

# 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, 2021**

Quantum Monte Carlo Methods

- 0. Lattice model of solids
- 1. QMC
  - Variational MC

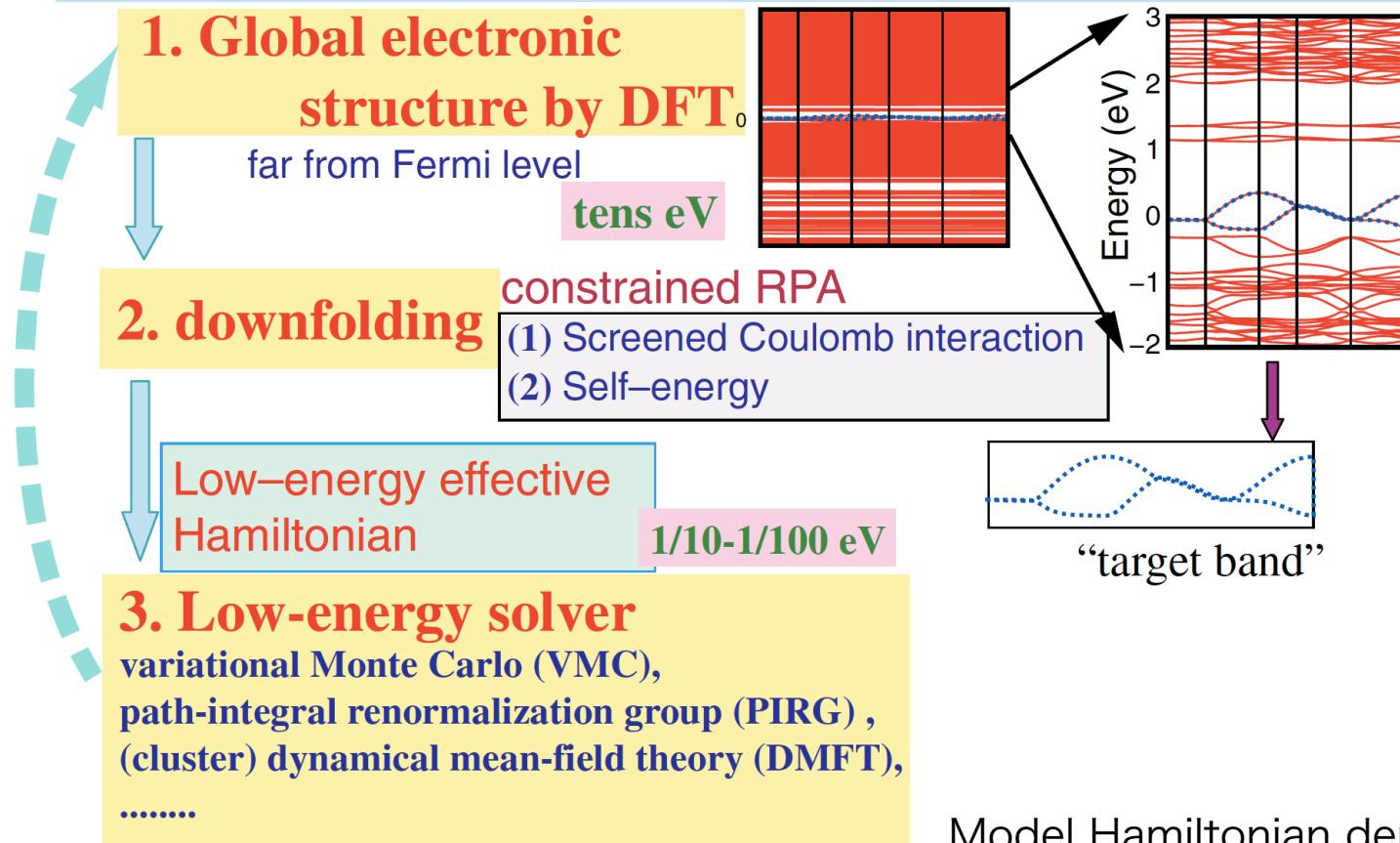
# Lattice Model of Solids

# Target of Model Calculations

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

# Model Construction

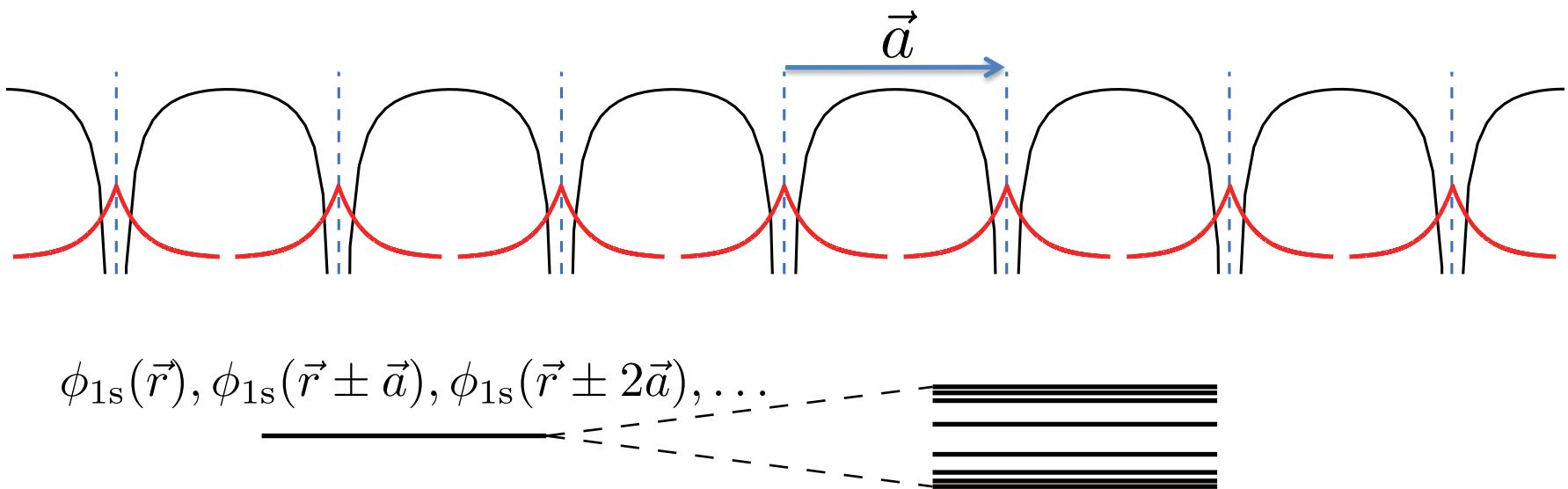
Schematic procedure of three-stage scheme  
thanks to energy hierarchy structure



Model Hamiltonian derived by  
DFT+DMFT, Wannier+cRPA  
G. Kotliar, et al., RMP 78, 865 (2006)  
M. Imada & T. Miyake, JPSJ 79, 112001 (2010)

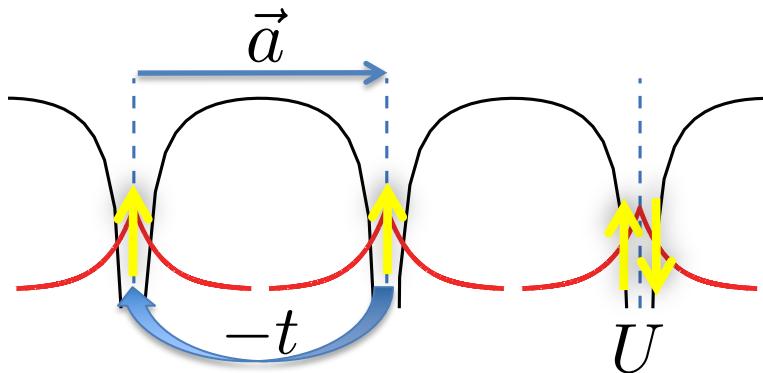
# Model of Many-Body Electrons

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



Gedankenexperiment of F. N. Mott

# One of the Simplest Model: 1D Hubbard Model



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

-Tunnelling among neighboring 1s orbitals

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

-Intra-atomic Coulomb in 1s orbitals

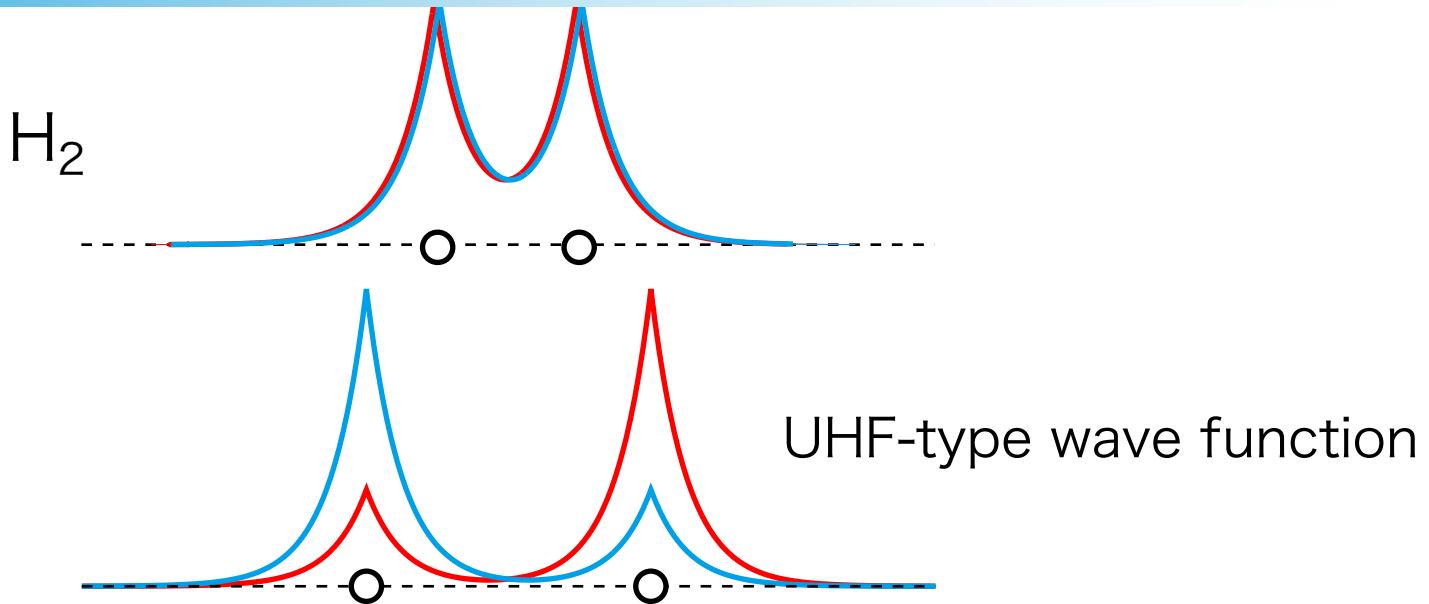
$$U = \int d^3r \int d^3r' \phi_{1s}^*(\vec{r}) \phi_{1s}^*(\vec{r}') \frac{e^2}{|\vec{r} - \vec{r}'|} \phi_{1s}(\vec{r}') \phi_{1s}(\vec{r})$$

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

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

cf.) Bethe ansatz, Tomonaga-Luttinger liquid

# Hydrogen Molecule



Hubbard model

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

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

Heisenberg model or  $J$ -coupling  $\hat{H} = J \left( \hat{S}_0^x \hat{S}_1^x + \hat{S}_0^y \hat{S}_1^y + \hat{S}_0^z \hat{S}_1^z \right)$



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

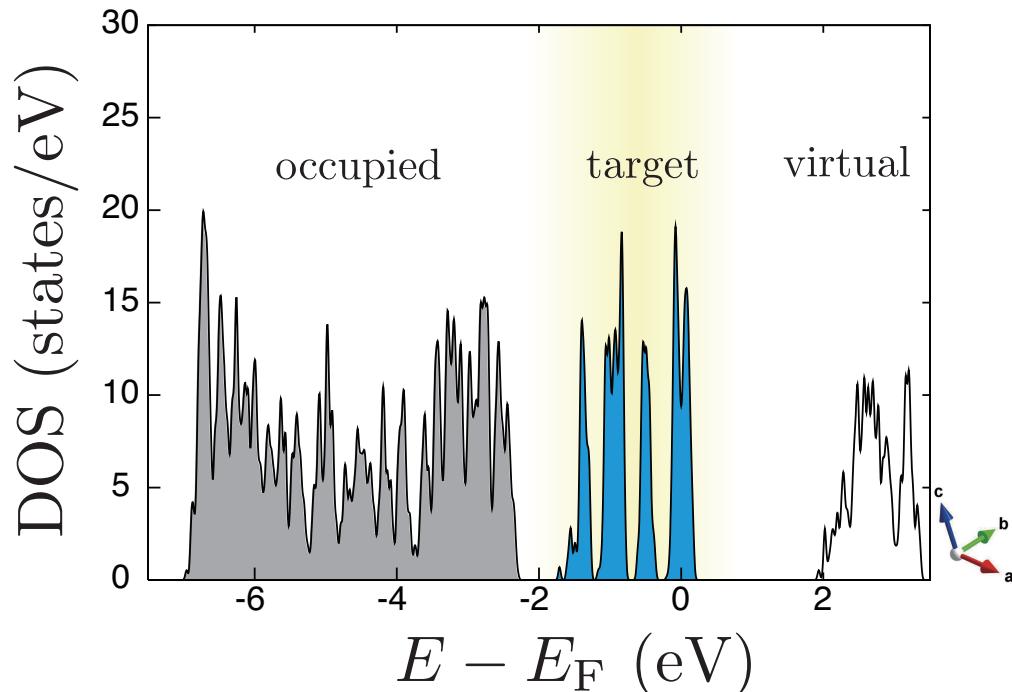


Singlet ground state

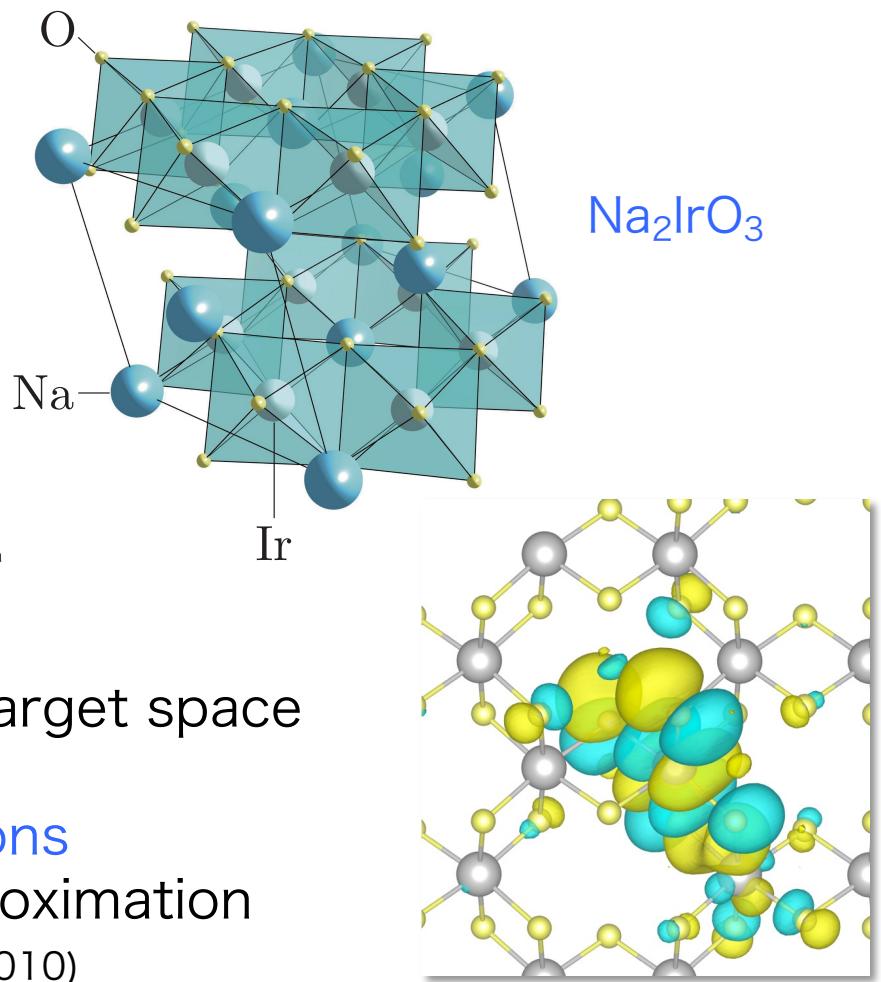
# Construction of Effective Hamiltonians: An Example

- Target Hilbert space expanded by localized Wannier orbitals

DFT result for energy spectrum



Souza-Marzari-Vanderbilt



- Effective Coulomb interactions in target space

Renormalization due to  
infinite virtual particle-hole excitations

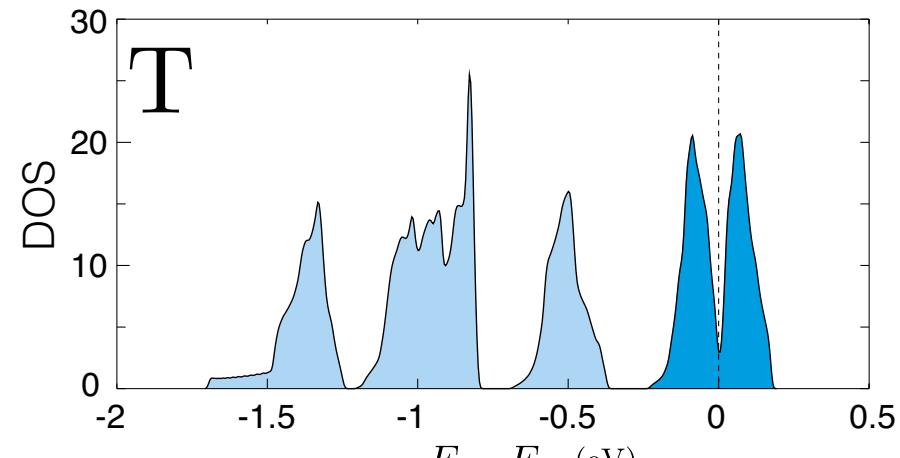
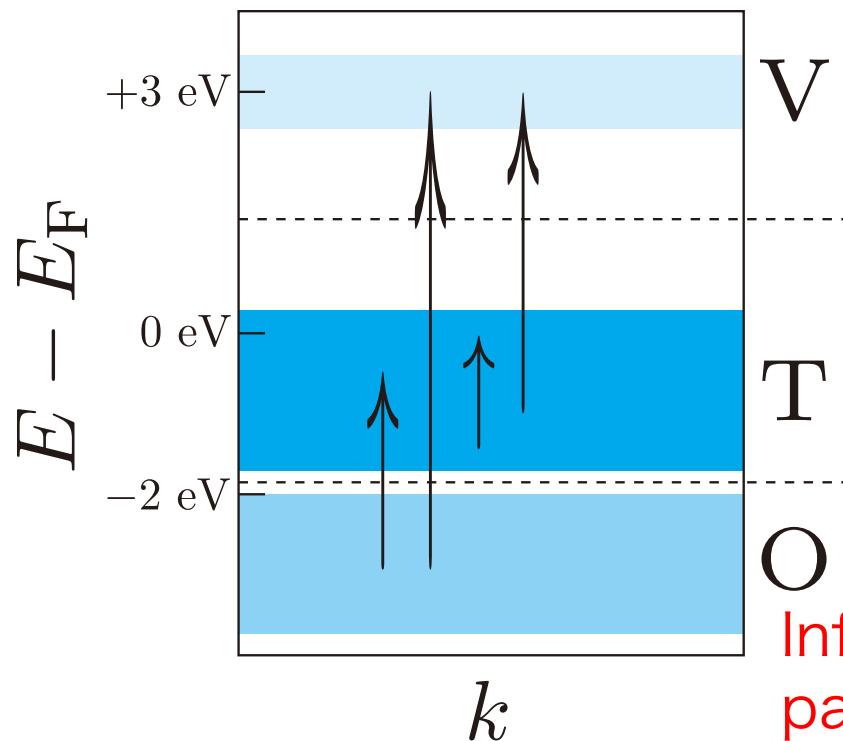
← Constrained random phase approximation

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

$$W^{\text{cRPA}} = \frac{V}{1 + V\chi^{\text{cRPA}}} \quad \leftarrow \text{Dielectric constant}$$

$$\chi^{\text{RPA}} = \chi_{O \rightarrow T} + \chi_{O \rightarrow V} + \chi_{T \rightarrow T} + \chi_{T \rightarrow V}$$

$$\chi^{\text{cRPA}} = \chi_{O \rightarrow T} + \chi_{O \rightarrow V} + \cancel{\chi_{T \rightarrow T}} + \chi_{T \rightarrow V}$$



Infinite number of RPA-type  
particle-hole excitations

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

Hopping

$$\hat{H}_0 = \sum_{\ell \neq m} \sum_{a,b=xy,yz,zx} \sum_{\sigma,\sigma'} t_{\ell,m;a,b}^{\sigma\sigma'} [\hat{c}_{\ell a\sigma}^\dagger \hat{c}_{mb\sigma'} + \text{h.c.}]$$

Trigonal+orbital-dependent  $\mu$

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

SOC

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

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

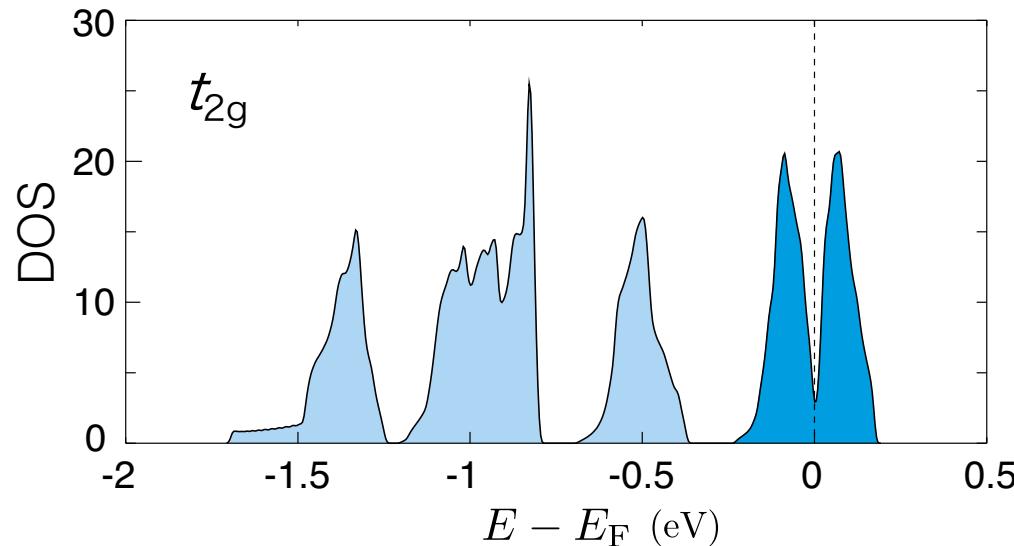
Coulomb

$$\begin{aligned} \hat{H}_U &= U \sum_{\ell} \sum_{a=yz,zx,xy} \hat{n}_{\ell a\uparrow} \hat{n}_{\ell a\downarrow} \\ &+ \sum_{\ell \neq m} \sum_{a,b} \frac{V_{\ell,m}}{2} (\hat{n}_{\ell a\uparrow} + \hat{n}_{\ell a\downarrow})(\hat{n}_{mb\uparrow} + \hat{n}_{mb\downarrow}) \\ &+ \sum_{\ell} \sum_{a < b} \sum_{\sigma} [U' \hat{n}_{\ell a\sigma} \hat{n}_{\ell b\bar{\sigma}} + (U' - J_H) \hat{n}_{\ell a\sigma} \hat{n}_{\ell b\sigma}] \\ &+ J_H \sum_{\ell} \sum_{a \neq b} [\hat{c}_{\ell a\uparrow}^\dagger \hat{c}_{\ell b\downarrow}^\dagger \hat{c}_{\ell a\downarrow} \hat{c}_{\ell b\uparrow} + \hat{c}_{\ell a\uparrow}^\dagger \hat{c}_{\ell a\downarrow}^\dagger \hat{c}_{\ell b\downarrow} \hat{c}_{\ell b\uparrow}] \end{aligned}$$

F. Aryasetiawan, *et al.*,

Phys. Rev. B 70, 195104 (2004)

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



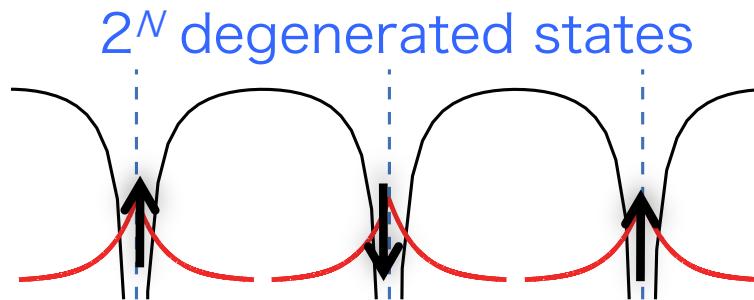
DFT: Elk (FLAPW)

<http://elk.sourceforge.net>  
Vxc: Perdew-Wang 1992

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

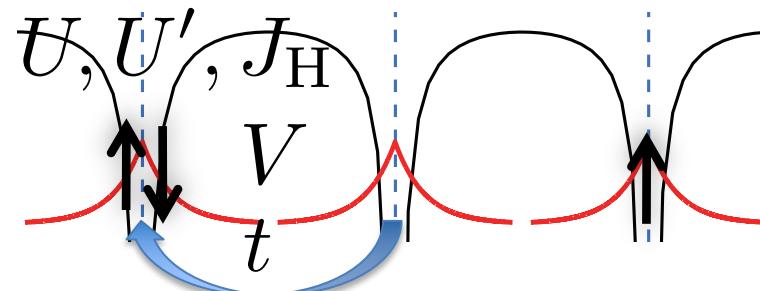
# Heisenberg (Spin) Hamiltonian from Strong Coupling Expansion

Unperturbed atomic Hamiltonian



Perturbation: Tunneling

virtual states lift the degeneracy



# Spin Hamiltonian

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

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

$$\mathcal{J}_X = \begin{bmatrix} -23.9 & -3.1 & -8.4 \\ -3.1 & 3.2 & 1.8 \\ -8.4 & 1.8 & 2.0 \end{bmatrix} \text{ (meV)}$$

$$\mathcal{J}_Y = \begin{bmatrix} 3.2 & -3.1 & 1.8 \\ -3.1 & -23.9 & -8.4 \\ 1.8 & -8.4 & 2.0 \end{bmatrix} \text{ (meV)}$$

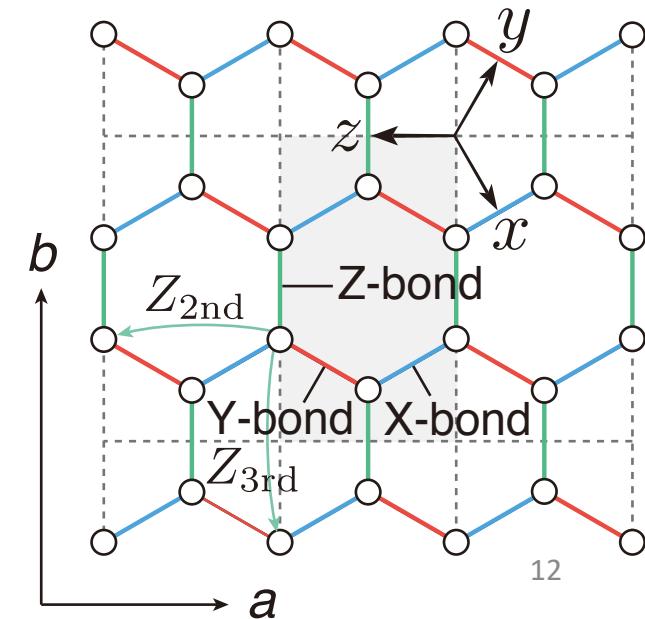
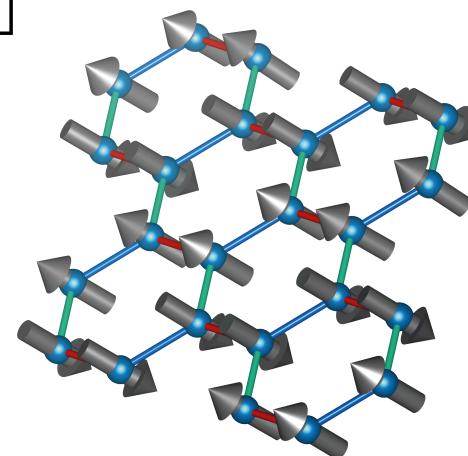
$$\mathcal{J}_Z = \begin{bmatrix} 4.4 & -0.4 & 1.1 \\ -0.4 & 4.4 & 1.1 \\ 1.1 & 1.1 & -30.7 \end{bmatrix} \text{ (meV)}$$

Ground state:  
Zigzag order

agrees with experiments

iPEPS, 2D DMRG, & ED:

T. Okubo, K. Shinjo, Y. Yamaji, *et al.*,



# 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 ( $^4\text{He}$ , 1965)

Ceperley-Chester-Kalos ( $^3\text{He}$ , 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

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

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

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

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

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

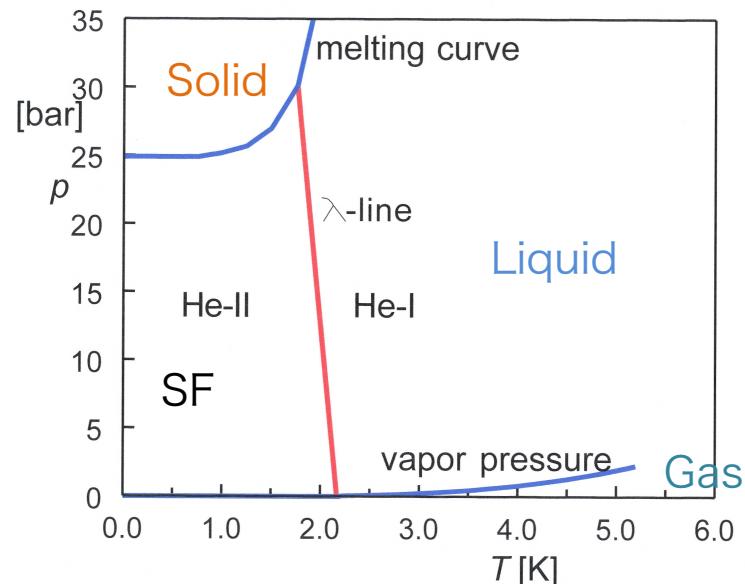
$$m_{^4}\text{He}/\hbar^2 = 0.597639 \times 10^{22} \text{ J}^{-1} \cdot \text{\AA}^{-2}$$

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

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

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

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

# 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

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

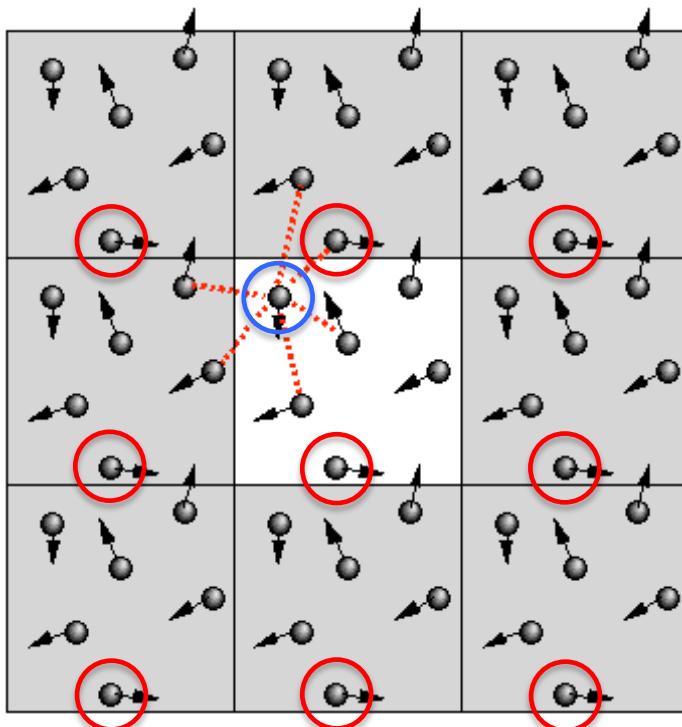
Weight/probability  $P_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \frac{1}{V^N} \frac{|\langle \vec{r}_1, \vec{r}_2, \dots, \vec{r}_N | \Psi \rangle|^2}{\langle \Psi | \Psi \rangle}$

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

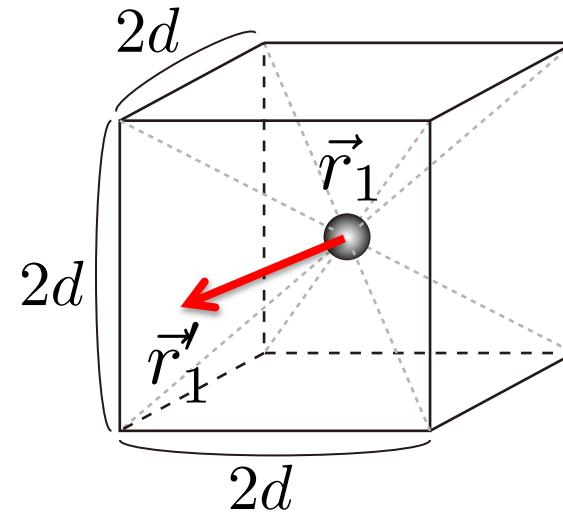
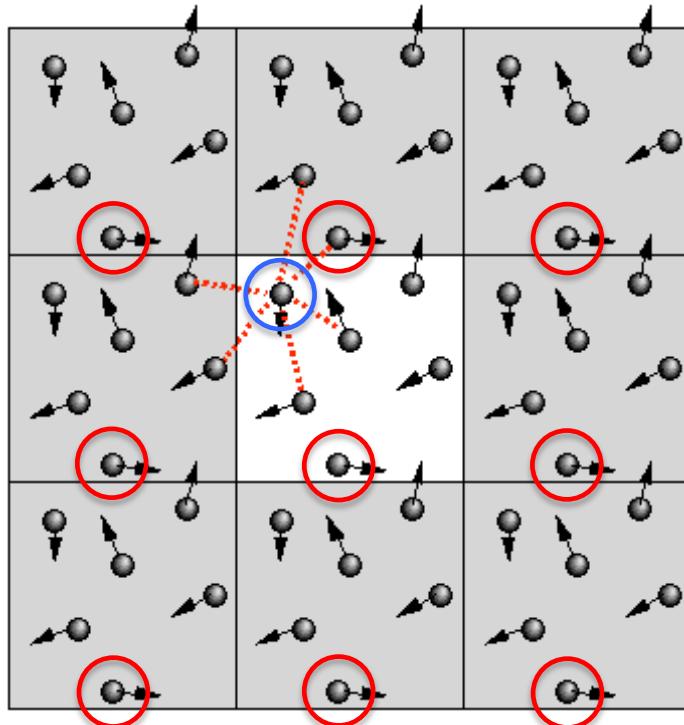
$$P_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \frac{|\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)|^2}{\int \prod_i d^3 r'_i |\psi(\vec{r}'_1, \vec{r}'_2, \dots, \vec{r}'_N)|^2}$$



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  $\rho = N/\Omega$ .

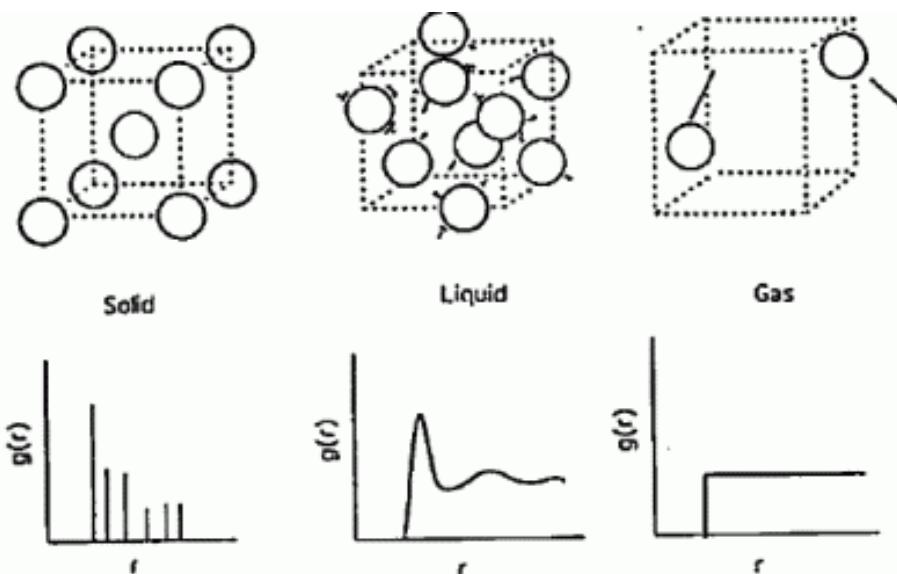
$$\begin{aligned} & \frac{1}{\Omega} \int d^3 R \int d(-\cos \theta) d\varphi \int_r^{r+\Delta r} dr' g(\vec{R} + \vec{r}', \vec{R}) \\ &= \rho^{-2} \frac{\frac{1}{\Omega} \int d^3 R \int d(-\cos \theta) d\varphi \int_r^{r+\Delta r} dr' \int \sum_{i \neq j} \psi(\vec{r}_1, \dots, \vec{r}_N)^2 |_{\vec{r}_i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

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

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  ${}^4\text{He}$

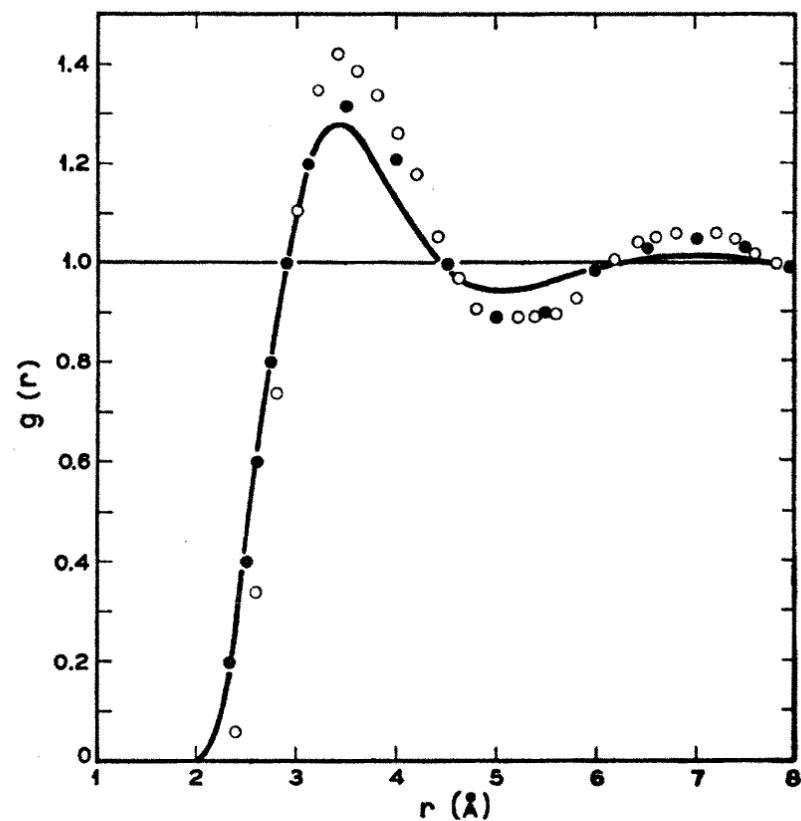
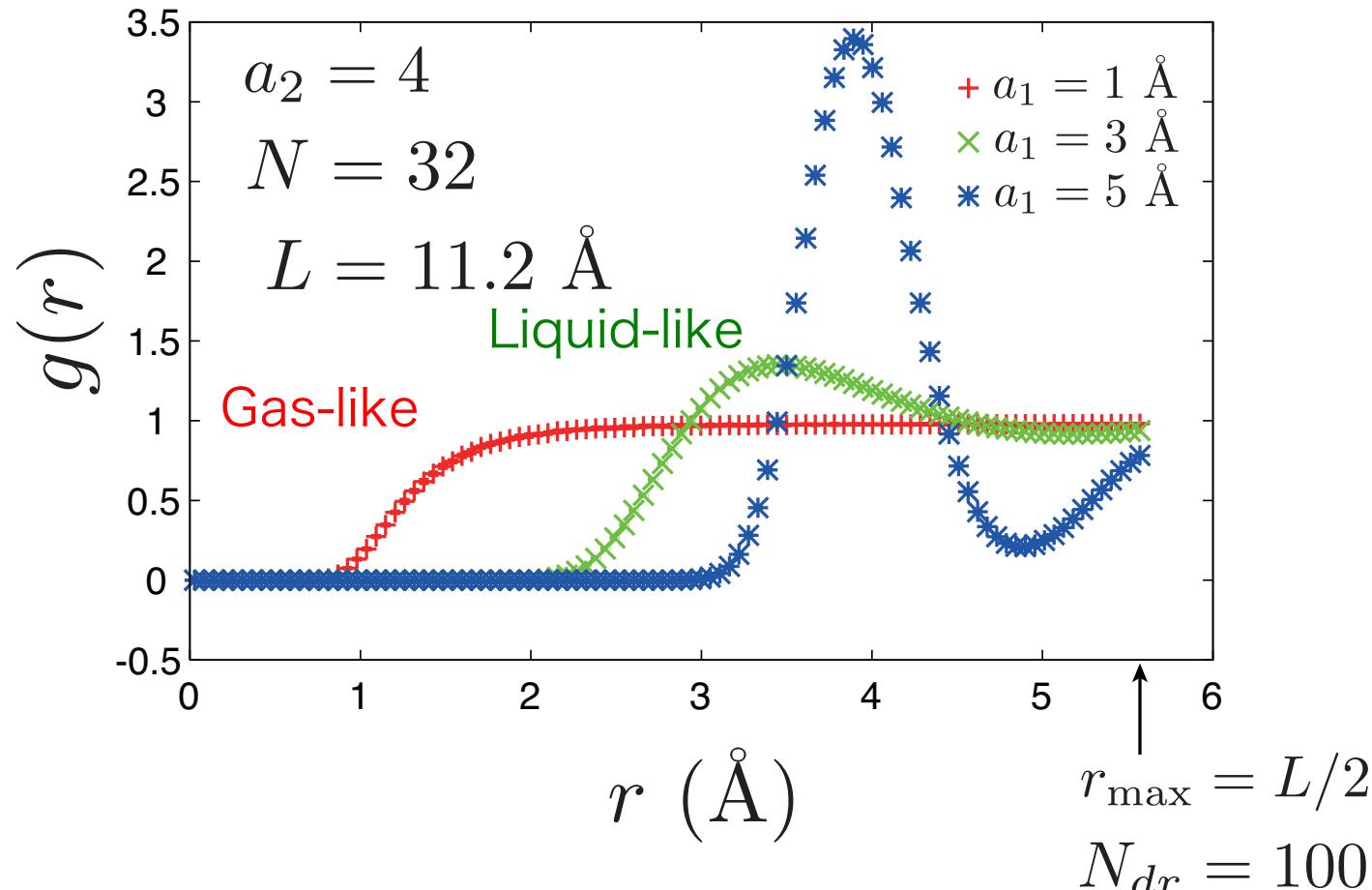


FIG. 5. Comparison of the two-body correlation function with experiment. The solid line is the theoretical curve, the solid circles are computed from the x-ray data of Gordon *et al.* (Ref. 26) and the open circles are computed from the neutron data of Henshaw (Ref. 27).

# 2 Point Distribution Function: $g(r)$



Volume per particle:  $43.904 \text{ \AA}^3$

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

# Comparison with Experiments

## 1. Energy

-Measure of accuracy

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

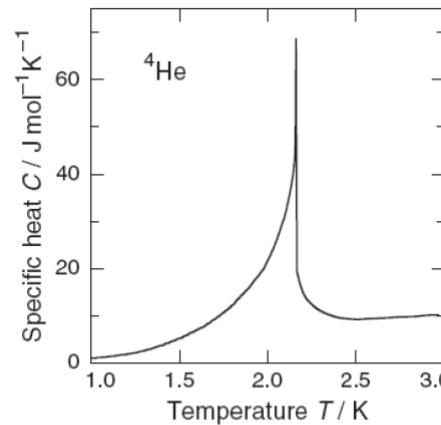
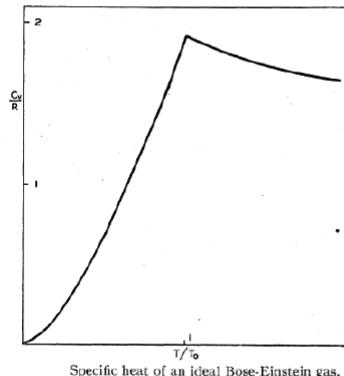
## 3. Structure factor (Fourier transformation of $g(r)$ )

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

## 4. Condensation fraction

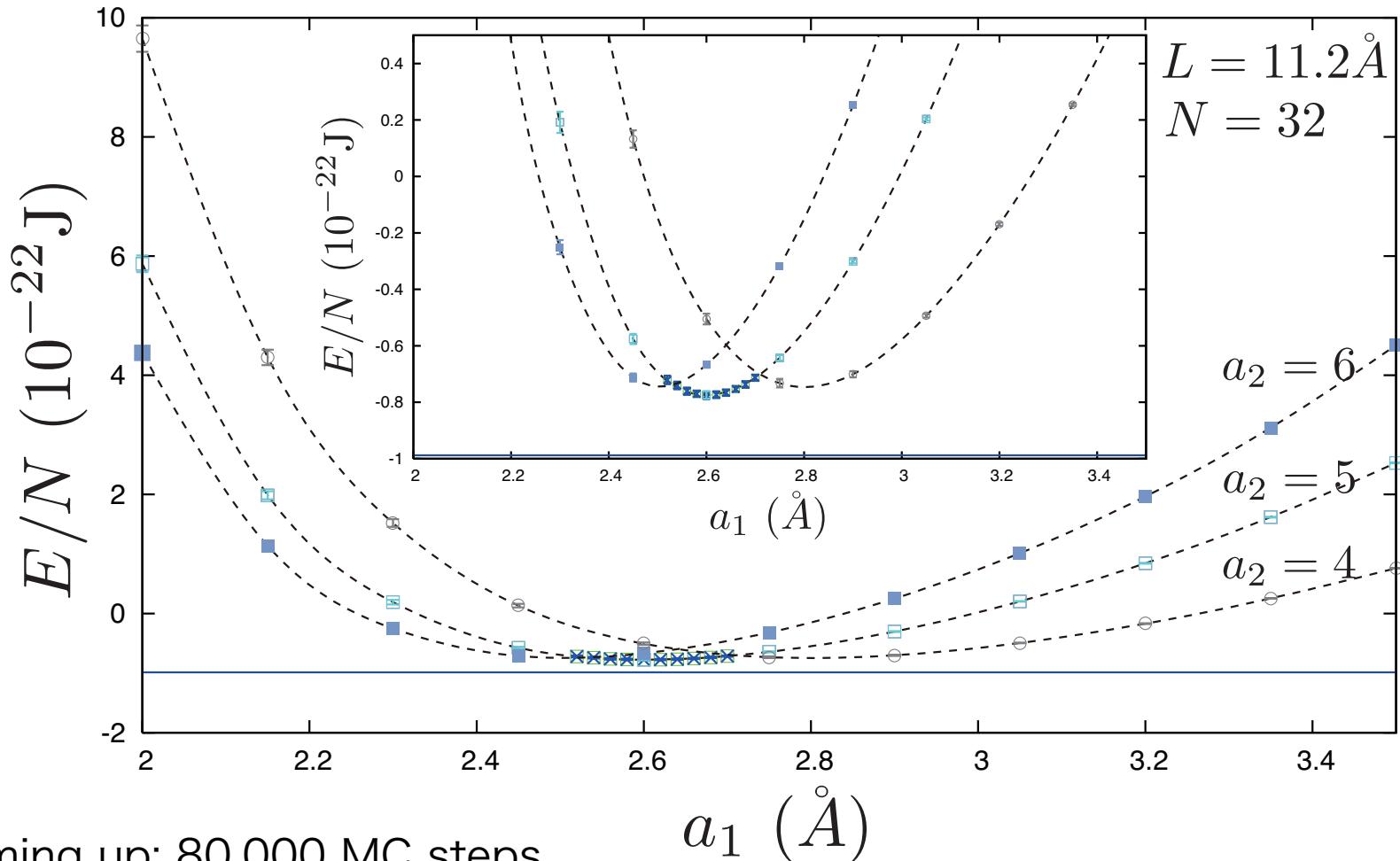
-Relation between Bose-Einstein condensation and He-II (superfluid phase)

Heat capacity: Ideal Bose gas and Liquid  $^4\text{He}$



# 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?

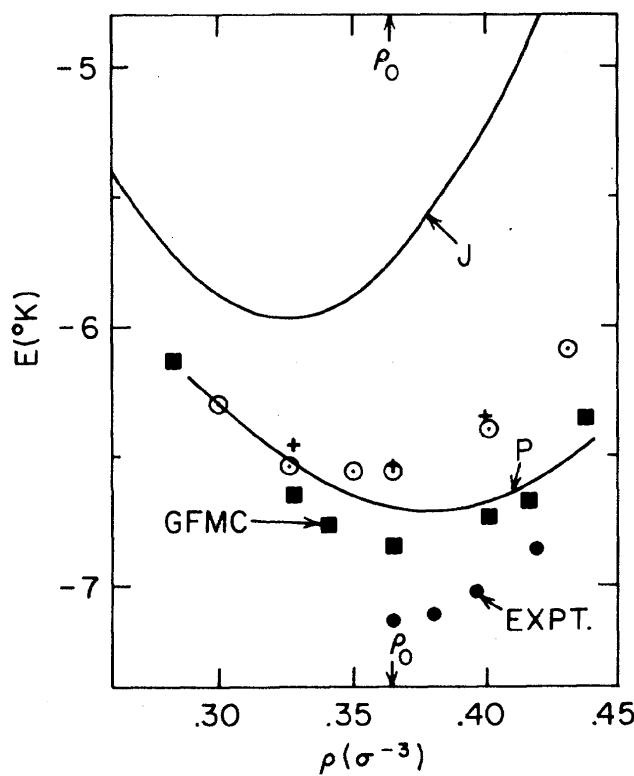


FIG. 1. Comparison of energy vs density. *J* indicates pure Jastrow results of Ref. 10; *P* indicates triplet calculations of Ref. 5; experimental results from Ref. 11; exact Lennard-Jones from Ref. 3; cross indicates present calculation; dot in circle indicates results from Ref. 4.

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

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

many-body\_vmc\_he4.zip

many-body\_vmc\_he4

| -main.f90

| -sub\_makesample.f90

| -sub\_measure.f90

| -mtfort90.f90

| -Makefile

Requirement:

gfortran or ifort

Compilation:

\$make mtmod

\$make

Parameters:

Defined in main.f90

Output:

$g(r)$  contained  
in gofr.dat

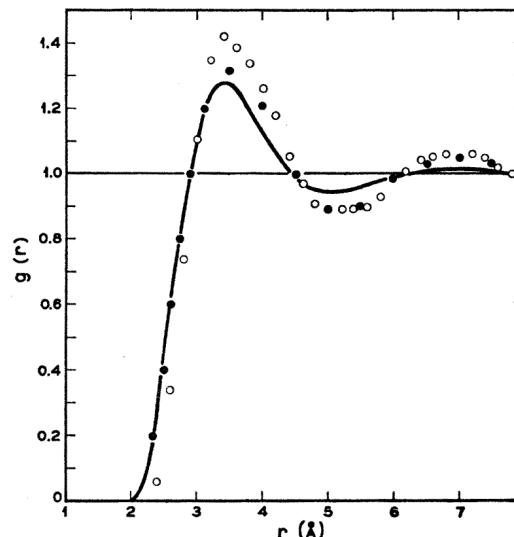


FIG. 5. Comparison of the two-body correlation function with experiment. The solid line is the theoretical curve, the solid circles are computed from the x-ray data of Gordon *et al.* (Ref. 26) and the open circles are computed from the neutron data of Henshaw (Ref. 27).

# Liquid Helium 3 (fermion): LJ Hamiltonian

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

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

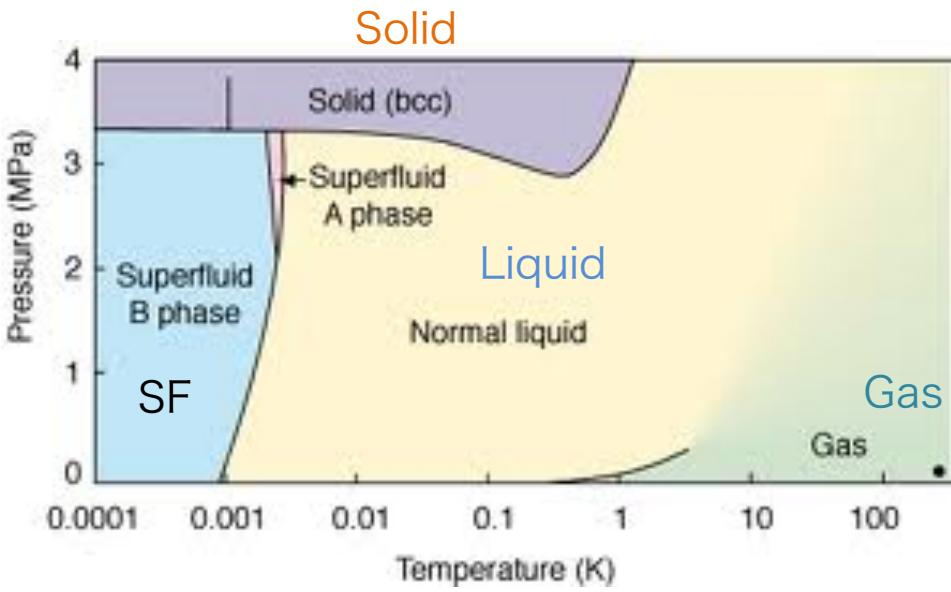
$$V(r) = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$$

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

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

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

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)

.

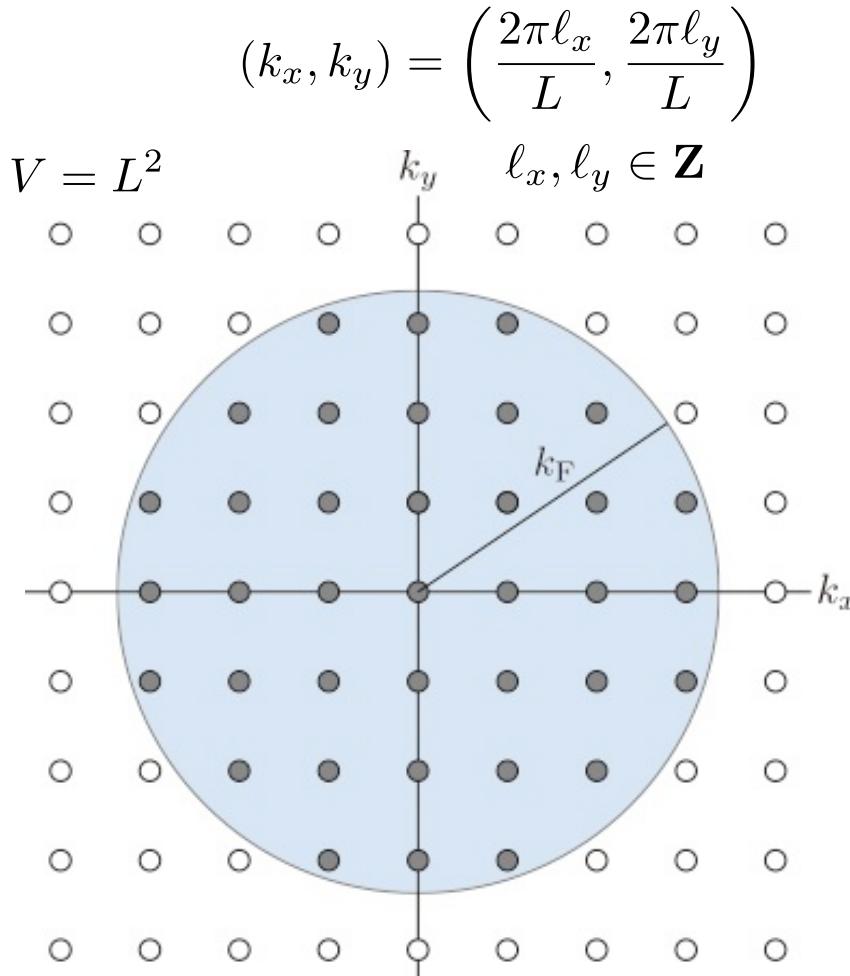
$$\begin{aligned}\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_\uparrow+N_\downarrow}) = & \psi_B(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_\uparrow+N_\downarrow}) \\ & \times D_\uparrow(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N_\uparrow}) D_\downarrow(\vec{r}_{N_\uparrow+1}, \dots, \vec{r}_{N_\uparrow+N_\downarrow})\end{aligned}$$

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

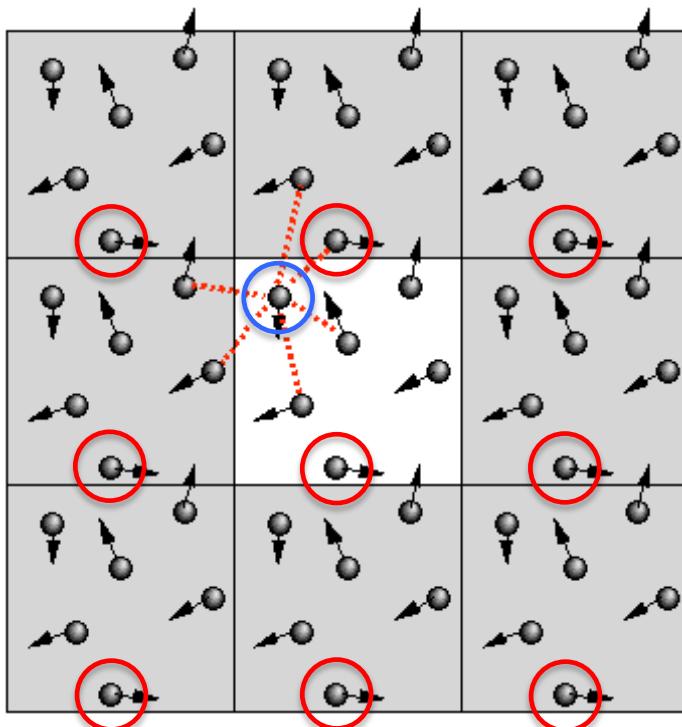
# Iteration Steps

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

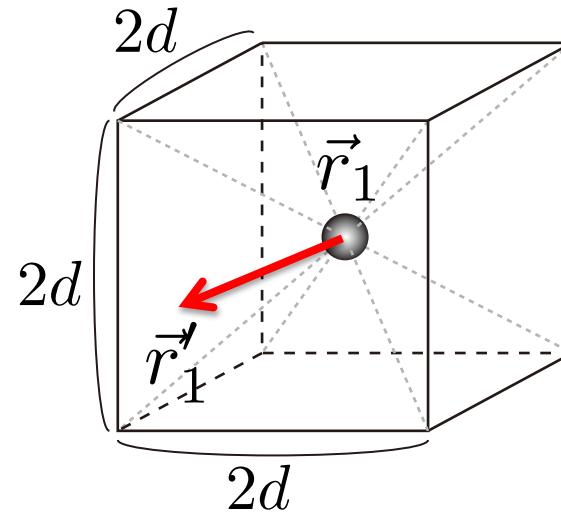
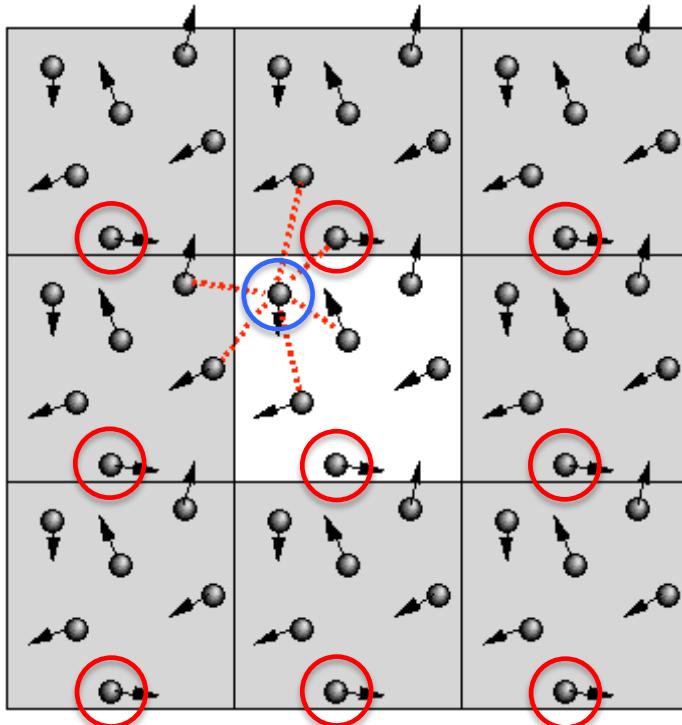
$$P_N(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \frac{|\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)|^2}{\int \prod_i d^3 r'_i |\psi(\vec{r}'_1, \vec{r}'_2, \dots, \vec{r}'_N)|^2}$$



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  $\uparrow \uparrow$

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

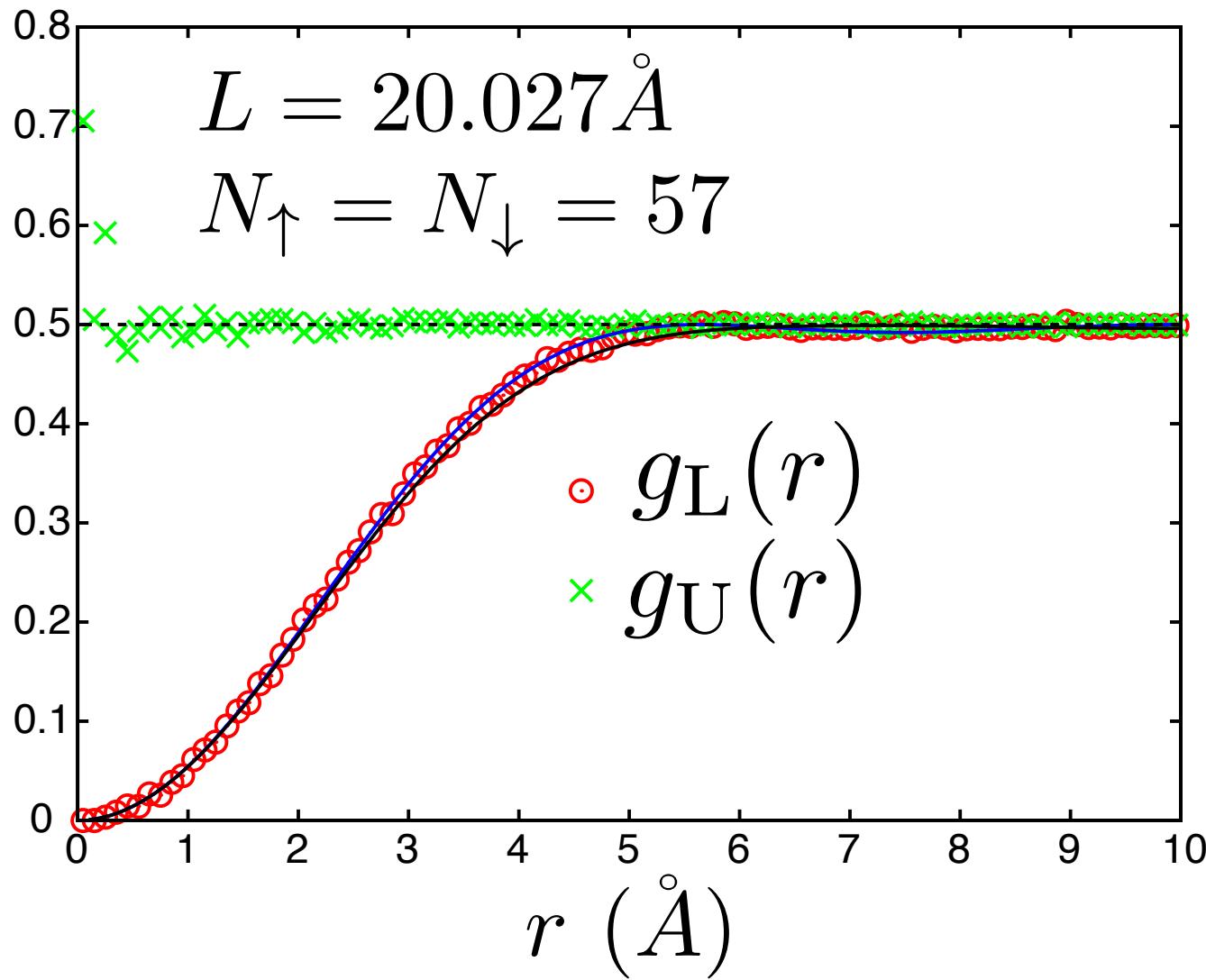
Antiparallel spins  $\uparrow \downarrow$

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

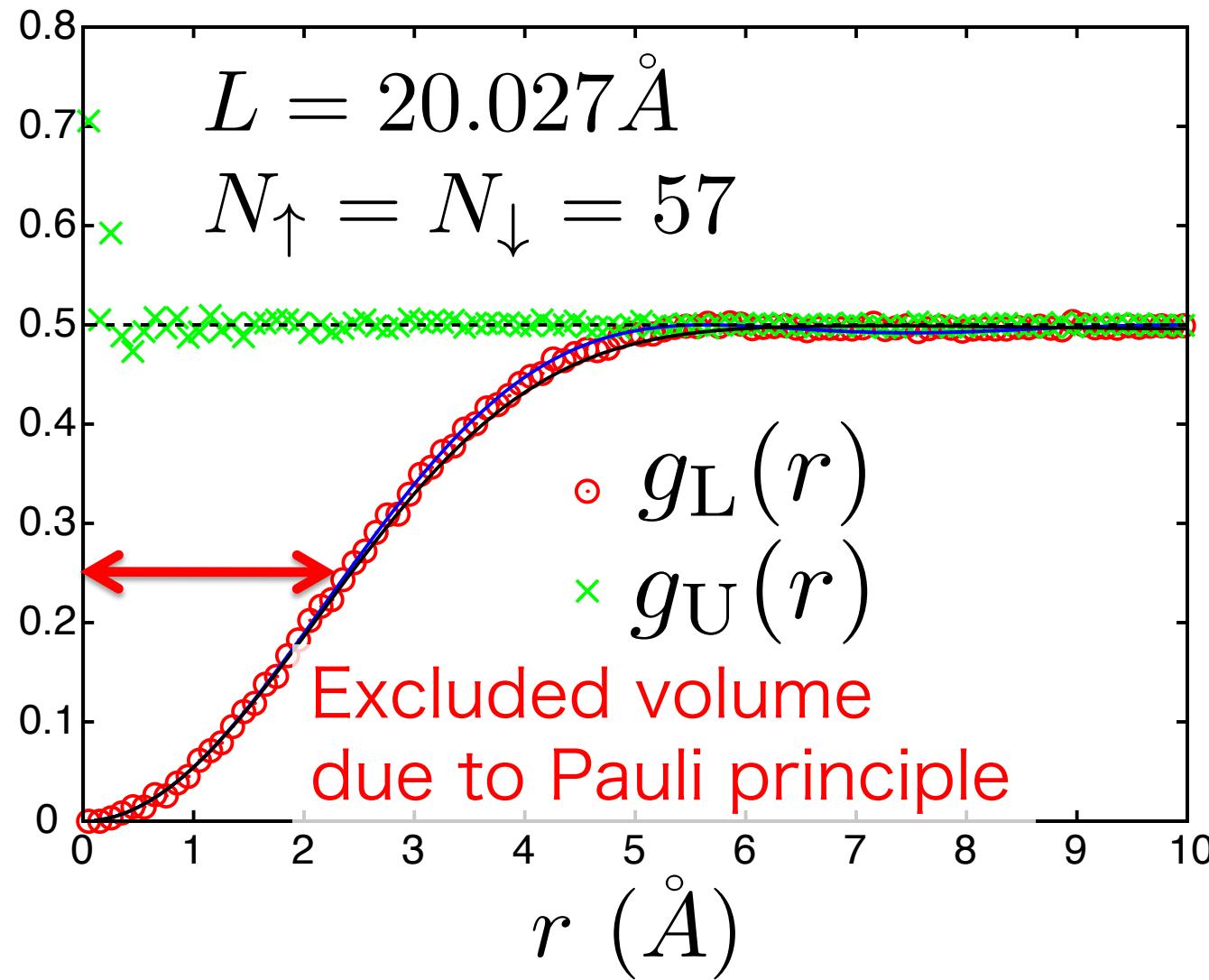
Expectation value

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

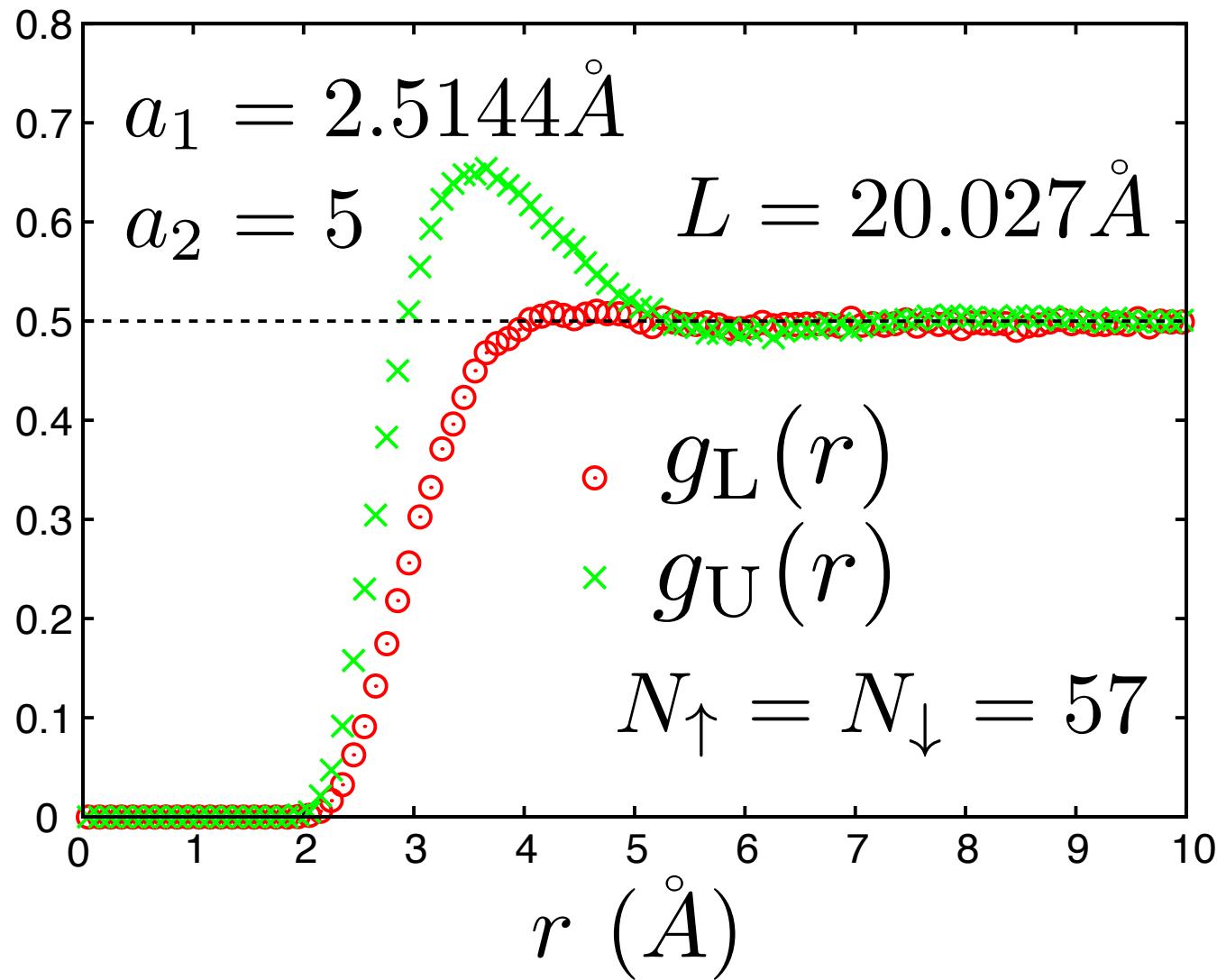
# Free Fermions



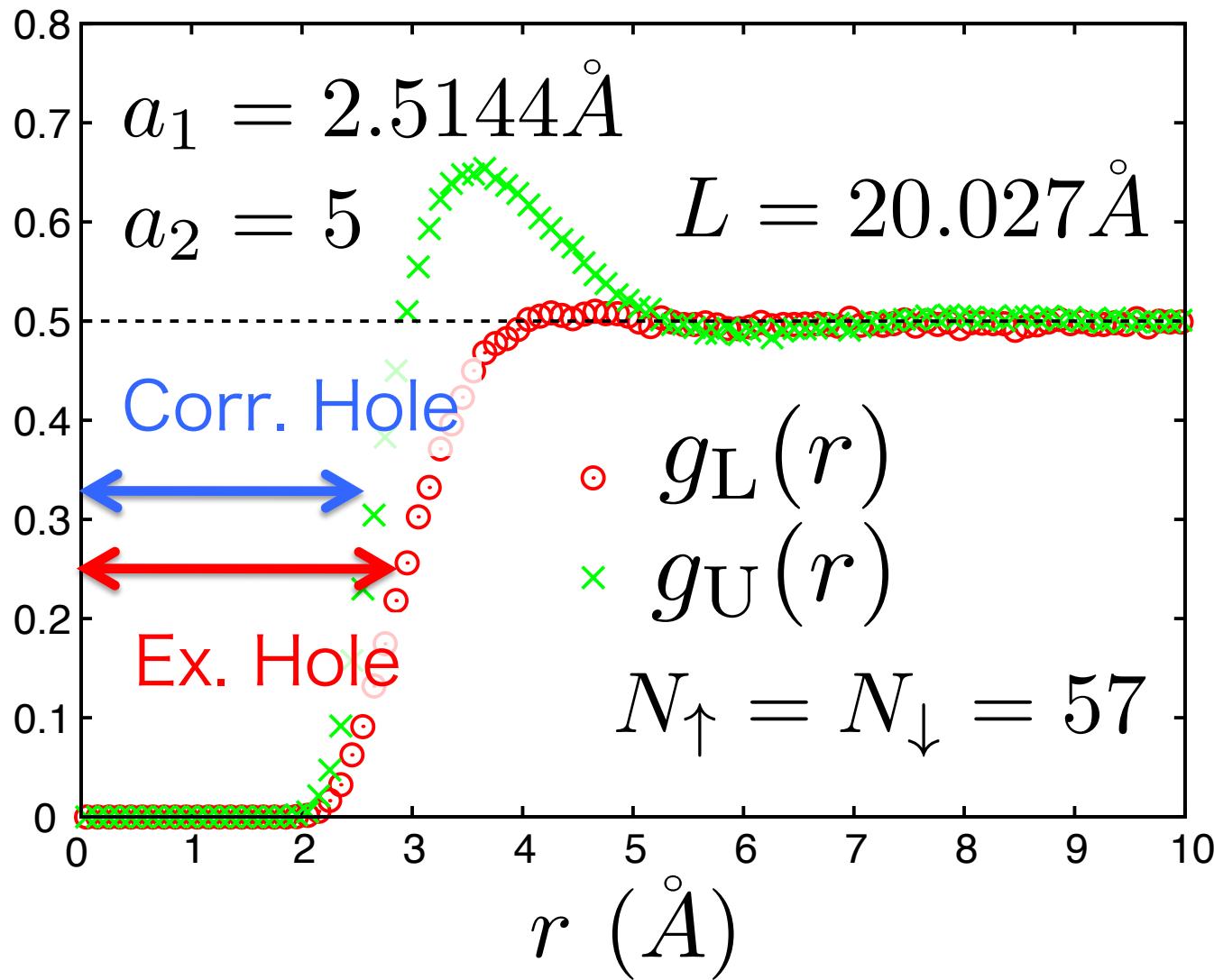
# Exchange Hole Due to Pauli Principle



# 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

$$\eta_{ij}(r_{ij}) = 0 \rightarrow E(k) = \frac{\Im m {}^4\text{He} G(k)}{k_3 k_3}$$

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)

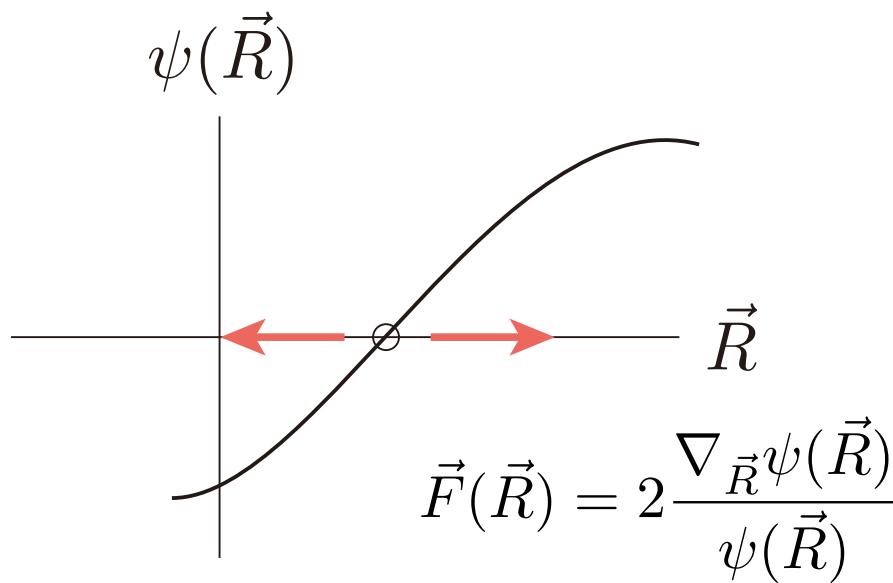
(邦訳) 計算物理学 (小柳義夫監訳, 朝倉書店)

# 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

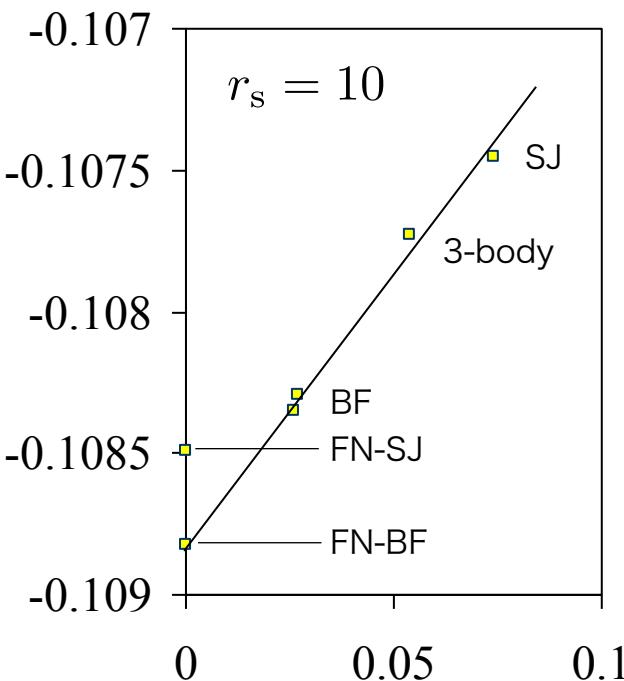
## Electron gas

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

# Lecture Schedule

Classical

Quantum

- #1 Many-body problems in physics
- #2 Why many-body problem is hard to solve
- #3 Classical statistical model and numerical simulation
- #4 Classical Monte Carlo method and its applications
- #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
  - Path integral & applications
- #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  $|\alpha\rangle \in \mathcal{F}$ ,  $\hat{O}|\alpha\rangle \in \mathcal{F}$

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