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 inpurities in alloys
  -Rare earth alloys

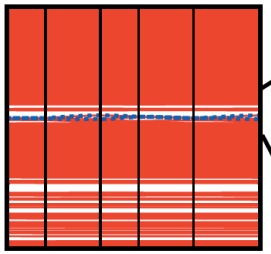
Model Construction

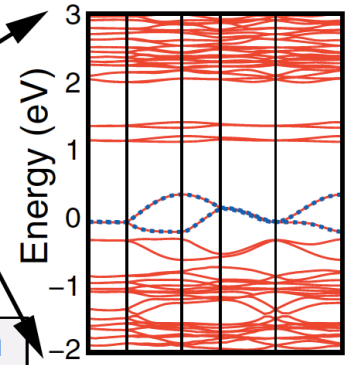
Schematic procedure of three–stage scheme thanks to energy hierarchy structure

1. Global electronic structure by DFT

far from Fermi level

tens eV





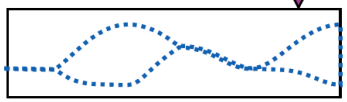
2. downfolding

constrained RPA

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

Low–energy effective Hamiltonian

1/10-1/100 eV



"target band"

3. Low-energy solver

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

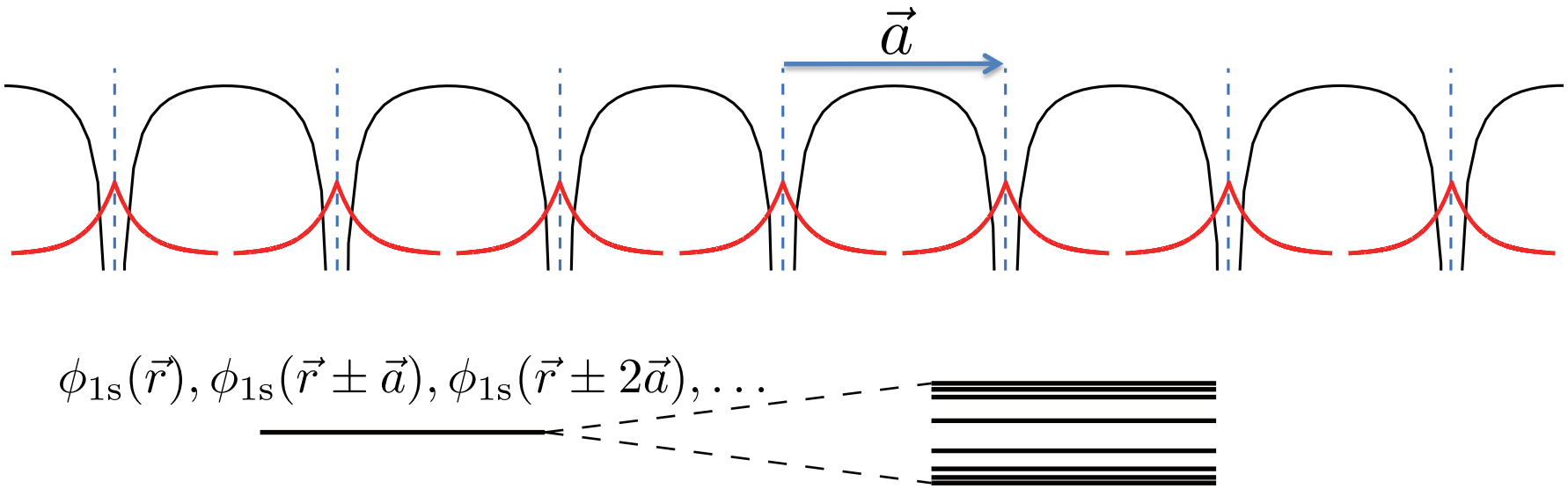
Model Hamiltonian derived by DFT+DMFT, Wannier+cRPA

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

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

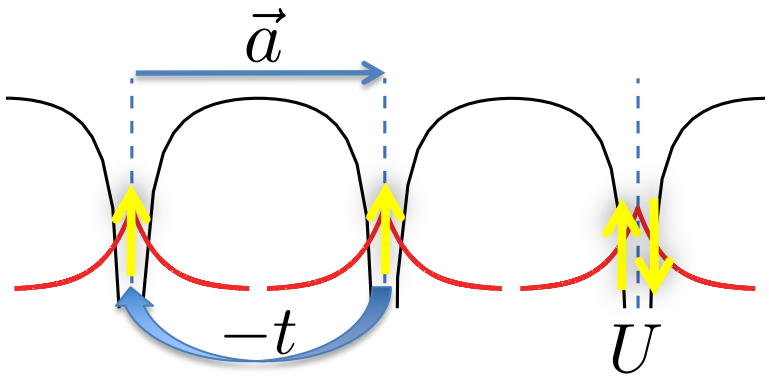
Model of Many-Body Electrons

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



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

-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

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

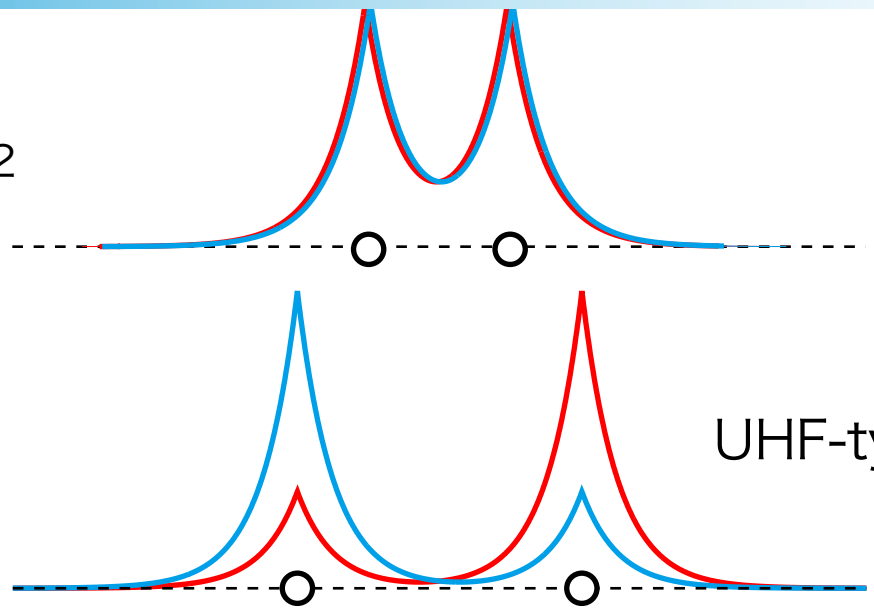
1D Hubbard model (periodic boundary condition, *L* site)

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

cf.) Bethe ansatz, Tomonaga-Luttinger liquid

Hydrogen Molecule

H_2

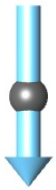


UHF-type wave function

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

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

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



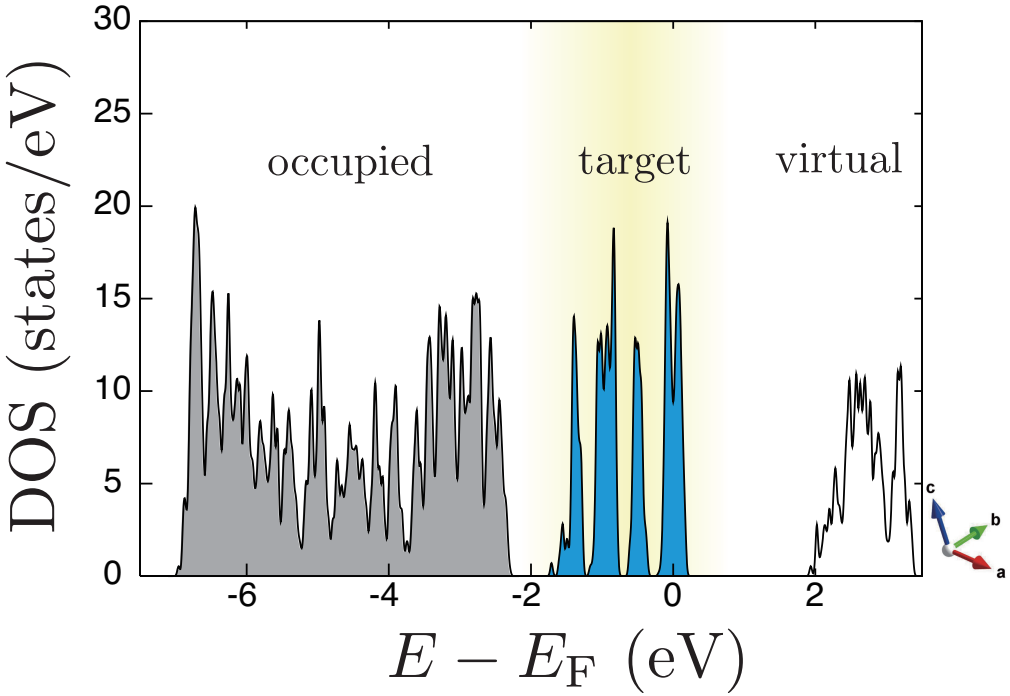
$$J = 4t^2/U$$

Singlet ground state

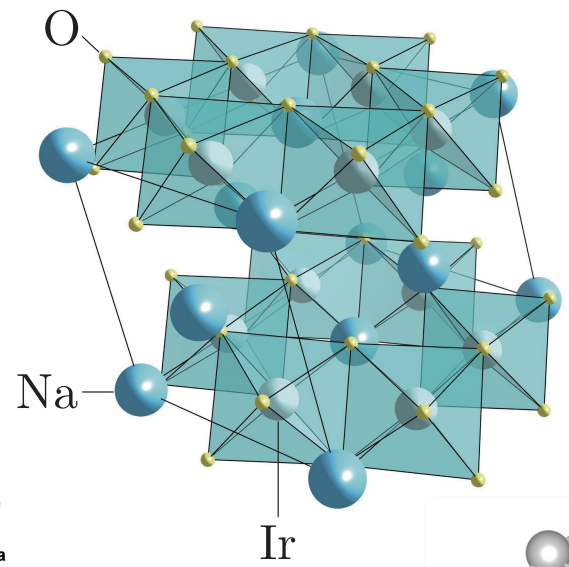
Construction of Effective Hamiltonians: An Example

- Target Hilbert space expanded by localized Wannier orbitals

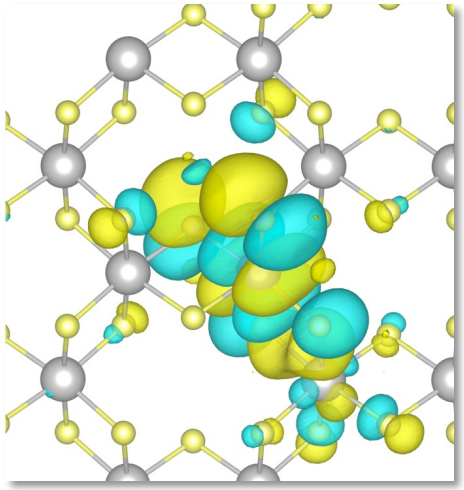
DFT result for energy spectrum



Souza-Marzari-Vanderbilt



Na_2IrO_3



- Effective Coulomb interactions in target space
  Renormalization due to
  infinite virtual particle-hole excitations
  ← Constrained random phase approximation

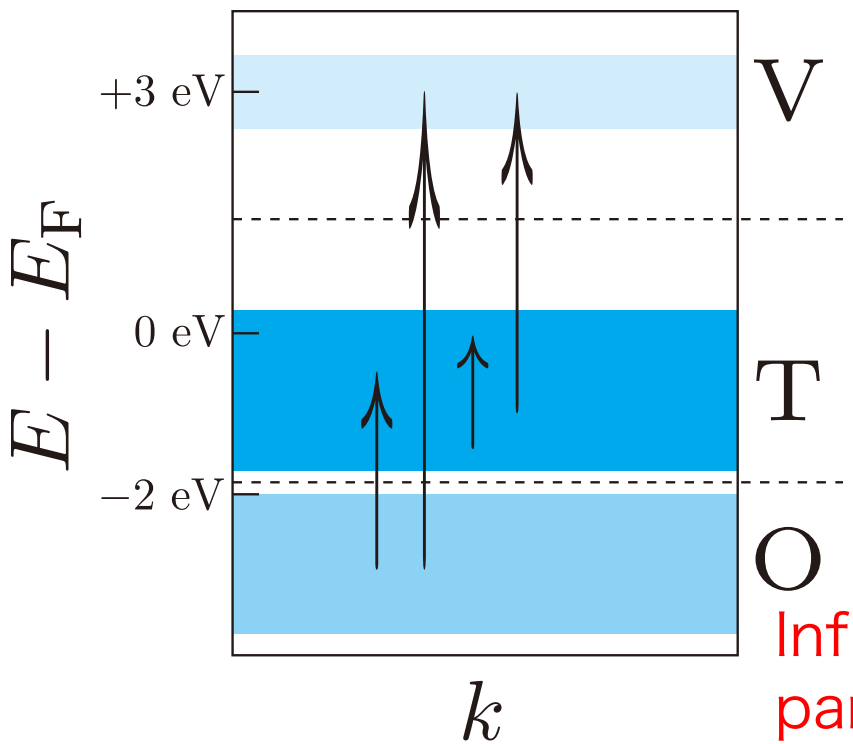
Imada & Miyake, J. Phys. Soc. Jpn. **79**, 112001 (2010)

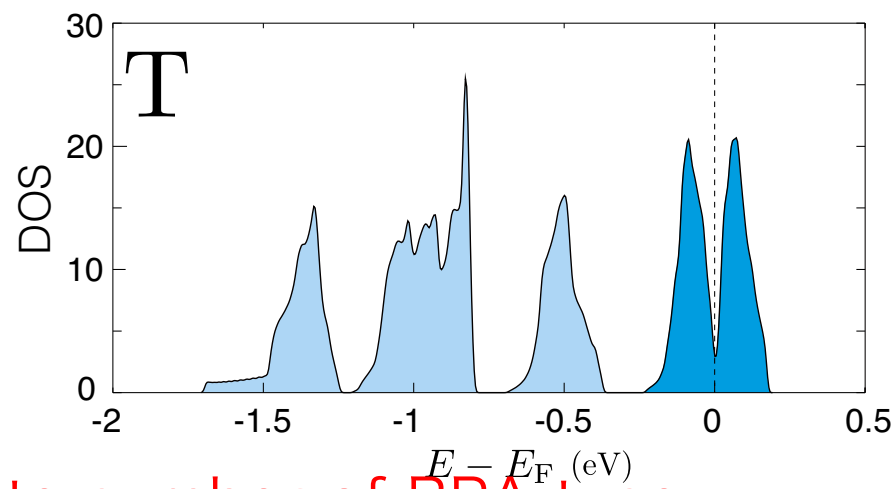
Constrained RPA Estimate on Coulomb Interaction of t_{2g}-Hubbard

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

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

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





Infinite number of RPA-type particle-hole excitations

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

Hopping

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

Trigonal+orbital-dependent μ

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

SOC

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

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

Coulomb

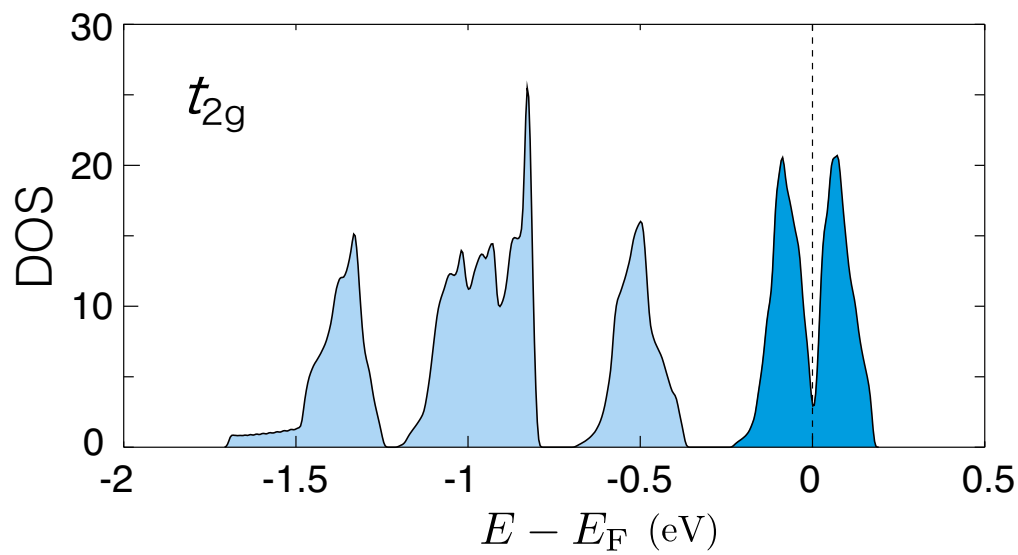
$$\hat{H}_U = U \sum_\ell \sum_{a=yz,zx,xy} \hat{n}_{\ell a\uparrow} \hat{n}_{\ell a\downarrow}$$

$$+ \sum_{\ell \neq m} \sum_{a,b} \frac{V_{\ell,m}}{2} (\hat{n}_{\ell a\uparrow} + \hat{n}_{\ell a\downarrow})(\hat{n}_{mb\uparrow} + \hat{n}_{mb\downarrow})$$

$$+ \sum_\ell \sum_{a<b} \sum_\sigma [U' \hat{n}_{\ell a\sigma} \hat{n}_{\ell b\overline{\sigma}} + (U' - J_{\text{H}}) \hat{n}_{\ell a\sigma} \hat{n}_{\ell b\sigma}]$$

$$+ J_{\text{H}} \sum_\ell \sum_{a \neq b} \left[\hat{c}^\dagger_{\ell a\uparrow} \hat{c}^\dagger_{\ell b\downarrow} \hat{c}_{\ell a\downarrow} \hat{c}_{\ell b\uparrow} + \hat{c}^\dagger_{\ell a\uparrow} \hat{c}^\dagger_{\ell a\downarrow} \hat{c}_{\ell b\downarrow} \hat{c}_{\ell b\uparrow} \right]$$

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



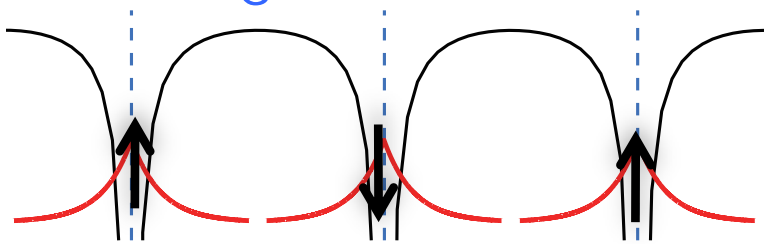
DFT: Elk (FLAPW)
http://elk.sourceforge.net
Vxc: Perdew-Wang 1992

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

Heisenberg (Spin) Hamiltonian from Strong Coupling Expansion

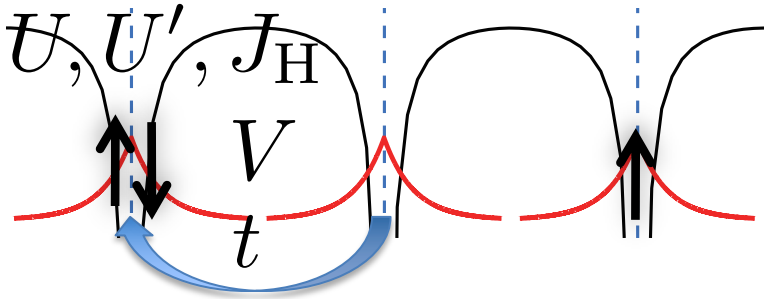
Unperturbed atomic Hamiltonian

2^N degenerated states



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).

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

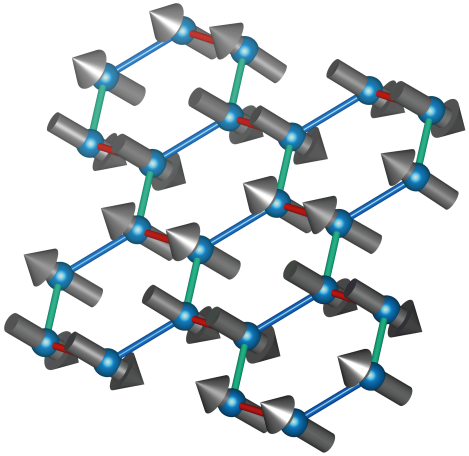
$$\mathcal{J}_X = \begin{bmatrix} \mathbf{-23.9} & -3.1 & -8.4 \\ -3.1 & 3.2 & 1.8 \\ -8.4 & 1.8 & 2.0 \end{bmatrix} (\mathrm{meV}) \qquad \mathcal{J}_{Z_{2\mathrm{nd}}} = \begin{bmatrix} -0.8 & 1.0 & -1.4 \\ 1.0 & -0.8 & -1.4 \\ -1.4 & -1.4 & -1.2 \end{bmatrix} (\mathrm{meV})$$

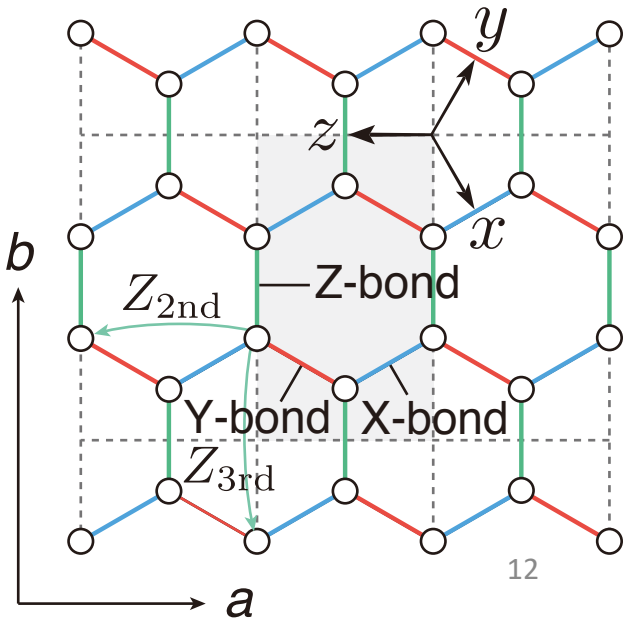
$$\mathcal{J}_Y = \begin{bmatrix} 3.2 & -3.1 & 1.8 \\ -3.1 & \mathbf{-23.9} & -8.4 \\ 1.8 & -8.4 & 2.0 \end{bmatrix} (\mathrm{meV}) \qquad \mathcal{J}_3 = \begin{bmatrix} 1.7 & 0.0 & 0.0 \\ 0.0 & 1.7 & 0.0 \\ 0.0 & 0.0 & 1.7 \end{bmatrix} (\mathrm{meV})$$

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

Ground state:
Zigzag order
agrees with experiments

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





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}He, 1965)
  Ceperley-Chester-Kalos (^{3}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: $\vec{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_M)$

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

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

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

$$E = -77.5 \text{ eV}$$

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

Screening of ionic Coulomb force by the other electrons

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

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

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: $\vec{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_M)$

When analytical methods are not available
→ Energy expectation values evaluated by MC

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

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

・Volume: L^3

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

MC for real space configuration instead of Riemann sum

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

Liquid Helium 4 (boson): LJ Hamiltonian

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

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

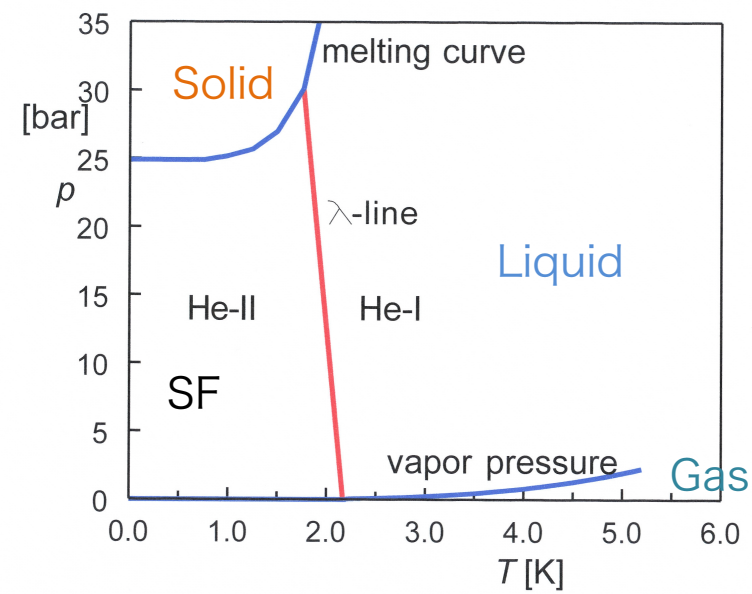
$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

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

$$\sigma = 2.556\ \mathring{A}$$
$$\epsilon = 1.41102 \times 10^{-22}\ \mathrm{J}$$

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

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

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

cf.) Partition function of classical gas & Boltzmann weight

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

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

VWF of Liquid Helium 4

How to choose vwf?

$$f(r) = \exp\left[-(a_1/r)^{a_2}\right] \qquad a_1, a_2 : \text{ variational parametres}$$

LJ interaction is repulsive at a short distance

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

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

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

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

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

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

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

Relation to WF in 1st quantization form

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

2nd Quantization Form

Hamiltonian

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

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

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

Expectation value

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

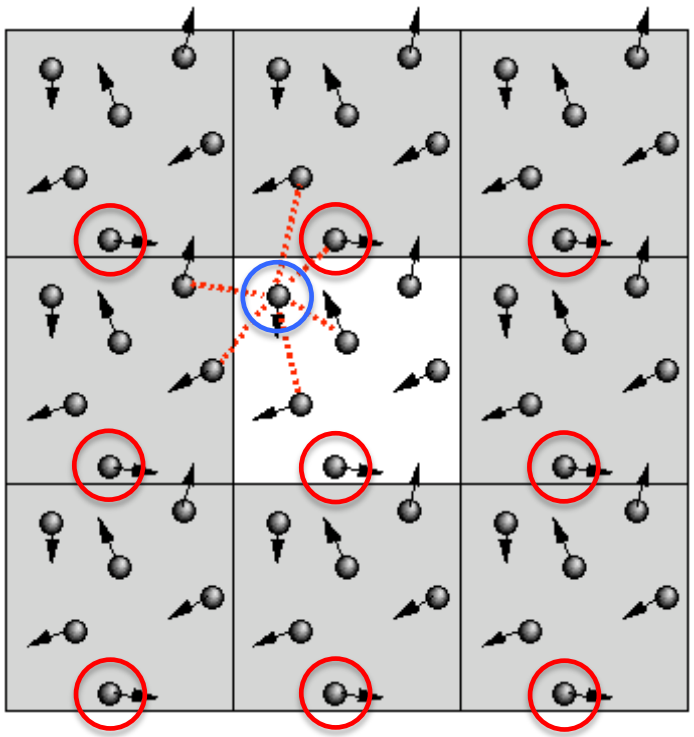
Weight/probability $P_N(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \frac{1}{V^N}\frac{|\langle\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle}$

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

Metropolis

Probability distribution, instead of Boltzmann weight

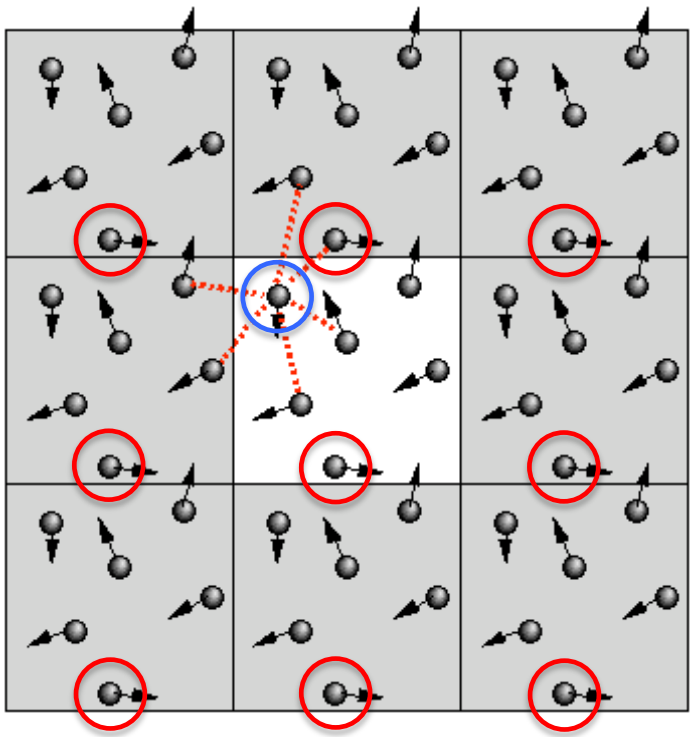
$$P_N(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N) = \frac{|\psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N)|^2}{\int \prod_i d^3 r'_i |\psi(\vec{r'}_1, \vec{r'}_2, \cdots, \vec{r'}_N)|^2}$$

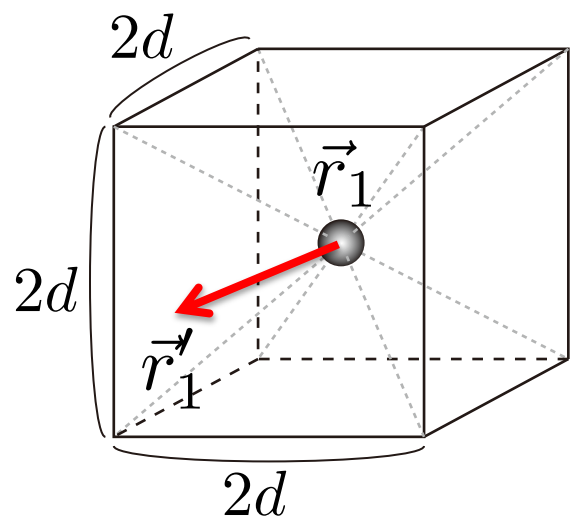


Short-ranged interactions
→Nearest neighbor mirror image

cf.) For electron gas, Ewald summation

Trial Configuration





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

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

→**Metropolis algorithm**

2 Point Distribution Function: $g(r)$

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

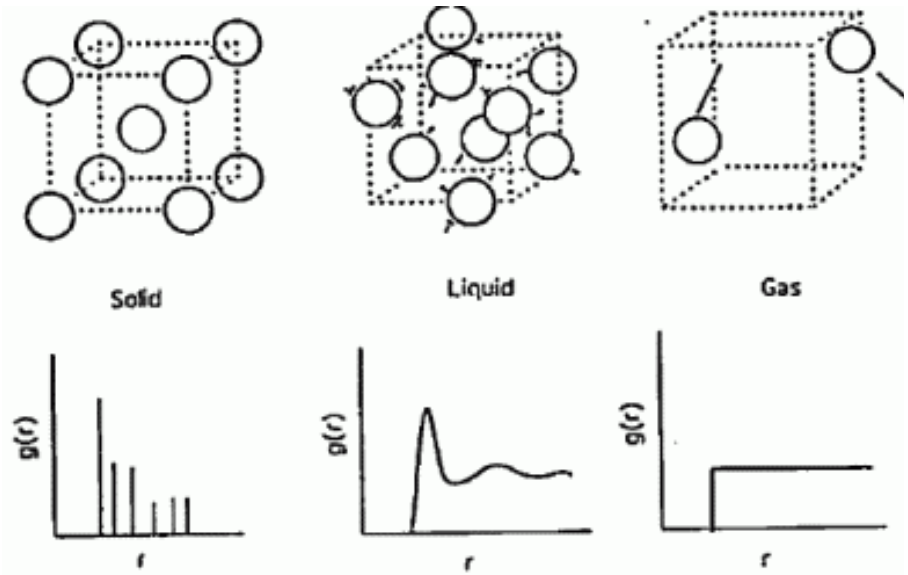
where $\rho = N/\Omega$.

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

where we suppose translational invariance of the system. Here $N^{(i)}_{[r,r+\Delta)}$ 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}He

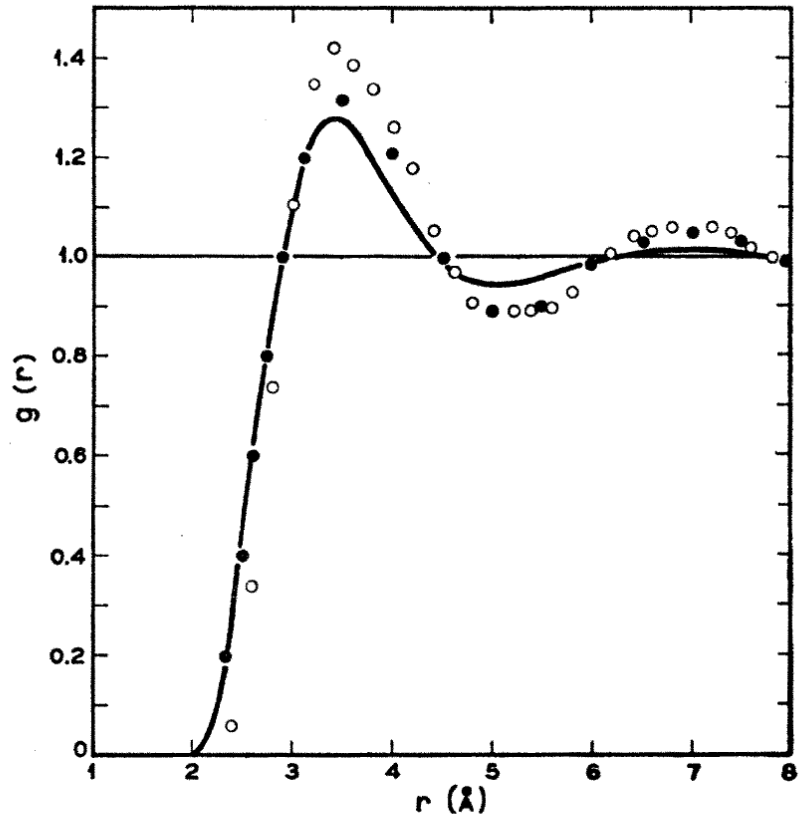
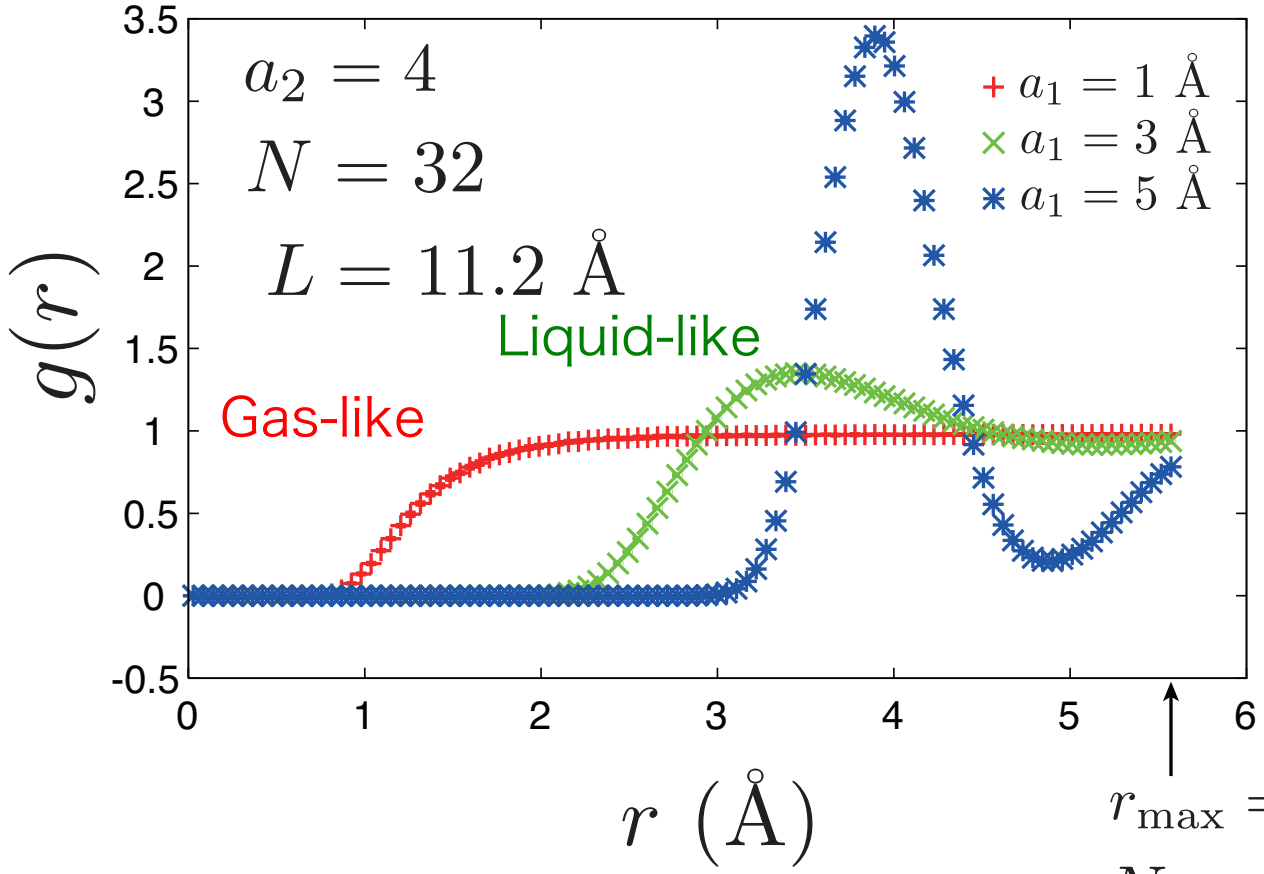


FIG. 5. Comparison of the two-body correlation function with experiment. The solid line is the theoretical curve, the solid circles are computed from the x-ray data of Gordon *et al.* (Ref. 26) and the open circles are computed from the neutron data of Henshaw (Ref. 27).

2 Point Distribution Function: $g(r)$



$r_{\max} = L/2$

$N_{dr} = 100$

Volume per perticle: 43.904 Å^3

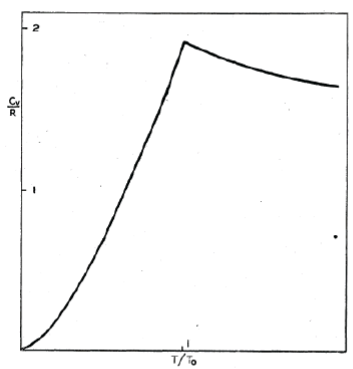
$$\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \prod_{i<j;i,j=1}^{N} f(r_{ij})$$

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

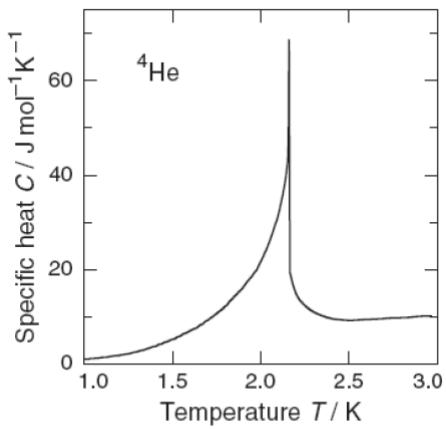
Comparison with Experiments

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}He

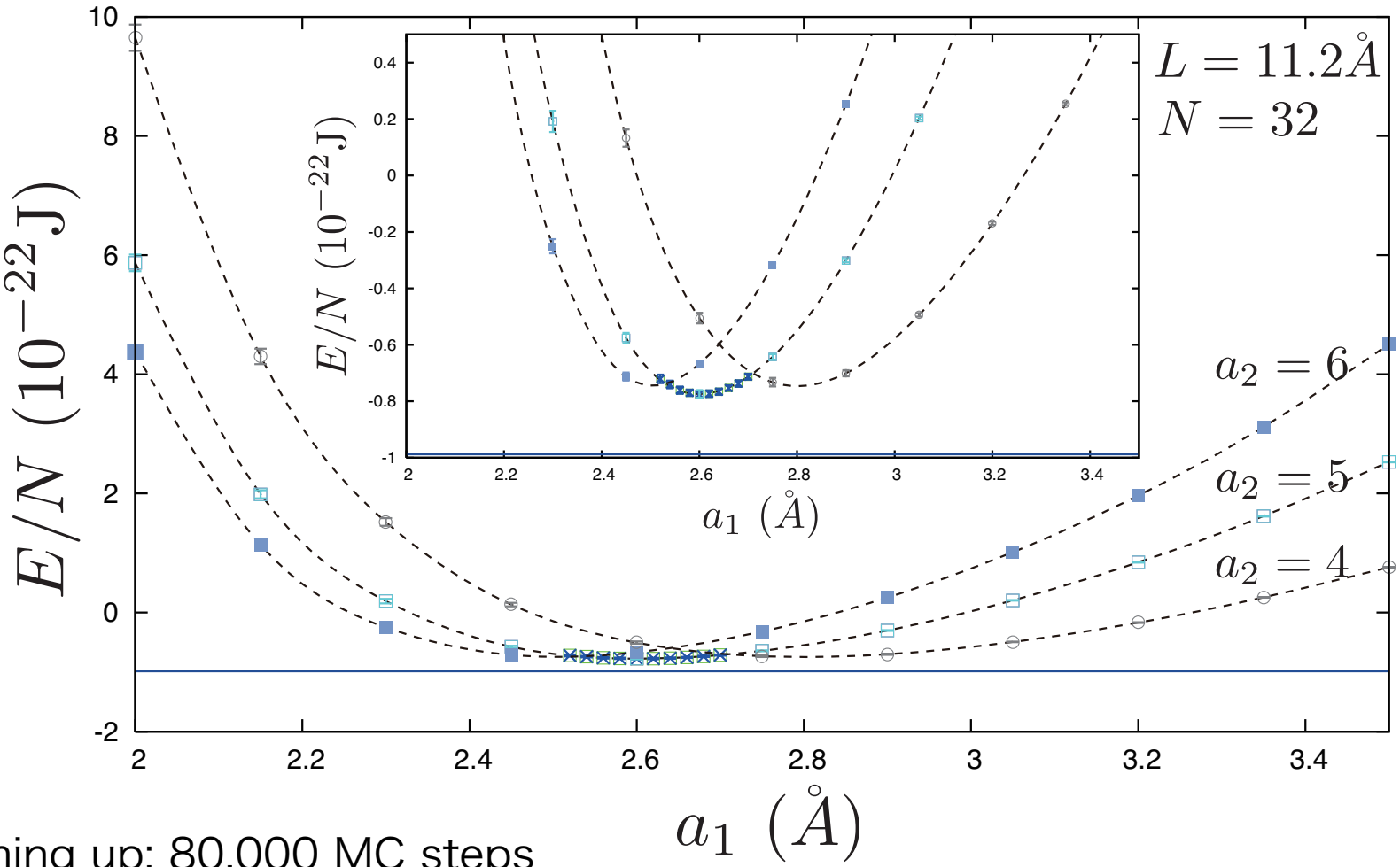


Specific heat of an ideal Bose-Einstein gas.



Energy

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



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

How Is VWF Accurate?

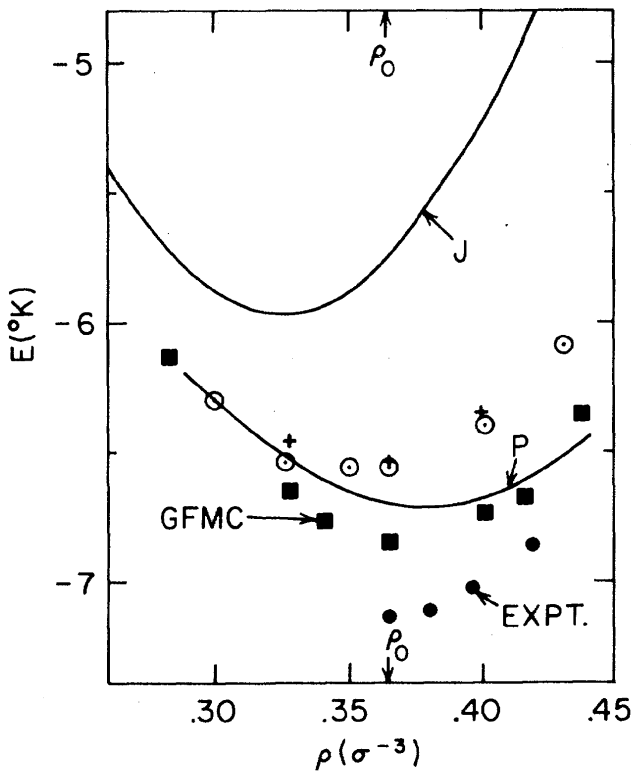


FIG. 1. Comparison of energy vs density. *J* indicates pure Jastrow results of Ref. 10; *P* indicates triplet calculations of Ref. 5; experimental results from Ref. 11; exact Lennard-Jones from Ref. 3; cross indicates present calculation; dot in circle indicates results from Ref. 4.

Origin of error:
- -Choice of vwf
- -LJ interaction

10^{-22} J = 7.246 K

$\rho_0 \sigma^3$=0.3648
(Stable volume in experiment at zero pressure)

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

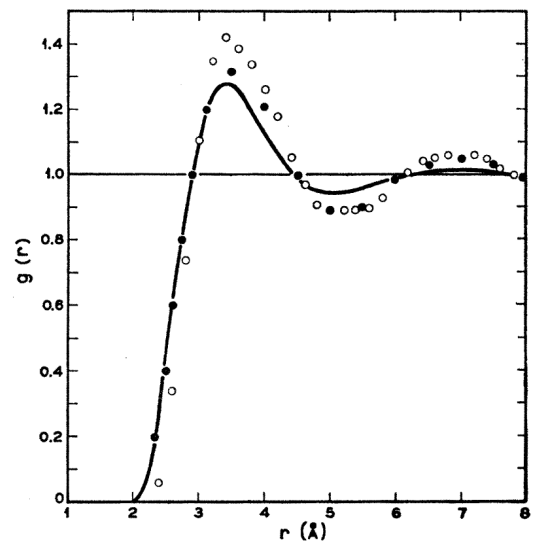
K. Schmidt, M. H. Kalos, M. A. Lee, and G. V. Chester, Phys. Lett. Rev. 45, 573 (1980)

Sample Code for ^{4}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)



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Liquid Helium 3 (fermion): LJ Hamiltonian

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

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

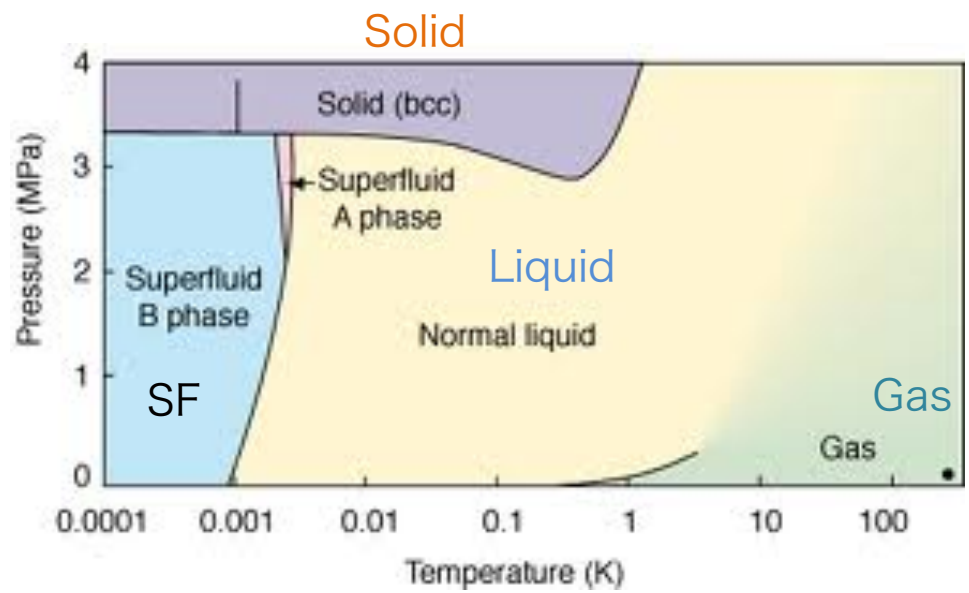
$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

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

$$\sigma = 2.556\ \mathring{A}$$

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

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}He, electron gas)

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

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

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

Relation to WF in 1st quantization form

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

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

1 st quantiztion VWF

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

Slater determinant originating from Fermi statistics

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

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

Jastrow VWF for Liquid Heliem 3

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

$$\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_\uparrow+N_\downarrow}) = \psi_{\mathrm{B}}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_\uparrow+N_\downarrow}) \times D_\uparrow(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_\uparrow}) D_\downarrow(\vec{r}_{N_\uparrow+1}, \ldots, \vec{r}_{N_\uparrow+N_\downarrow})$$

Bosonic wf:

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

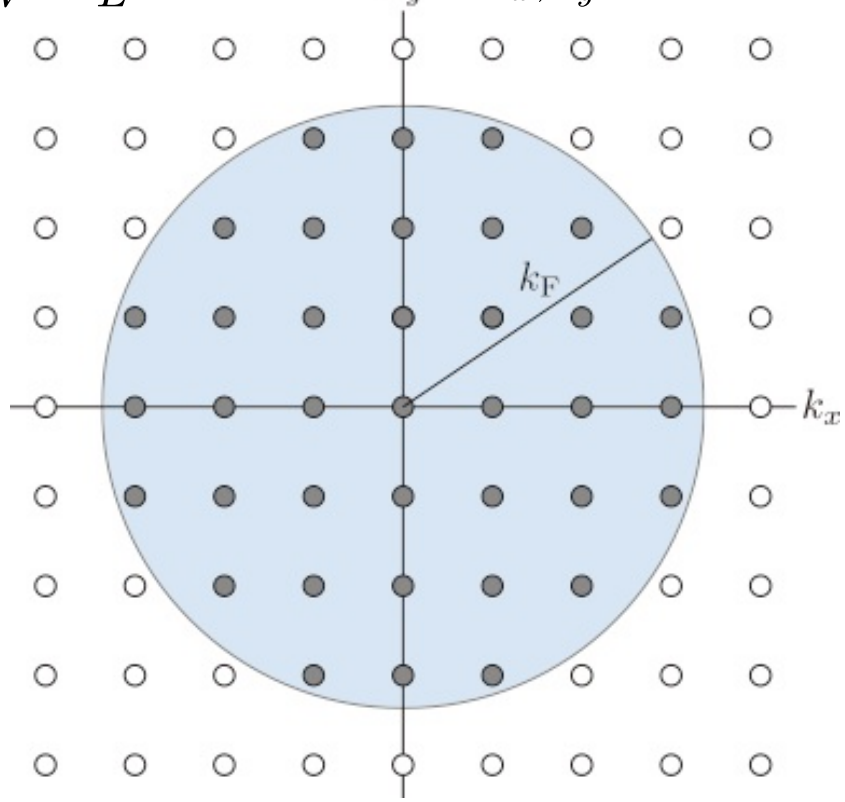
Fermi Sea

Fermi sea: WF for free fermions

$$(k_x, k_y) = \left(\frac{2\pi\ell_x}{L}, \frac{2\pi\ell_y}{L}\right)$$

$$V = L^2 \qquad \ell_x, \ell_y \in \mathbf{Z}$$

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

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

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

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

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

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

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

$$A = D_\uparrow$$

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

$$\vec{u}^T = (1,0,\ldots,0)$$

$$\vec{v}^T = (e^{i\vec{k}_1\cdot\vec{r}_1'}, e^{i\vec{k}_2\cdot\vec{r}_1'}, \ldots, e^{i\vec{k}_{N_\uparrow}\cdot\vec{r}_1'}) - (e^{i\vec{k}_1\cdot\vec{r}_1}, e^{i\vec{k}_2\cdot\vec{r}_1}, \ldots, e^{i\vec{k}_{N_\uparrow}\cdot\vec{r}_1})$$

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

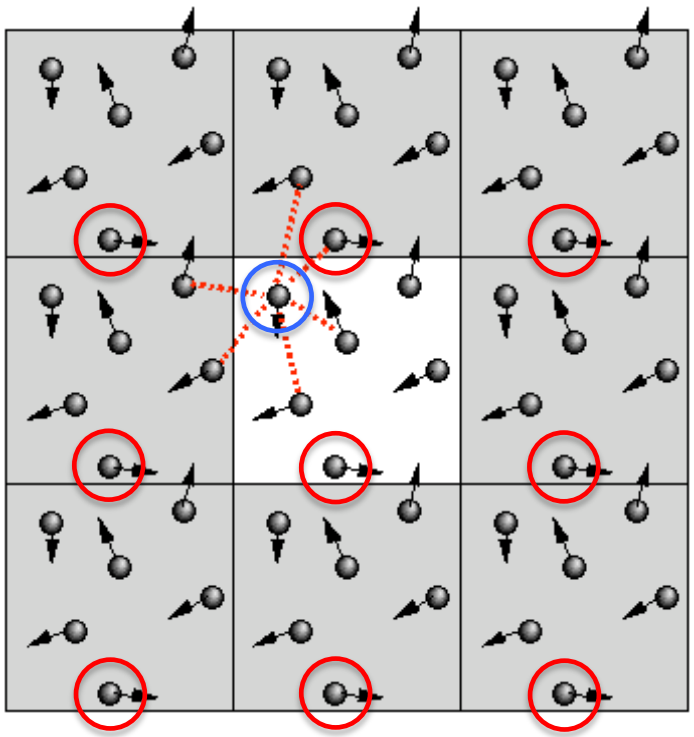
Iteration Steps

1. Generate an initial configuration and $D_\uparrow$ & $D_\downarrow$
2. do loop $1 \leqq i \leqq (N_\uparrow + N_\downarrow)^* M_{\text{warmup}}$
   Generate a new config. from old one by Metropolis
   Update $D_\uparrow$ & $D_\downarrow$ by Sherman-Morrison
3. do loop $1 \leqq i \leqq N_\uparrow + N_\downarrow$
   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

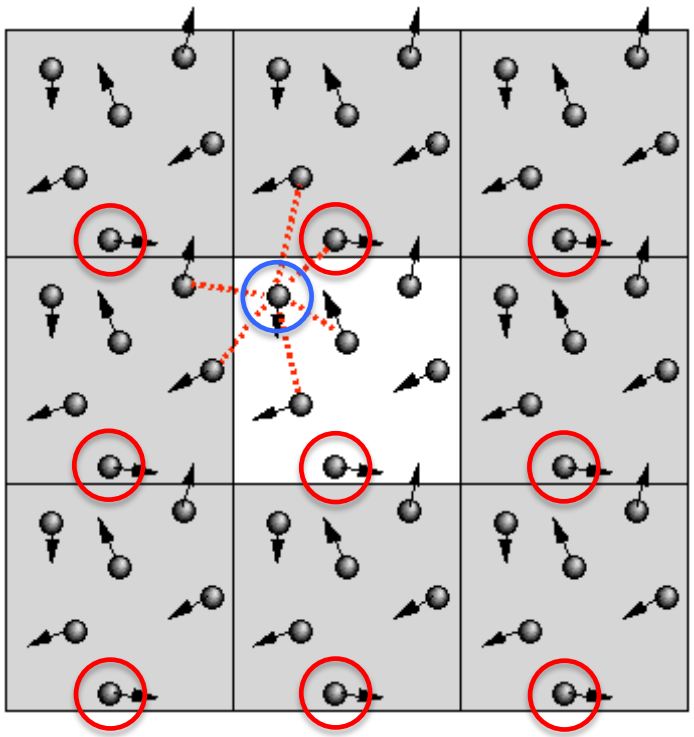
$$P_N(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N) = \frac{|\psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N)|^2}{\int \prod_i d^3 r'_i |\psi(\vec{r'}_1, \vec{r'}_2, \cdots, \vec{r'}_N)|^2}$$

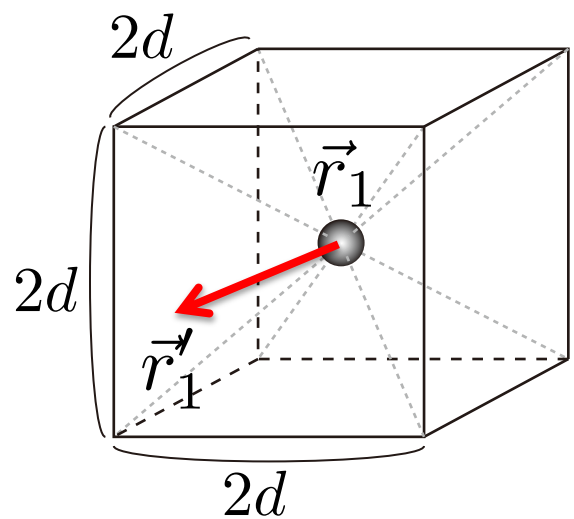


Short-ranged interactions
→Nearest neighbor mirror image

cf.) For electron gas, Ewald summation

Trial Configuration





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

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

→**Metropolis algorithm**

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

Parallel spins ↑ ↑

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

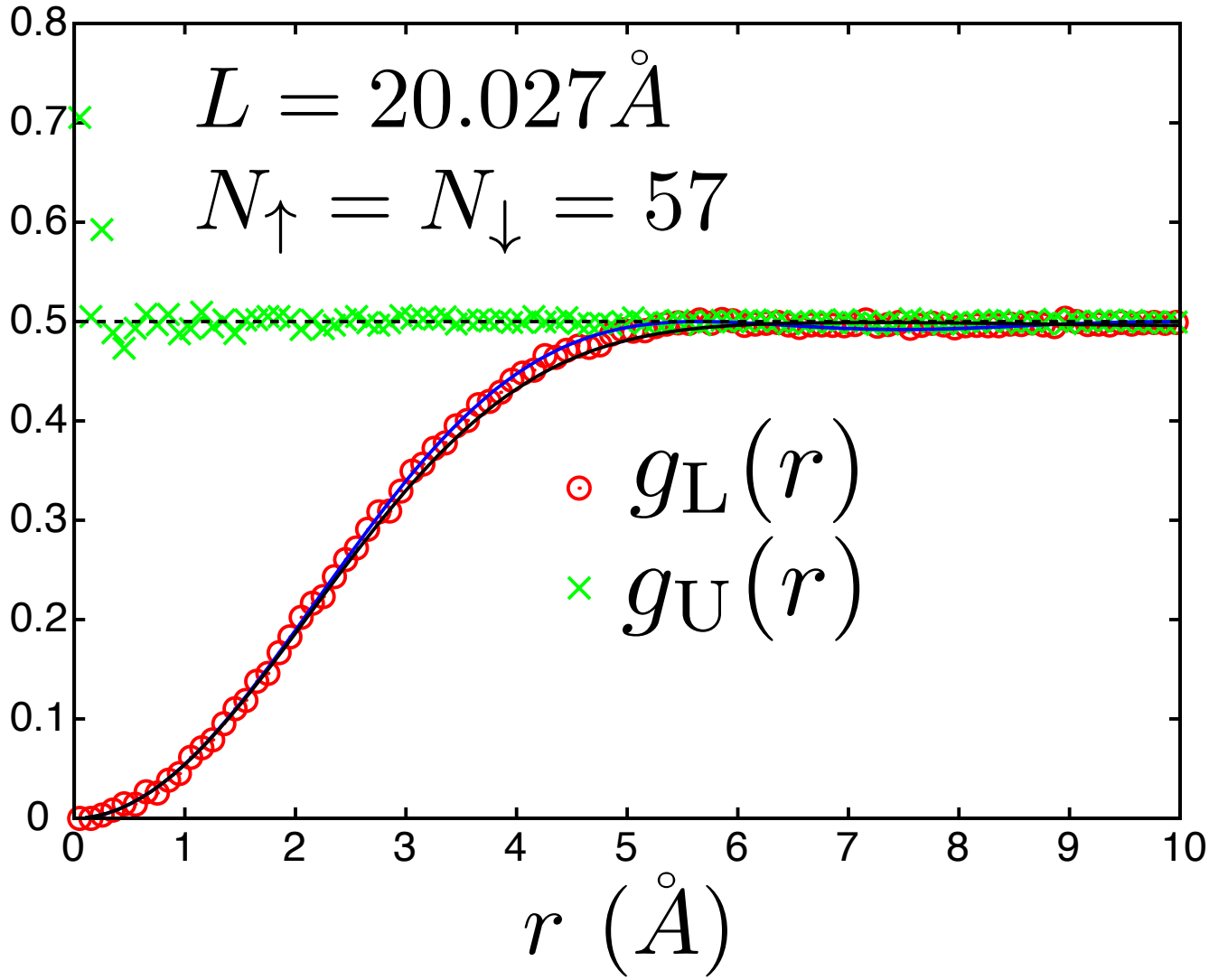
Antiparallel spins ↑ ↓

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

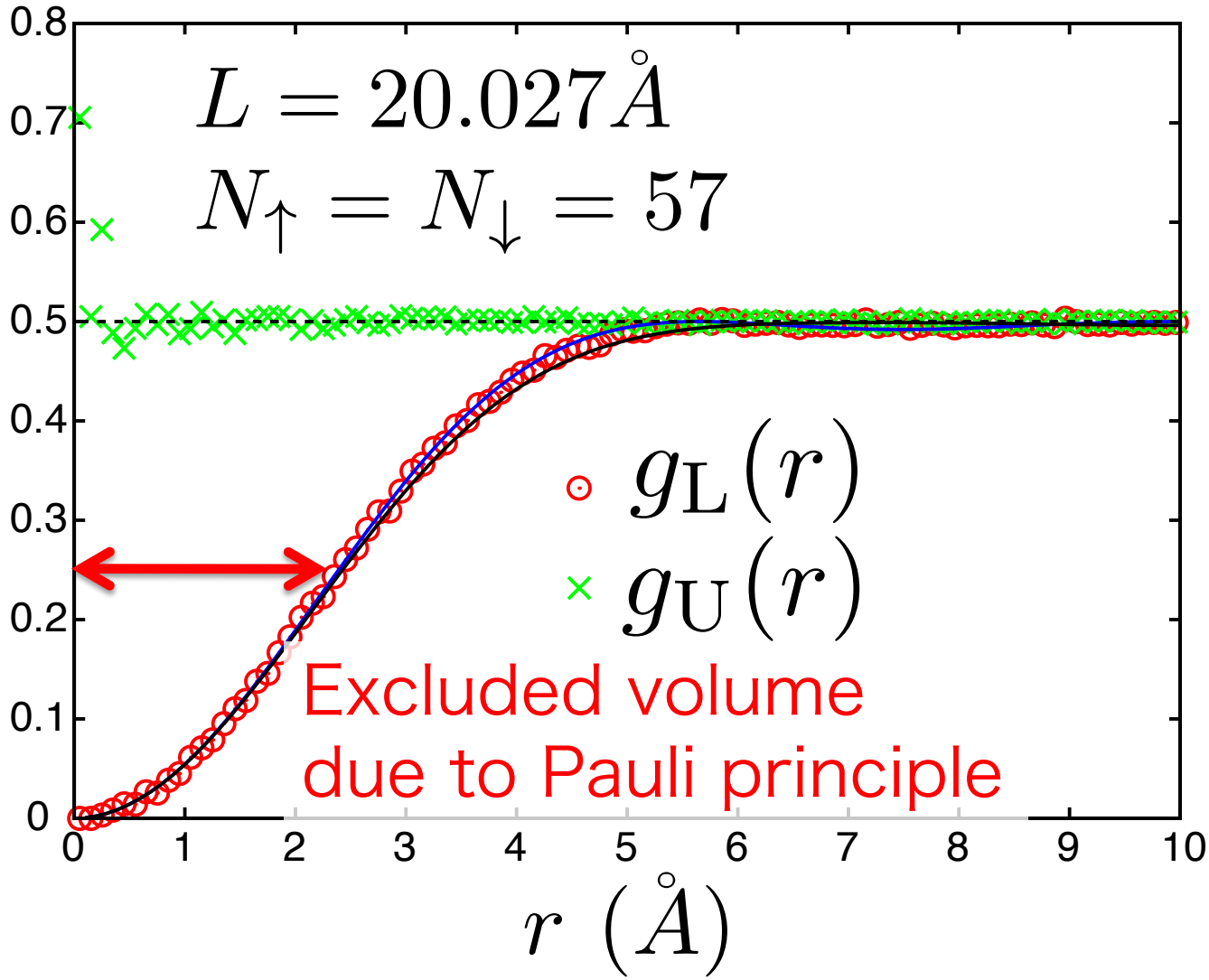
Expectation value

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

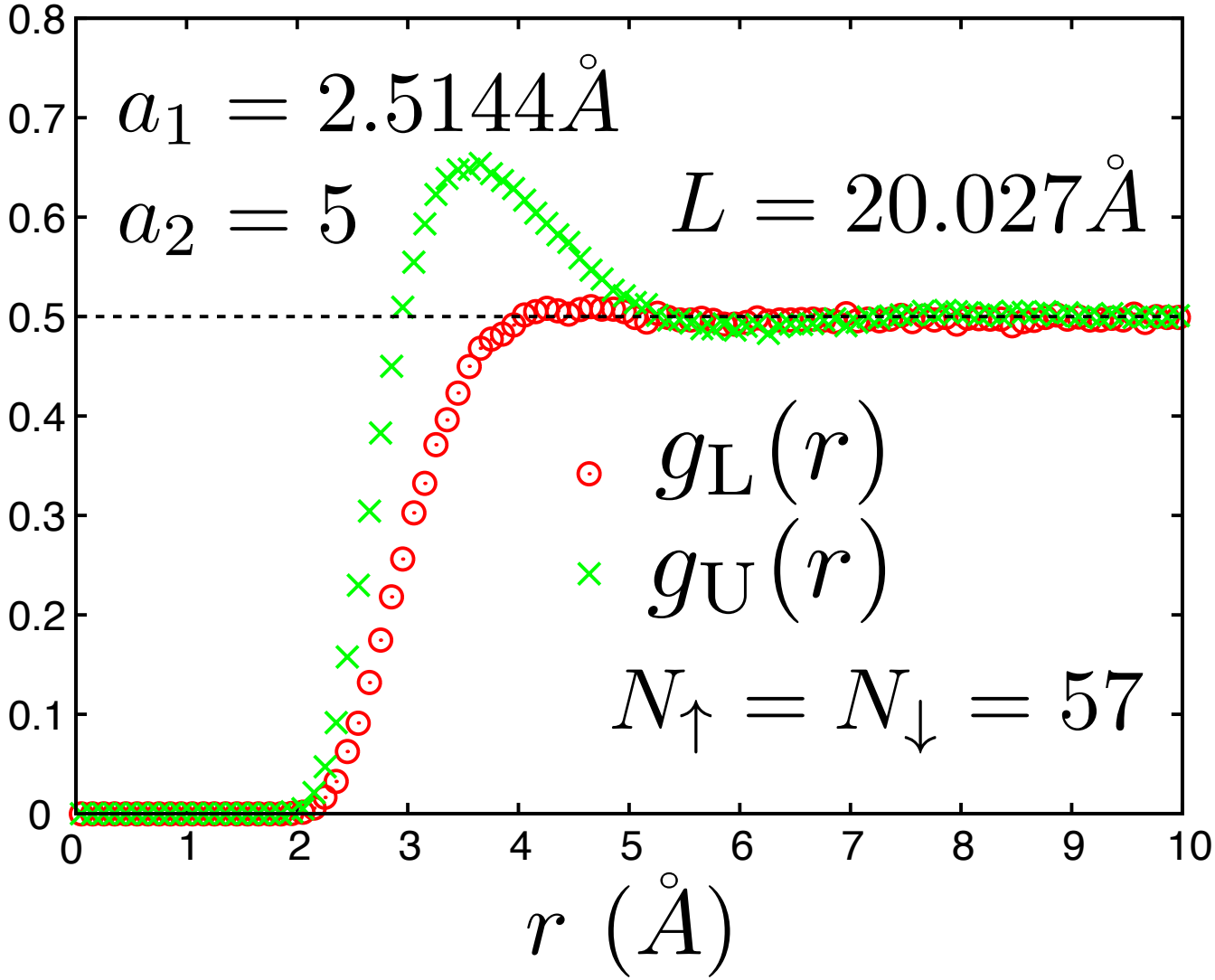
Free Fermions



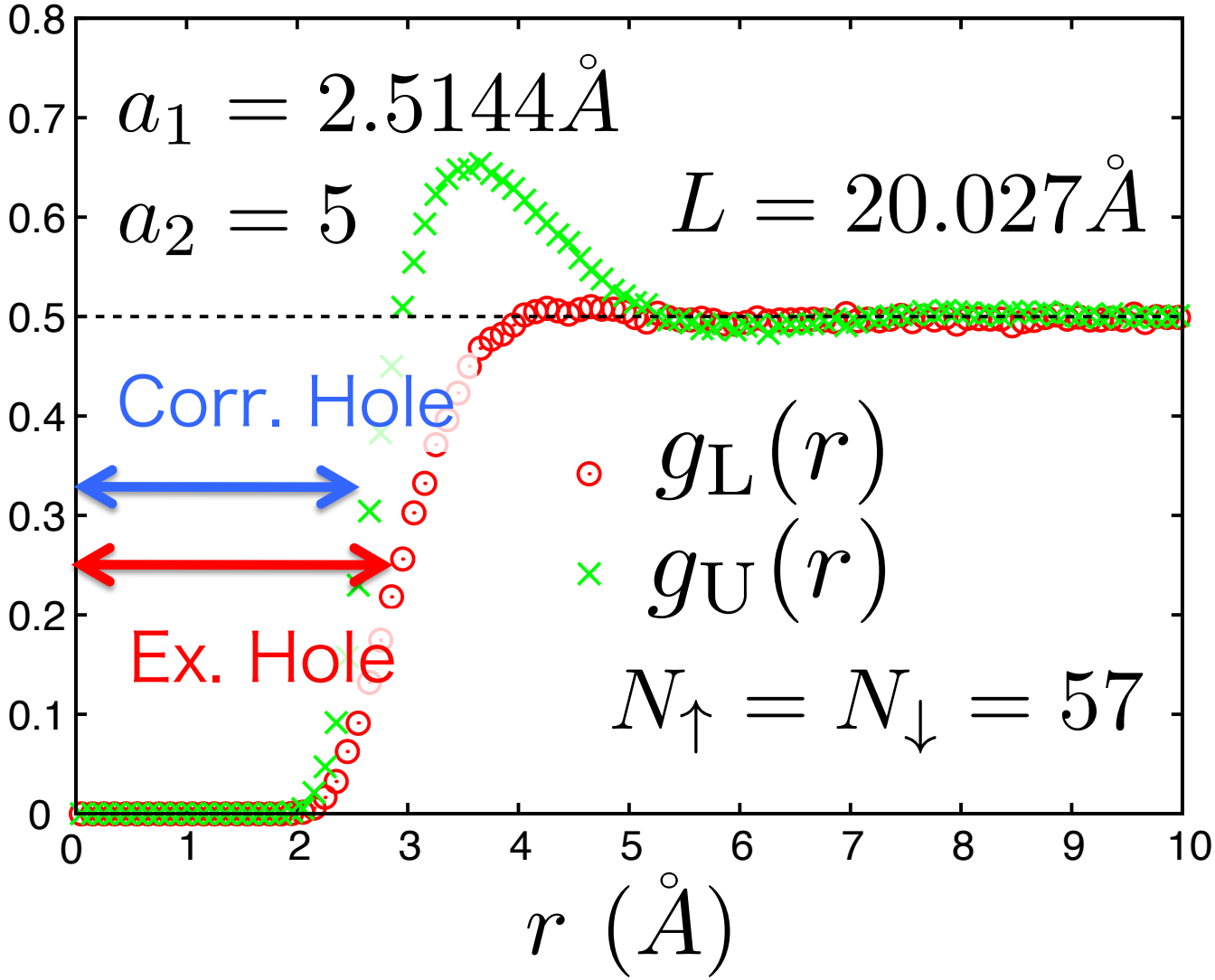
Exchange Hole Due to Pauli Principle



Liquid Helium 3



Many-Body Effect: Correlation Hole



Refinement VWF

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

Short range properties are enough?

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

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

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 ($r \to +\infty$)

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

Important for reproducing acoustic modes

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

Feynman-Cohen's back flow wf for excited states

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

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

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

Bijl-Feynman spectrum

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

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

Removal of Bias: Diffusion MC (Not a MCMC)

Imaginary-time evolution

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

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

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

$$\nabla^2_{\vec{R}} = \sum_i \nabla^2_i$$

Instead of direct imaginary-time evolution

Diffusion MC

$$f(\vec{R},\tau) = \psi(\vec{R})\Psi(\vec{R},\tau)$$

←Product of vwf and imaginary-time wf

Diffusion Driving force

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

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

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

Outline of Diffusion Equation

Diffusion equation

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

$$f(\vec{R}',\tau+\Delta\tau) = \int d^{3N}R\; G(\vec{R}',\vec{R},\Delta\tau) f(\vec{R},\tau)$$

$$G(\vec{R}',\vec{R},\Delta\tau) = \langle \vec{R}' | \exp\left[-\Delta\tau \hat{A}\right] | \vec{R}\rangle$$

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)

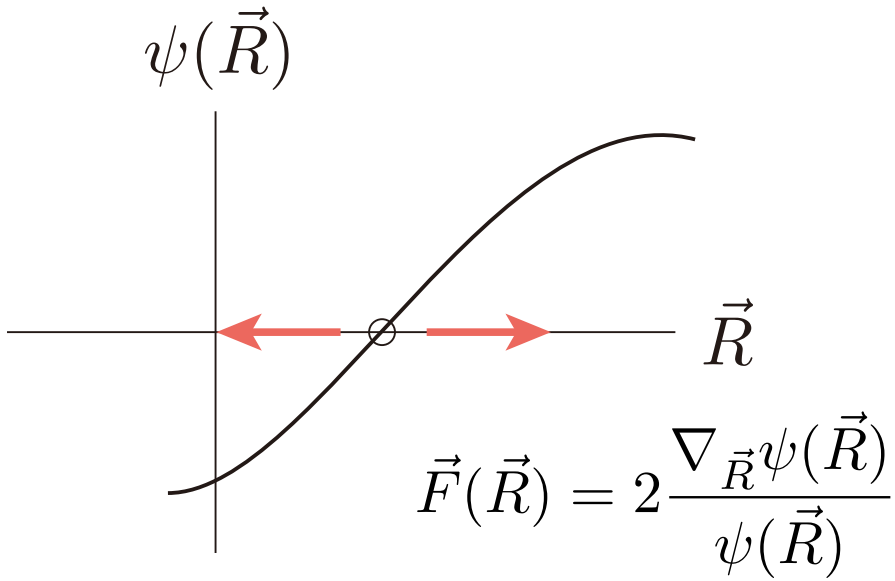
Introduction to numerical path integral (with a sample code):
Rubin H. Landau and M. J. Paez Mejia, Computational Physics
(John Wiley & Sons, Inc., 1997)
(邦訳) 計算物理学 (小柳義夫監訳, 朝倉書店)

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

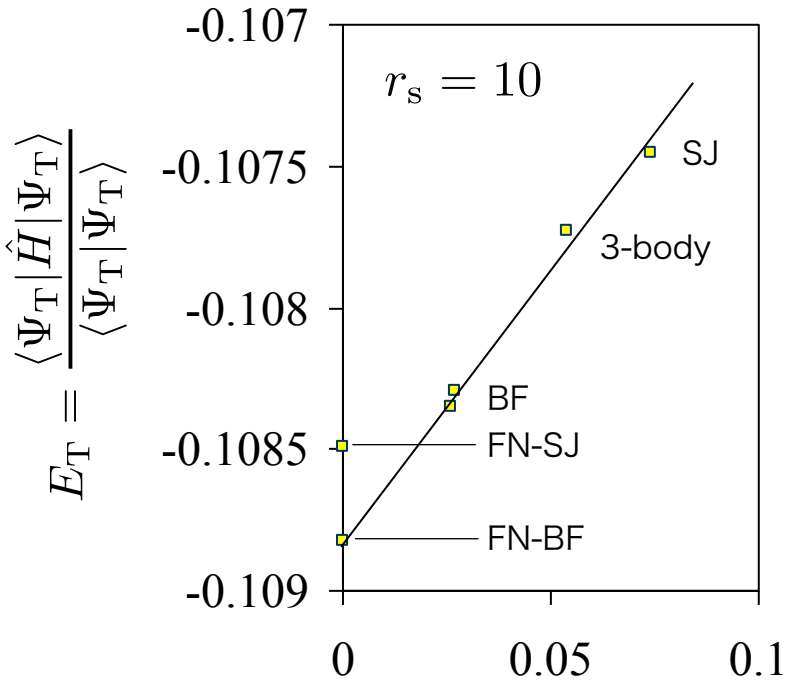
Kwon, Ceperley, & Martin, Phys. Rev. B 58, 6800 (1998);
Lecture materials of Prof. Ceperley

Electron gas

Density

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

Bohr radius:
$a_{\mathrm{B}} = 0.529$ Å



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

$$\mathrm{var}\ E_{\mathrm{T}} = \frac{\langle \Psi_{\mathrm{T}} | [\hat{H} - E_0]^2 | \Psi_{\mathrm{T}} \rangle}{\langle \Psi_{\mathrm{T}} | \Psi_{\mathrm{T}} \rangle}$$

$E=E(r_s)$ is used in LDA/GGA Perdew & Zunger, Phys. Rev. B 23, 5048 (1981)

Lecture Schedule

Classical

#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

Quantum

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

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

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

Hilbert space/Fock space (vector space)

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

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

(complex conjugate + transpose)

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

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

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

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