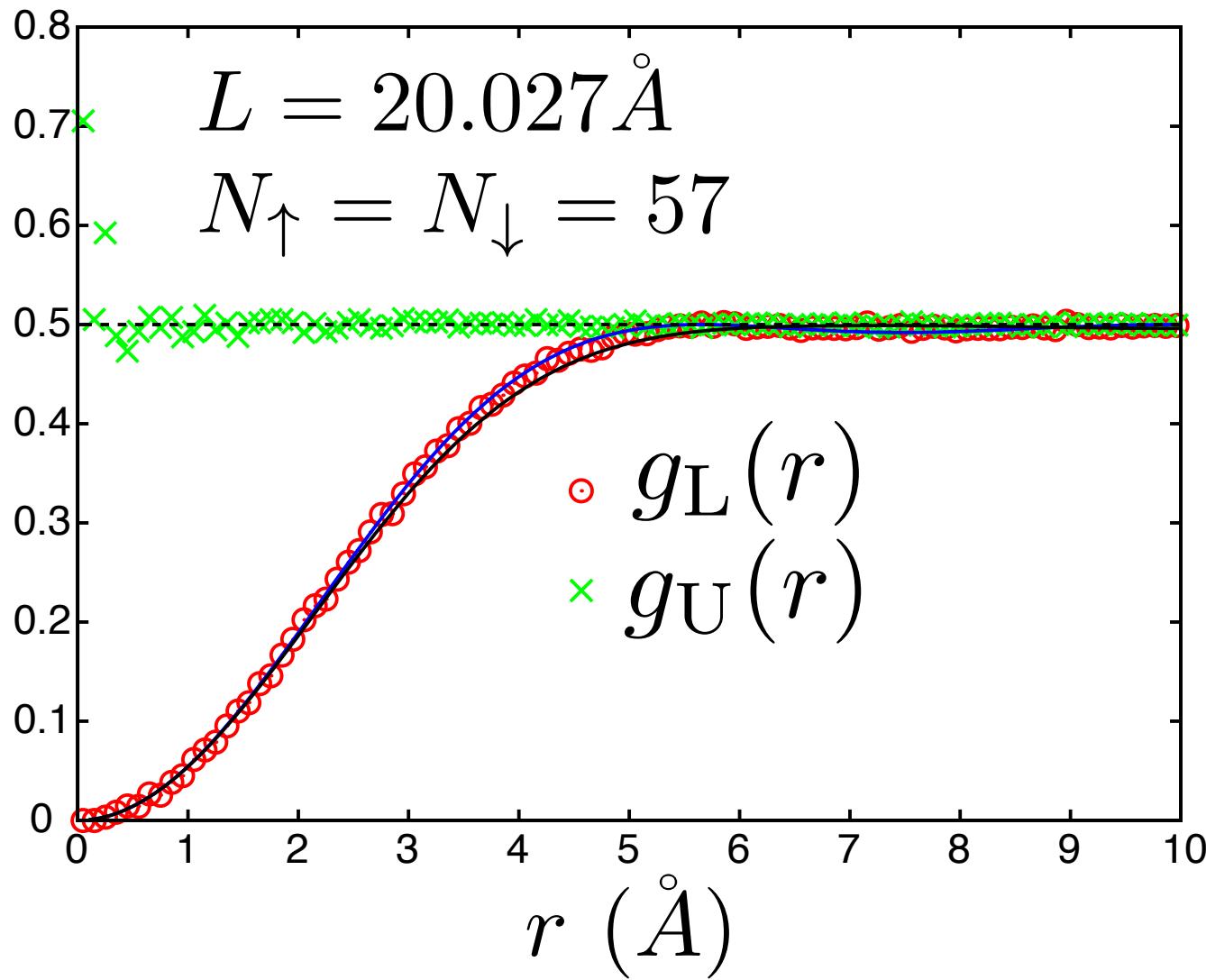
Antiparallel spins $\uparrow \downarrow$

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

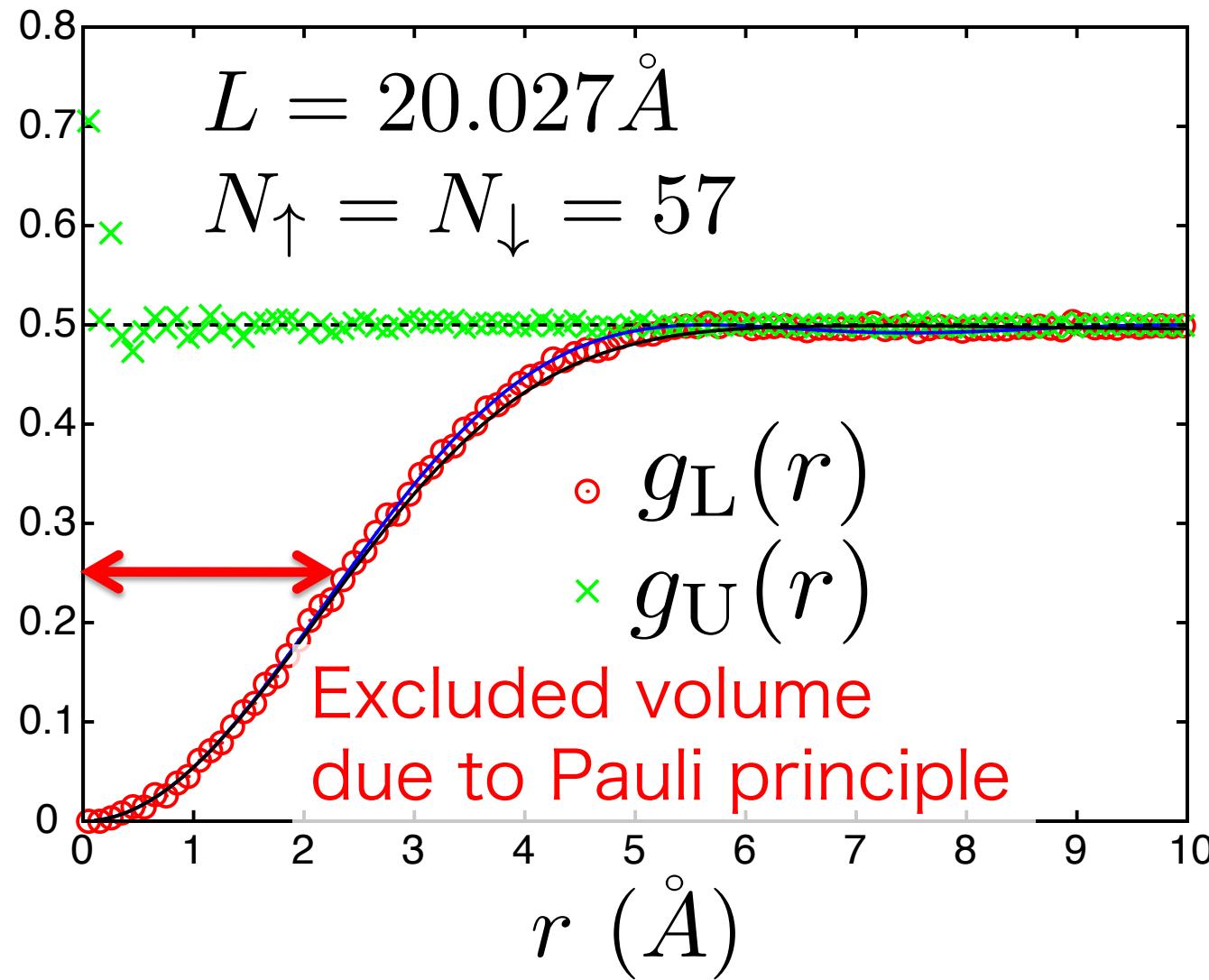
Expectation value

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

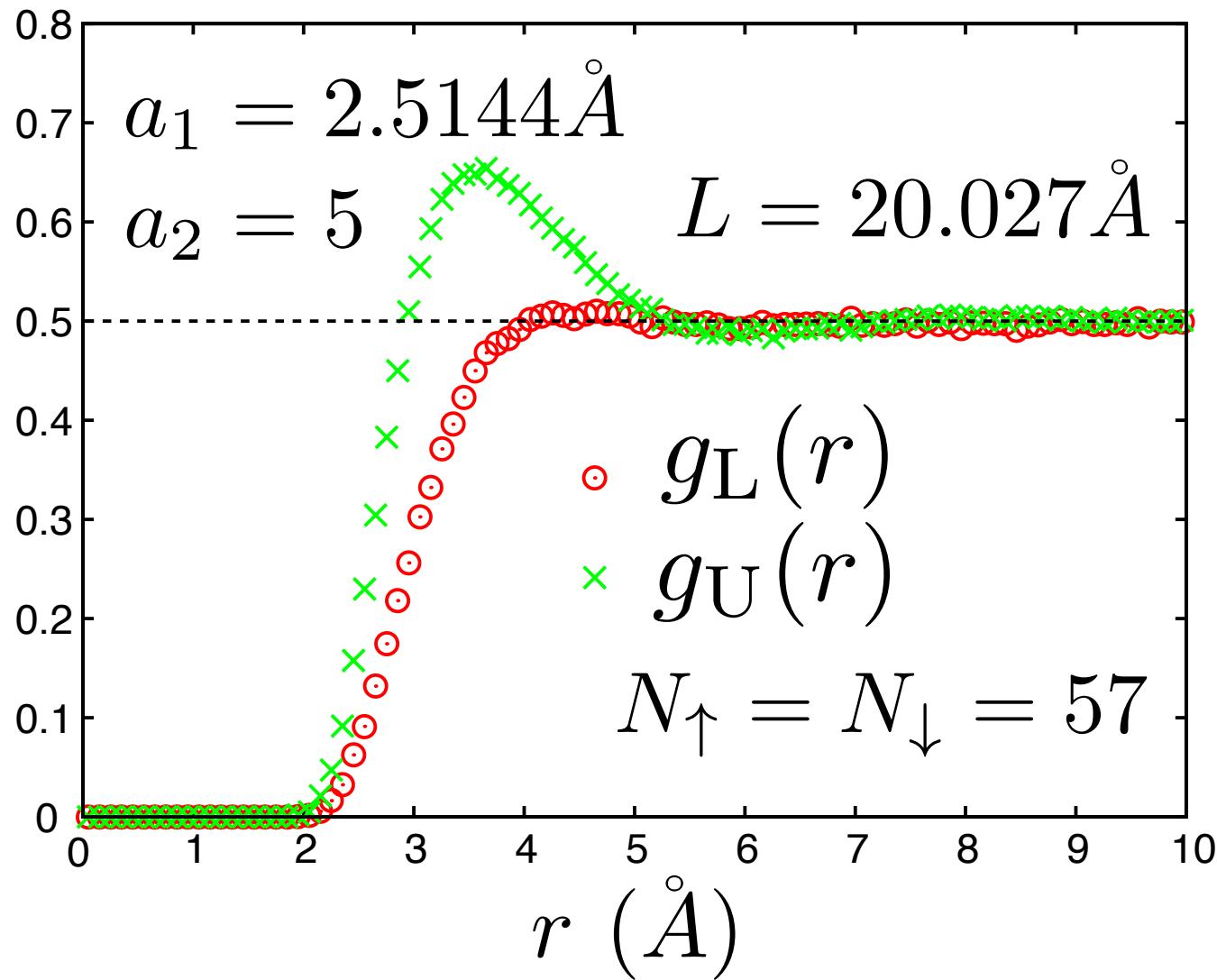
Free Fermions



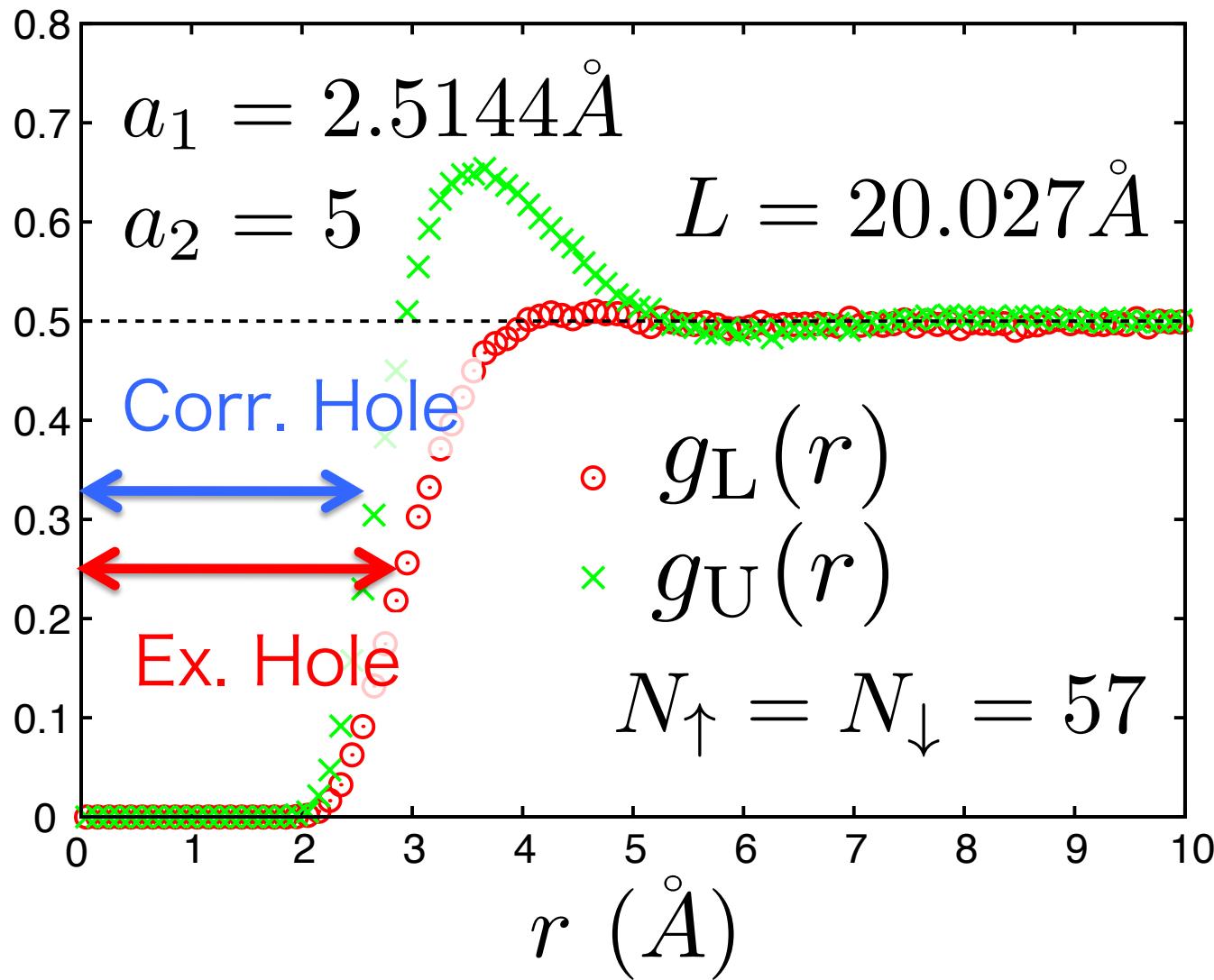
Exchange Hole Due to Pauli Principle



Liquid Helium 3



Many-Body Effect: Correlation Hole



Refinement VWF

Refinement of VWF for ${}^4\text{He}$ 1: Long-Range Part

Short range properties are enough?

Asymptotic form at a short distance ($r \rightarrow 0$)

$$f(r) = \exp [-(a_1/r)^{a_2}] \quad a_2 = 5$$

Ceperley, D.M., and Kalos, M.H.,

Quantum Many-Body Problems in Monte Carlo Methods in Statistical Physics,
ed. K. Binder, Springer-Verlag, 1979

Asymptotic form at a long distance ($r \rightarrow +\infty$)

$$f(r) \simeq \exp [-C/r^2] \quad (r \rightarrow +\infty)$$

Important for reproducing acoustic modes

Refinement of VWF for ${}^4\text{He}$ 2: 3-body Term

2 particle properties are enough?

Function of distance between 2 particles $f(r) = \exp[-u(r)]$

Example of 3-body terms:

$$\psi = \exp \left[- \sum_{i < j} u'(r_{ij}) - \lambda \sum_{\ell} \sum_{m, n \neq \ell} \xi(r_{\ell m}) \xi(r_{\ell n}) \vec{r}_{\ell m} \cdot \vec{r}_{\ell n} \right]$$

Refinement of VWF for ${}^4\text{He}$ 3: Back Flow

Feynman-Cohen's back flow wf for excited states

$$\psi_{\text{ex}} = \psi \sum_i \exp \left[i \vec{k} \cdot \left\{ \vec{r}_i + \sum_j \eta_{ij}(r_{ij})(\vec{r}_i - \vec{r}_j) \right\} \right]$$

Feynman-Cohen: $\eta_{ij}(r_{ij}) = A/r_{ij}^3$

R. P. Feynman and M. Cohen, Phys. Rev. 102, 1189 (1956)

Bijl-Feynman spectrum

$$\eta_{ij}(r_{ij}) = 0 \rightarrow E(k) = \frac{\hbar^2 k^2}{2m_{{}^4\text{He}} S(k)}$$

D. Pines, Phys. Today 42(2), 61 (1989)

Removal of Bias: Diffusion MC (Not a MCMC)

Imaginary-time evolution

$$-\frac{\partial \Psi(\vec{R}, \tau)}{\partial \tau} = (\hat{H} - E) \Psi(\vec{R}, \tau)$$

$$\hat{H} = -\frac{\hbar^2}{2m_{^4\text{He}}} \nabla_{\vec{R}}^2 + V(\vec{R})$$

$$\vec{R} = (\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$$

$$\nabla_{\vec{R}}^2 = \sum_i \nabla_i^2$$

Instead of direct imaginary-time evolution

Diffusion MC

$$f(\vec{R}, \tau) = \psi(\vec{R}) \Psi(\vec{R}, \tau) \quad \leftarrow \text{Product of vwf and imaginary-time wf}$$

$$-\frac{\partial f(\vec{R}, \tau)}{\partial \tau} = \text{Diffusion} \quad \text{Driving force} \\ -D \nabla_{\vec{R}}^2 f(\vec{R}, \tau) + D \nabla_{\vec{R}} \left[\vec{F}(\vec{R}) f(\vec{R}, \tau) \right] + \left[E_\ell(\vec{R}) - E \right] f(\vec{R}, \tau)$$

$$D = \frac{\hbar^2}{2m_{^4\text{He}}} \quad \vec{F}(\vec{R}) = 2 \frac{\nabla_{\vec{R}} \psi(\vec{R})}{\psi(\vec{R})} \quad E_\ell(\vec{R}) = \frac{1}{\psi(\vec{R})} \left[\hat{H} \psi(\vec{R}) \right]$$

Optimization of amplitude at each real-space configuration \vec{R}

Outline of Diffusion Equation

Diffusion equation

$$-\frac{\partial f(\vec{R}, \tau)}{\partial \tau} = -D \nabla_{\vec{R}}^2 f(\vec{R}, \tau) + D \nabla_{\vec{R}} \left[\vec{F}(\vec{R}) f(\vec{R}, \tau) \right] + \left[E_\ell(\vec{R}) - E \right] f(\vec{R}, \tau)$$
$$= \hat{A} f(\vec{R}, \tau)$$

$$f(\vec{R}', \tau + \Delta\tau) = \int d^{3N} R \ G(\vec{R}', \vec{R}, \Delta\tau) f(\vec{R}, \tau)$$
$$G(\vec{R}', \vec{R}, \Delta\tau) = \langle \vec{R}' | \exp \left[-\Delta\tau \hat{A} \right] | \vec{R} \rangle$$

Mutidimensional diffusion equation can be solved numerically by multi-walker path integral MC

Reference (Not the first publication of DMC):

J. Boronat and J. Casulleras, Phys. Rev. B, 49, 8920 (1994)

Introduction to numerical path integral (with a sample code):

Rubin H. Landau and M. J. Paez Mejia, Computational Physics
(John Wiley & Sons, Inc., 1997)

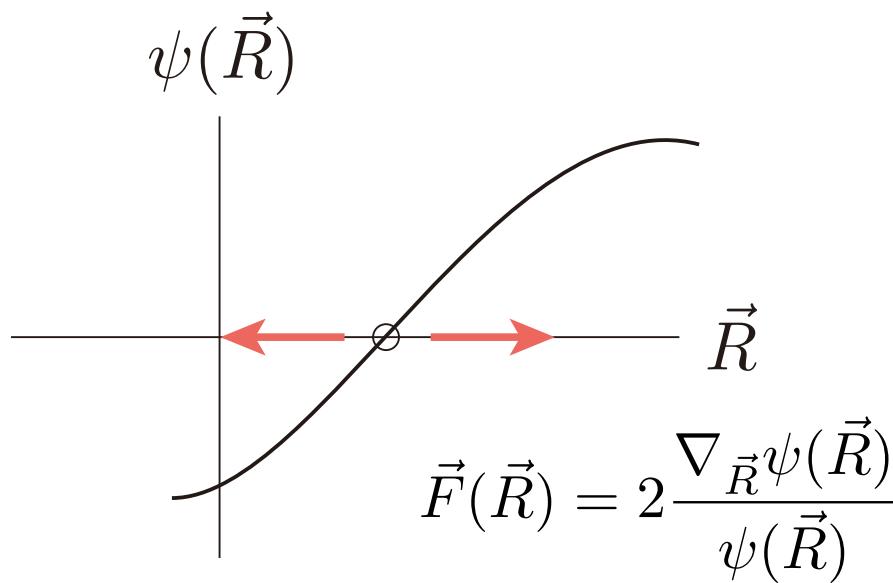
(邦訳) 計算物理学 (小柳義夫監訳, 朝倉書店)

Problem in Many-Body Fermions

DMC does not guarantee
numerically exact solution in many-body fermions

DMC = Fixed node approximation

DMC does not modify locations of nodes



Walkers feel repulsive force from nodes
and can not sample amplitude around the nodes

Needs for Refinement of VWF

Initial vwf dependence of DMC results

Kwon, Ceperley, & Martin, Phys. Rev. B 58, 6800 (1998);
Lecture materials of Prof. Ceperley

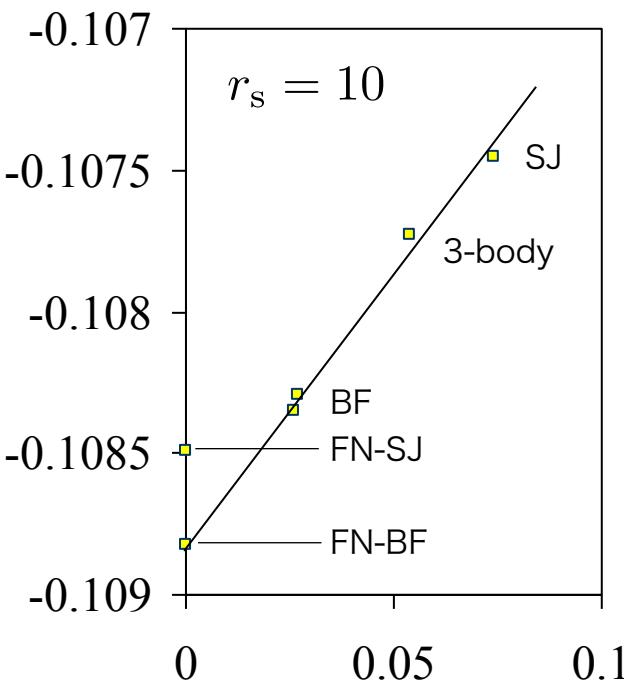
Electron gas

Density

$$n = \left(\frac{4\pi}{3} r_s^3 a_B^3 \right)^{-1}$$

Bohr radius:
 $a_B = 0.529 \text{ \AA}$

$$E_T = \frac{\langle \Psi_T | \hat{H} | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$



$$\text{var } E_T = \frac{\langle \Psi_T | [\hat{H} - E_0]^2 | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$

$E = E(r_s)$ is used in LDA/GGA

Perdew & Zunger, Phys. Rev. B 23, 5048 (1981)

SJ: Slater-Jastrow
BF: Back flow
FN: Fixed node

Correlation Factors by Neural Network

N -body correlation by neural network

$$|\psi\rangle = \int \prod_{\ell} d^d r_{\ell} \mathcal{N}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) |\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N\rangle \langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N | \psi_0 \rangle$$
$$|\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N\rangle = \hat{\phi}^\dagger(\vec{r}_1) \hat{\phi}^\dagger(\vec{r}_2) \cdots \hat{\phi}^\dagger(\vec{r}_N) |0\rangle$$

-Restricted Boltzmann machine for quantum spins/qubits

G. Carleo & M. Troyer, Science 355, 602 (2017).

-Restricted Boltzmann machine for fermions

For example,

Y. Nomura, A. S. Darmawan, Y. Yamaji, & M. Imada,
Phys. Rev. B 83, 205152 (2017).

N -body backflow

$$|\psi\rangle = \int \prod_{\ell} d^d \rho_{\ell} \prod_m d^d r_m \mathcal{N}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N; \vec{\rho}_1, \vec{\rho}_2, \dots, \vec{\rho}_N)$$
$$\times |\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N\rangle \langle \vec{\rho}_1, \vec{\rho}_2, \dots, \vec{\rho}_N | \psi_0 \rangle$$

H. Xie, L. Zhang, and L. Wang,
Journal of Machine Learning 1, 38 (2022).

Lecture Schedule

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

Appendix: Operators and Hilbert space

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

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

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)

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

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

(complex conjugate + transpose)

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

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

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

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