多体問題の計算科学

Computational Science for Many-Body Problems

#7 Quantum lattice models and numerical approaches

15:10-16:40 May 31, 2022

Quantum lattice models and numerical approaches

1. Quantum many-body physics
2. Description of quantum many-body (QMB) systems
3. Numerical approaches for QMB systems

Quantum Many-Body Physics

First Principle for quantum many-body systems

Principles that <u>elementary particles</u> (electrons,···) & <u>composite particles</u> (atoms, nuclei,···) follow

-Schrödinger/Dirac equation
 Hamiltonian
-Path integral
 Lagrangian (in 8th lecture and others)

Please be careful of applicability:
They could be approximations and effective ones.

For low-energy degrees of freedom:
spins, Cooper pairs, circuit,···

→Effective Hamiltonian/Lagrangian approach

An Example of Quantum Many-Body Systems

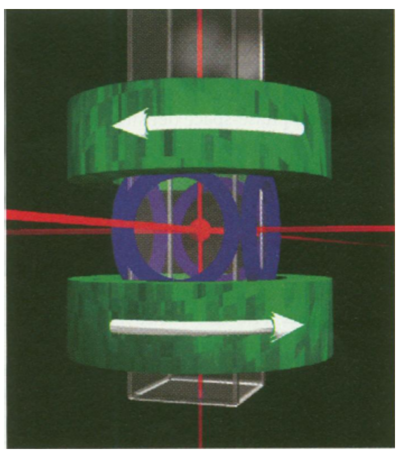
Cold atoms trapped in potential well

“Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor”
M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell,
Science 269, 198 (1995).

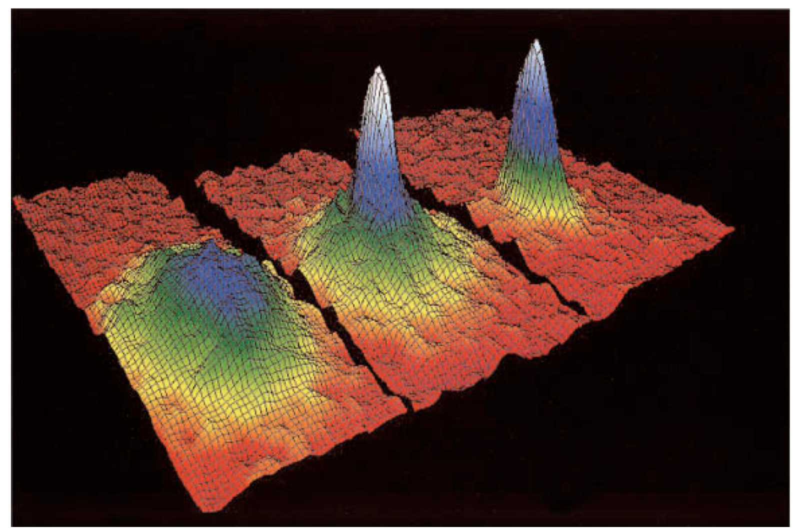
^{87}Rb

density: 2.5×10^{12} cm^{-3}
temperature: 170 nK

Magneto-optical trap



velocity distribution



“Theory of Bose-Einstein condensation in trapped gases”
F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari,
Rev. Mod. Phys. 71, 463 (1999).

A free particle in harmonic potential

Schrödinger equation $\hat{H}\phi(x) = E\phi(x)$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{k}{2}x^2\right]\phi(x) = E\phi(x)$$

$$k = m\omega^2$$

Given: Hamiltonian $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{k}{2}x^2$

Unknown: Wave function and energy $\phi(x),\ E$

A free particle in harmonic potential

-Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{k}{2}x^2$$

$$k = m\omega^2$$

-Wave function

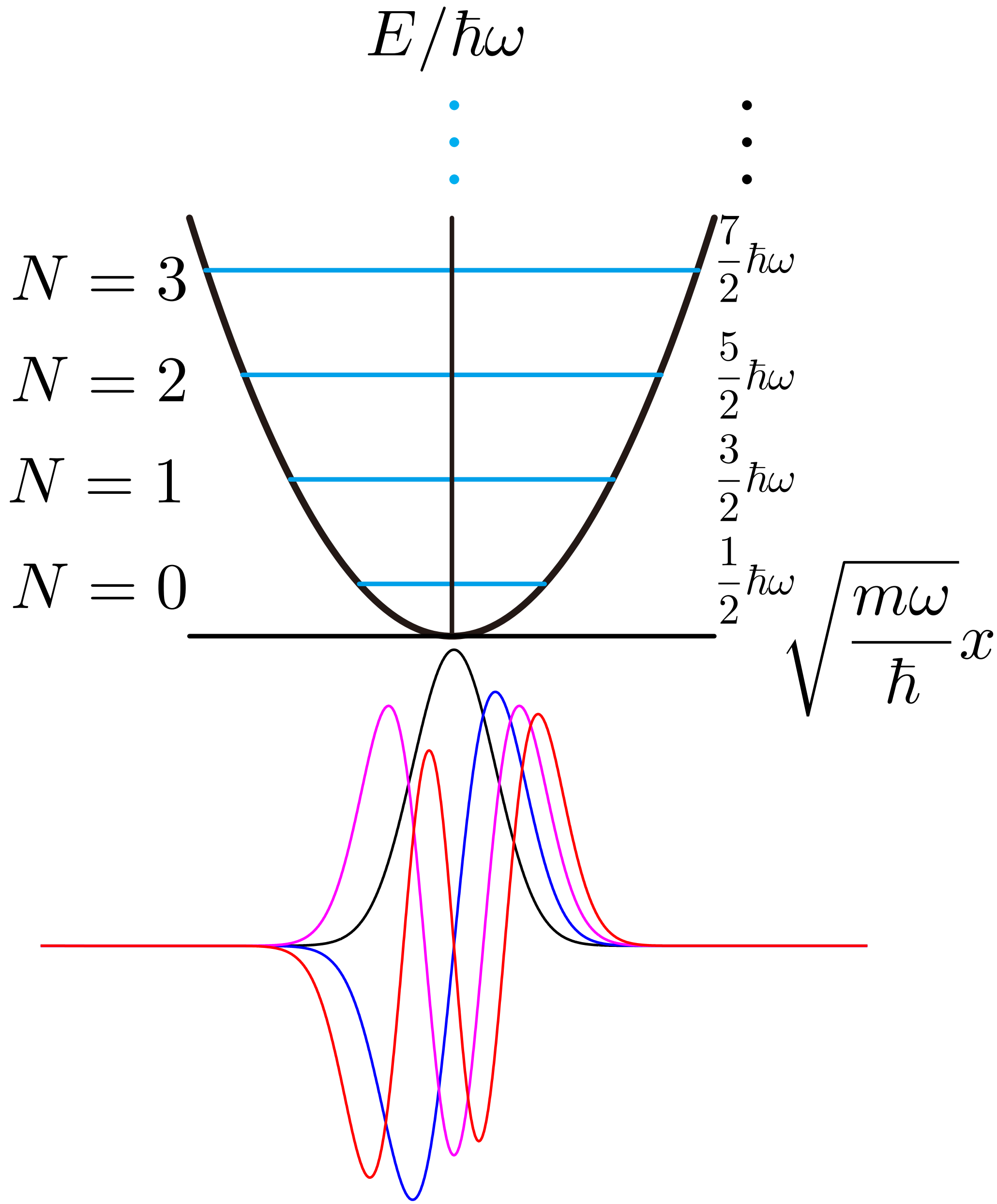
$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\phi_N(x) = \frac{1}{\sqrt{N!}}(\hat{\ell}^+)^N \phi_0(x)$$

ladder operator

$$\hat{\ell}^- = \sqrt{\frac{\hbar}{2m\omega}}\left(-\frac{\partial}{\partial x} + \frac{m\omega}{\hbar}x\right)$$

$$\hat{\ell}^+ = \sqrt{\frac{\hbar}{2m\omega}}\left(+\frac{\partial}{\partial x} + \frac{m\omega}{\hbar}x\right)$$



velocity distribution of ϕ_0 $\quad e^{-\frac{mv^2}{2\hbar\omega}}$

Indistinguishable → Particle statistics

Classical: Tracking particle positions
Quantum: Tracking occupation of bases

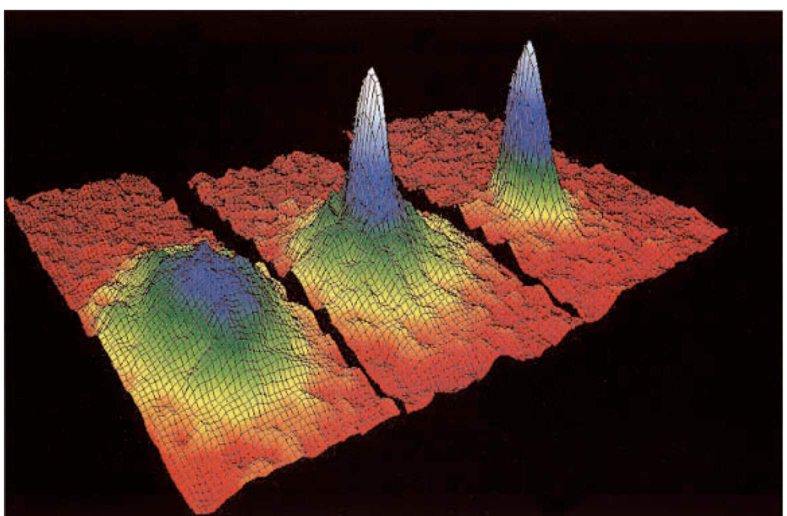
$$\hat{H} = \sum_j \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_j^2} + \frac{k}{2}x_j^2 \right)$$

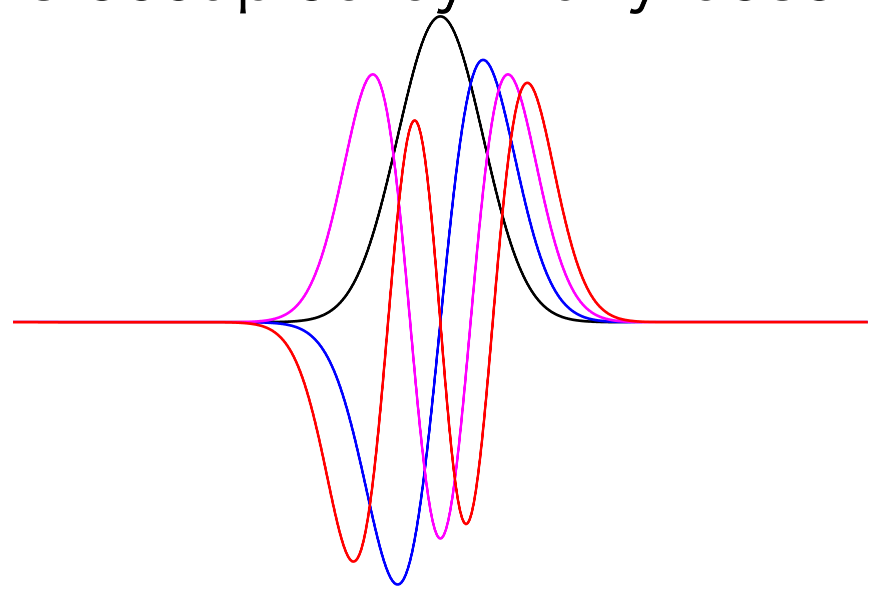
The indices cannot identify the individual particle

non-interacting system

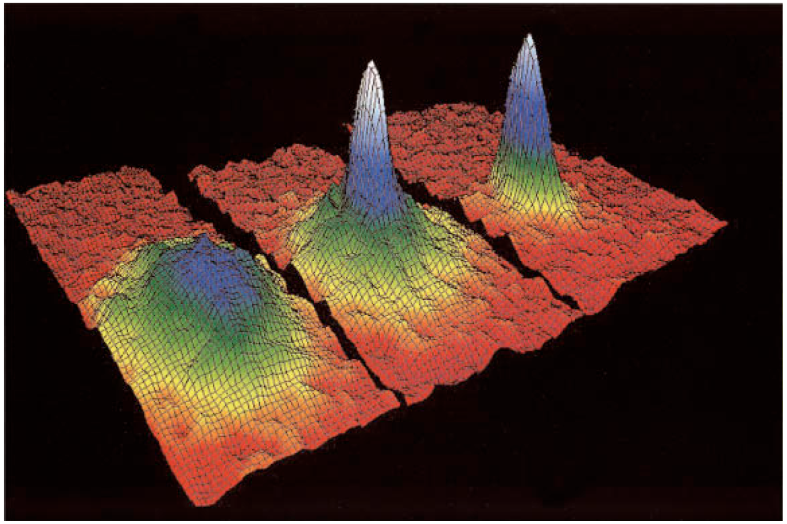
Example of Quantum phase: Bose-Einstein condensation

-A single state (ground state)is occupied by many bosons





Note: The distribution is wider than that estimated for non-interacting bosons



$$\hat{H} \neq \sum_j \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_j^2} + \frac{k}{2}x_j^2 \right)$$

Interaction among particles is relevant

Quantum Many-Body Problems in Physics

-Quantum chromodynamics
-Nuclear physics
-Condensed matter physics
-Quantum chemistry

Nucleus: Many-body systems consist of protons and neutrons

Hadrons (bryons and mesons): Quarks, antiquarks, and gluons

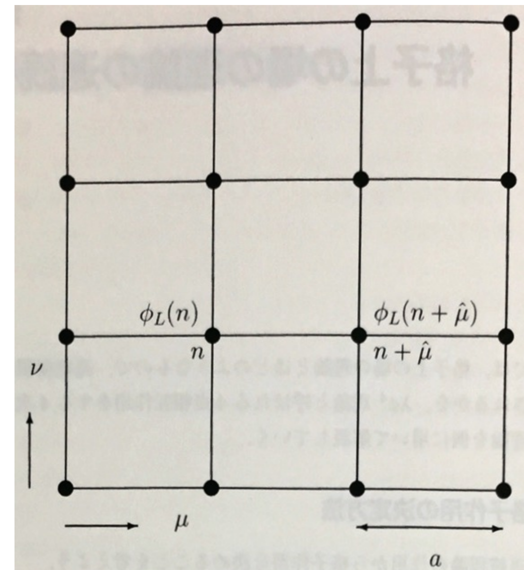
Lattice QCD: A Lattice Field Theory

Lattice QCD: Gauge & matter fields

A quantum field theory on a lattice

To define quantum field theory exactly
To regularize ultraviolet divergence

$$p/\hbar \leq \pi/a$$



Monte Carlo for guage and matter fields

SU(3) non-abelian gauge field

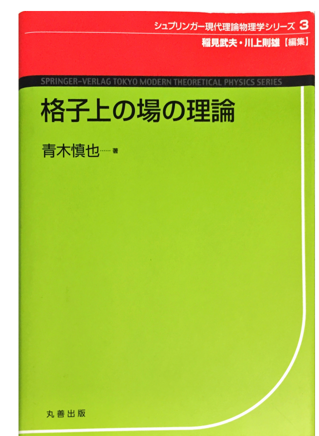
Applications:

-Nucleon-nucleon interaction Yukawa's pion
(Interaction among protons & neutrons)

"Nuclear Force from Lattice QCD"
N. Ishii, S. Aoki, and T. Hatsuda, Phys. Rev. Lett. 99, 022001 (2007)

-Mass of hadron consist of quark, antiquark, and gluon

"Light hadron masses from lattice QCD"
Z. Fodor and C. Hoelbling, Rev. Mod. Phys. 84, 449 (2012)



Lattice Field Theory for Condensed Matter

Lattice field theory:
Coulomb fields and massless Dirac electrons

Monte Carlo for guage and matter fields

Application to condensed matter physics:

-Mass generation due to chiral symmetry breakings
 in Dirac electrons in graphene

"Lattice field theory simulations of graphene"
J. E. Drut and T. A. Lähde, Phys. Rev. B 79, 165425 (2009)

Coulomb gauge field

Field theory: Massless to massive
Condensed matter: Semimetal to insulator

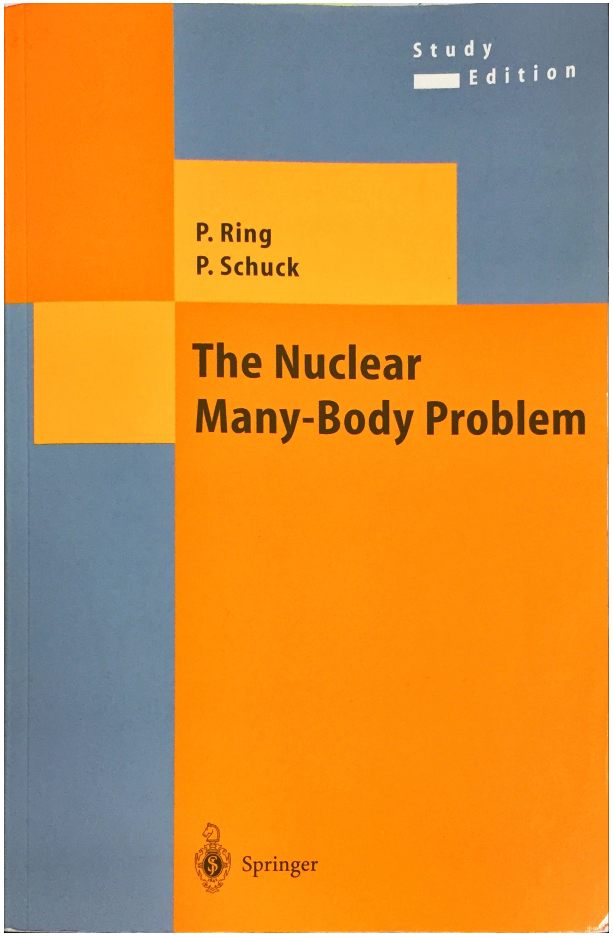
Nuclear Physics

Many-body systems with finite number of nucleons

-No derivation for the nucleon-nucleon force other than lattice QCD
-Models have been used

Effective Hamiltonian approach is common to condensed matter physics

Numerical technique common to condensed matter physics:
-Hartree-Fock/Hartree-Fock-Bogoliubov
-Time-dependent HF/HFB
-Random phase approximation
-Quantum number projection



Condensed Matter Physics and Quantum Chemistry

Many-body electrons and ions

Not feasible to simulate in general

- Born-Oppenheimer approximation:
  Decoupling electrons and ions

→Many-body electrons

cf.) *ab initio* MD

Note that density functional theory *captures* many-body physics
(will be explained in the Quantum Monte Carlo part)

P. Hohenberg & W. Kohn, Phys. Rev. 136, B864 (1964).
W. Kohn & L. J. Sham, Phys. Rev. 140, A1133 (1965).

Other many-body systems: Cold atoms, qubits,⋯

“Density functional theory for atomic Fermi gases”
P. N. Ma, S. Pilati, M. Troyer, & X. Dai, Nat. Phys. 8, 601 (2012).

Mathematical Description of Quantum Many-Body Systems: Bosons & Fermions

Description of Quantum Many-Body Systems 1.

Building blocks of many-body quantum theory

-Complete orthonormal basis set of 1-body wave functions

An example:
Plane wave

$$\frac{e^{+i\vec{k}\cdot\vec{r}}}{\sqrt{L^3}} \quad \left(\vec{k}^T = \left(\frac{2\pi\ell_x}{L}, \frac{2\pi\ell_y}{L}, \frac{2\pi\ell_z}{L}\right), \ \ell_{x,y,z} \in \mathbb{Z}\right)$$

-Creation & annihilation operators

Non-commutative
→ Quantum fluctuations

boson

$$\left[\,\hat{a}_{\vec{k}},\ \hat{a}^\dagger_{\vec{k}'}\,\right] = \hat{a}_{\vec{k}}\hat{a}^\dagger_{\vec{k}'} - \hat{a}^\dagger_{\vec{k}'}\hat{a}_{\vec{k}} = \delta_{\vec{k},\vec{k}'}$$

$$\left[\,\hat{a}_{\vec{k}},\ \hat{a}_{\vec{k}'}\,\right] = \left[\,\hat{a}^\dagger_{\vec{k}},\ \hat{a}^\dagger_{\vec{k}'}\,\right] = 0$$

fermion

$$\left\{\hat{c}_{\vec{k}\sigma},\ \hat{c}^\dagger_{\vec{k}'\sigma'}\right\} = \hat{c}_{\vec{k}\sigma}\hat{c}^\dagger_{\vec{k}'\sigma'} + \hat{c}^\dagger_{\vec{k}'\sigma'}\hat{c}_{\vec{k}\sigma} = \delta_{\vec{k},\vec{k}'}\delta_{\sigma,\sigma'}$$

$$\left\{\hat{c}_{\vec{k}\sigma},\ \hat{c}_{\vec{k}'\sigma'}\right\} = \left\{\hat{c}^\dagger_{\vec{k}\sigma},\ \hat{c}^\dagger_{\vec{k}'\sigma'}\right\} = 0$$

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

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$$

-Vacuum (kernel of annihilation operators)

$$\hat{a}_{\vec{k}}|0\rangle = 0$$

$$\hat{c}_{\vec{k}\sigma}|0\rangle = 0$$

Description of Quantum Many-Body Systems 2.

Fock space: Hilbert space for many-body systems

-Vector space expanded by
products of operators and vacuum

ket vectors $|\Psi\rangle = |0\rangle, \hat{A}|0\rangle, \hat{A}\hat{B}|0\rangle, \ldots$

-Inner product $\langle 0|\hat{D}^\dagger \hat{C}^\dagger \cdot \hat{A}\hat{B}|0\rangle \in \mathbb{C}$

bra vectors $\left(\hat{A}\hat{B}|0\rangle\right)^\dagger = \langle 0|\hat{B}^\dagger \hat{A}^\dagger$

Hermitian conjugate $\left(\hat{A}^\dagger\right)^\dagger = \hat{A}$

Usually we normalize the vacuum $\langle 0| \cdot |0\rangle = \langle 0|0\rangle = 1$

2-norm of $|\Psi\rangle = \hat{A}\hat{B}|0\rangle$ $\sqrt{\langle 0|\hat{B}^\dagger \hat{A}^\dagger \hat{A}\hat{B}|0\rangle}$

Description of Quantum Many-Body Systems 3.

Many-body bosons

Exercise 1. Particle number operator $\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}$

Confirm the following identity:

$$\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}\left(\hat{a}^\dagger_{\vec{k}}\right)^N|0\rangle = N\left(\hat{a}^\dagger_{\vec{k}}\right)^N|0\rangle$$

Exercise 2. Norm of a *N* boson wave function

Evaluate the following inner product:

$$\langle 0|\left(\hat{a}_{\vec{k}}\right)^N\left(\hat{a}^\dagger_{\vec{k}}\right)^N|0\rangle$$

$$\left(\left(\hat{a}^\dagger_{\vec{k}}\right)^N|0\rangle\right)^\dagger = \langle 0|\left(\hat{a}_{\vec{k}}\right)^N$$

Answer to the exercises

Exercise 1. Particle number operator $\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}$

Confirm the following identity:

$$\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}\left(\hat{a}^\dagger_{\vec{k}}\right)^N|0\rangle = N\left(\hat{a}^\dagger_{\vec{k}}\right)^N|0\rangle$$

$$\begin{aligned}
\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}\left(\hat{a}^\dagger_{\vec{k}}\right)^N|0\rangle &= \hat{a}^\dagger_{\vec{k}}\cdot\hat{a}_{\vec{k}}\hat{a}^\dagger_{\vec{k}}\cdot\left(\hat{a}^\dagger_{\vec{k}}\right)^{N-1}|0\rangle \\
&= \hat{a}^\dagger_{\vec{k}}\left(\hat{a}^\dagger_{\vec{k}}\hat{a}_{\vec{k}}+1\right)\left(\hat{a}^\dagger_{\vec{k}}\right)^{N-1}|0\rangle \\
&= \left(\hat{a}^\dagger_{\vec{k}}\right)^2\hat{a}_{\vec{k}}\left(\hat{a}^\dagger_{\vec{k}}\right)^{N-1}|0\rangle + \left(\hat{a}^\dagger_{\vec{k}}\right)^N|0\rangle \\
&= \left(\hat{a}^\dagger_{\vec{k}}\right)^3\hat{a}_{\vec{k}}\left(\hat{a}^\dagger_{\vec{k}}\right)^{N-2}|0\rangle + 2\left(\hat{a}^\dagger_{\vec{k}}\right)^N|0\rangle \\
&\vdots \\
&= N\left(\hat{a}^\dagger_{\vec{k}}\right)^N|0\rangle
\end{aligned}$$

Answer to the exercises

Exercise 2. Norm of a *N* boson wave function

Evaluate the following inner product:

$$\langle 0| \left(\hat{a}_{\vec{k}}\right)^{N} \left(\hat{a}^{\dagger}_{\vec{k}}\right)^{N} |0\rangle$$

$$\left(\left(\hat{a}^{\dagger}_{\vec{k}}\right)^{N} |0\rangle\right)^{\dagger} = \langle 0| \left(\hat{a}_{\vec{k}}\right)^{N}$$

$$\begin{aligned}
\langle 0| \left(\hat{a}_{\vec{k}}\right)^{N} \left(\hat{a}^{\dagger}_{\vec{k}}\right)^{N} |0\rangle &= \langle 0| \left(\hat{a}_{\vec{k}}\right)^{N-1} \left(\hat{a}^{\dagger}_{\vec{k}}\hat{a}_{\vec{k}} + 1\right) \left(\hat{a}^{\dagger}_{\vec{k}}\right)^{N-1} |0\rangle \\
&= N\langle 0| \left(\hat{a}_{\vec{k}}\right)^{N-1} \left(\hat{a}^{\dagger}_{\vec{k}}\right)^{N-1} |0\rangle \\
&= N(N-1)\langle 0| \left(\hat{a}_{\vec{k}}\right)^{N-2} \left(\hat{a}^{\dagger}_{\vec{k}}\right)^{N-2} |0\rangle \\
&\vdots \\
&= N!
\end{aligned}$$

Description of Quantum Many-Body Systems 4.

1st quantization and 2nd quantization in bosons

Field operator $\hat{\phi}(\vec{r}) = \sum_{\vec{k}} \frac{e^{+i\vec{k}\cdot\vec{r}}}{\sqrt{L^3}} \hat{a}_{\vec{k}}$

A non-interacting many-body wave function

$$|\Psi\rangle = \prod_{\nu} \frac{1}{\sqrt{N_\nu !}} \left(\hat{a}^\dagger_{\vec{k}_\nu} \right)^{N_\nu} |0\rangle \qquad \langle \Psi | \Psi \rangle = 1$$

A 2-body wave function:

2nd quantization $|\Psi\rangle = \hat{a}^\dagger_{\vec{k}_1} \hat{a}^\dagger_{\vec{k}_2} |0\rangle$

1st quantization $\psi(\vec{r}_1, \vec{r}_2) = \langle 0 | \hat{\phi}(\vec{r}_2) \hat{\phi}(\vec{r}_1) | \Psi \rangle$

$$\langle 0 | \hat{\phi}(\vec{r}_2) \hat{\phi}(\vec{r}_1) | \Psi \rangle = \left(\frac{1}{\sqrt{L^3}} \right)^2 \left(e^{i\vec{k}_1\cdot\vec{r}_1 + i\vec{k}_2\cdot\vec{r}_2} + e^{i\vec{k}_2\cdot\vec{r}_1 + i\vec{k}_1\cdot\vec{r}_2} \right)$$

Symmetrized

Indistinguishable particles $\psi(\vec{r}_1, \vec{r}_2) = +\psi(\vec{r}_2, \vec{r}_1)$

Description of Quantum Many-Body Systems 5.

1st quantization and 2nd quantization in fermions

Field operator $\hat{\phi}_\sigma(\vec{r}) = \sum_{\vec{k}} \frac{e^{+i\vec{k}\cdot\vec{r}}}{\sqrt{L^3}} \hat{c}_{\vec{k}\sigma}$

A non-interacting many-body wave function

$$|\Psi\rangle = \prod_\mu \hat{c}^\dagger_{\vec{k}_\mu\uparrow} \prod_\nu \hat{c}^\dagger_{\vec{k}_\nu\downarrow} |0\rangle \qquad \langle\Psi|\Psi\rangle = 1$$

A 2-body wave function:

2nd quantization $|\Psi\rangle = \hat{c}^\dagger_{\vec{k}_1\sigma} \hat{c}^\dagger_{\vec{k}_2\sigma} |0\rangle$

1st quantization $\psi(\vec{r}_1\sigma, \vec{r}_2\sigma) = \langle 0|\hat{\phi}_\sigma(\vec{r}_2)\hat{\phi}_\sigma(\vec{r}_1)|\Psi\rangle$

$$\langle 0|\hat{\phi}_\sigma(\vec{r}_2)\hat{\phi}_\sigma(\vec{r}_1)|\Psi\rangle = \left(\frac{1}{\sqrt{L^3}}\right)^2 \left(e^{i\vec{k}_1\cdot\vec{r}_1 + i\vec{k}_2\cdot\vec{r}_2} - e^{i\vec{k}_2\cdot\vec{r}_1 + i\vec{k}_1\cdot\vec{r}_2}\right)$$

Anti-symmetrized

Indistinguishable particles $\psi(\vec{r}_1\sigma, \vec{r}_2\sigma) = -\psi(\vec{r}_2\sigma, \vec{r}_1\sigma)$

Description of Quantum Many-Body Systems 6.

Hamiltonian in 2nd quantization form

Spin independent

$$\hat{H} = \int d^3r \hat{\phi}^\dagger(\vec{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 + v(\vec{r}) \right) \hat{\phi}(\vec{r})$$
$$+ \frac{1}{2} \int d^3r \int d^3r' \hat{\phi}^\dagger(\vec{r}) \hat{\phi}(\vec{r}) V(|\vec{r} - \vec{r}'|) \hat{\phi}^\dagger(\vec{r}') \hat{\phi}(\vec{r}')$$

Spin dependent

$$\hat{H} = \sum_{\sigma,\sigma'} \int d^3r \hat{\phi}_\sigma^\dagger(\vec{r}) \left(-\delta_{\sigma,\sigma'} \frac{\hbar^2}{2m} \nabla^2 + v_{\sigma\sigma'}(\vec{\nabla}, \vec{r}) \right) \hat{\phi}_{\sigma'}(\vec{r})$$
$$+ \frac{1}{2} \sum_{\sigma,\sigma'} \int d^3r \int d^3r' \hat{\phi}_\sigma^\dagger(\vec{r}) \hat{\phi}_\sigma(\vec{r}) V(|\vec{r} - \vec{r}'|) \hat{\phi}_{\sigma'}^\dagger(\vec{r}') \hat{\phi}_{\sigma'}(\vec{r}')$$

Wave Function of Non-Interacting Fermions (S=1/2): Slater Determinant

1st quantization

$$\psi(\vec{r}_1\uparrow,\vec{r}_2\uparrow,\cdots,\vec{r}_{N_\uparrow}\uparrow;\vec{r}_{N_\uparrow+1}\downarrow,\vec{r}_{N_\uparrow+2}\downarrow,\cdots,\vec{r}_{N_\uparrow+N_\downarrow}\downarrow)$$
$$=(L^3)^{-(N_\uparrow+N_\downarrow)/2}D_\uparrow D_\downarrow$$

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

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

2nd quantization

$$|\Psi\rangle=\prod_{\mu=1}^{N_\uparrow}\hat{c}^\dagger_{\vec{k}_\mu\uparrow}\prod_{\nu=N_\uparrow+1}^{N_\uparrow+N_\downarrow}\hat{c}^\dagger_{\vec{k}_\nu\downarrow}|0\rangle$$

Numerical Approaches for Quantum Many-Body Systems

Numerical Methods for Quantum Many-Body Problems in CMP

- Numerical exact diagonalization: Lanczos method (Krylov subspace)

  Ground state and low-lying excited states (equivalent to full CI)

- Quantum Monte Carlo:
  Hirsch-Fye, World line, CTQMC, AFQMC, PQMC, DQMC, ···

  Negative sign problem

- Matrix/Tensor Product State:
  DMRG, NRG, MPS, TN, MERA, ···

- Negative-sign-free Quantum Monte Carlo:
  Green's function Monte Carlo
  Fixed node *DFT/LDA $E_{XC}[\rho]$ was derived by these techniques
  Variational Monte Carlo

  Biased by initial wave function

- Dynamical mean-field theory:
  Lanczos method, Hirsch-Fye QMC, CTQMC, NRG, ···

  No spatial fluctuations (Similar to MRCI?)

- One-body approximation or mean-field (Hartree-Fock, ···)

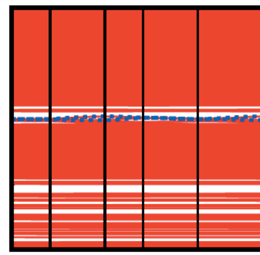
Target of Model Calculations

- 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

Effective Hamiltonian Construction

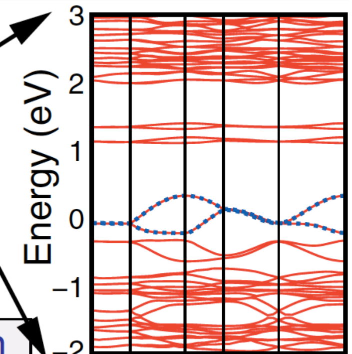
Schematic procedure of three–stage scheme thanks to energy hierarchy structure

1. Global electronic structure by DFT



far from Fermi level

tens eV

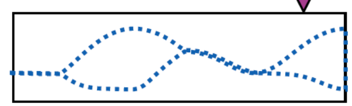


2. downfolding

constrained RPA

(1) Screened Coulomb interaction

(2) Self–energy



“target band”

Low–energy effective Hamiltonian

1/10-1/100 eV

3. Low-energy solver

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

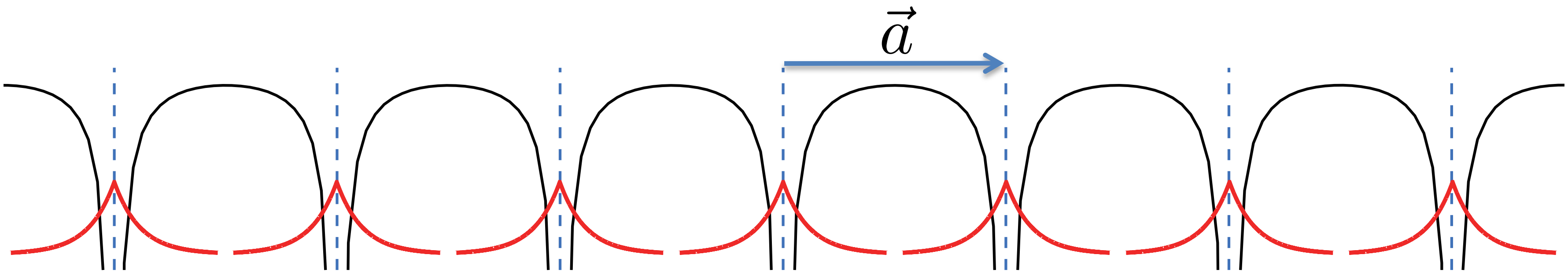
Model Hamiltonian derived by
DFT+DMFT, Wannier+cRPA

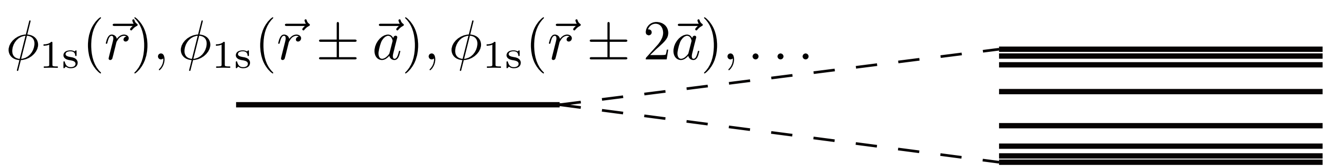
G. Kotliar, et al., RMP 78, 865 (2006)

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

Effective Hamiltonian of Many-Body Electrons

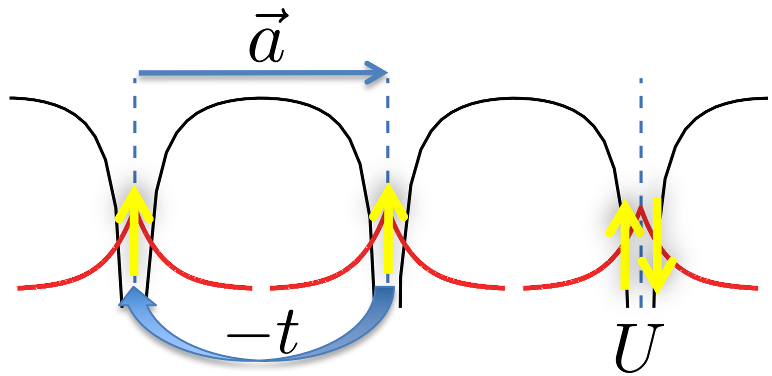
One of the simplest many-body electrons in Crystalline solids: Hydrogen solid





Gedankenexperiment of F. N. Mott

One of the Simplest Hamiltonian: 1D Hubbard Model



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

-Tunnelling among neighboring 1s orbitals

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

-Intra-atomic Coulomb in 1s orbitals

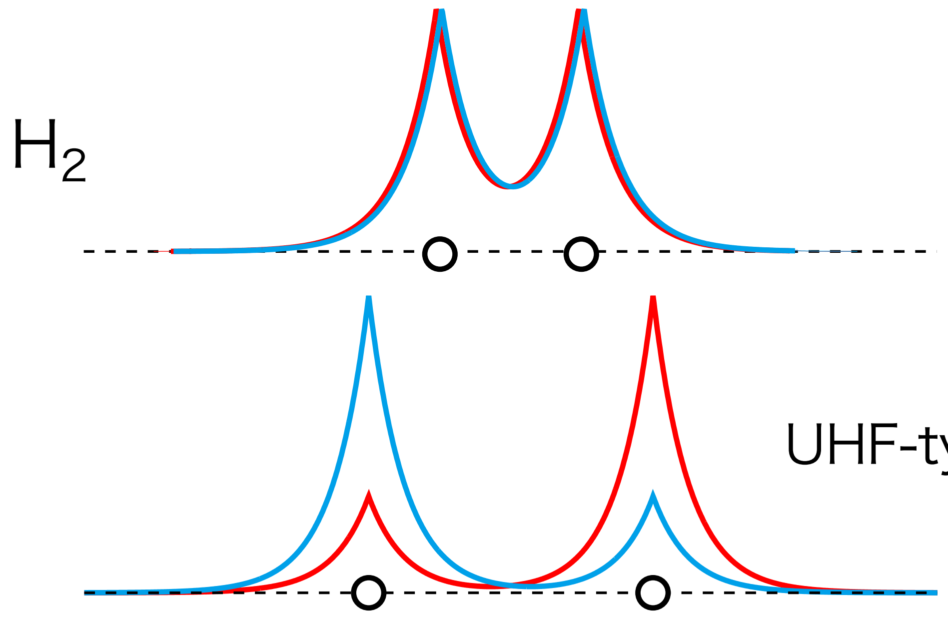
$$U = \int d^3 r \int d^3 r' \phi^*_{1\mathrm{s}}(\vec{r}) \phi^*_{1\mathrm{s}}(\vec{r'}) \frac{e^2}{\left|\vec{r} - \vec{r'}\right|} \phi_{1\mathrm{s}}(\vec{r'}) \phi_{1\mathrm{s}}(\vec{r})$$

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

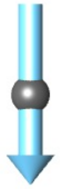
Hydrogen Molecule to Two Interacting Spins



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

Example of Approximation: LCAO

Linear Combination of Atomic Orbitals (LCAO)

$$\phi_{\mathrm{B}}(\vec{r}) = \frac{\phi_{1\mathrm{s}}(\vec{r}-\vec{r}_a) + \phi_{1\mathrm{s}}(\vec{r}-\vec{r}_b)}{\sqrt{2+2S_{12}}}$$

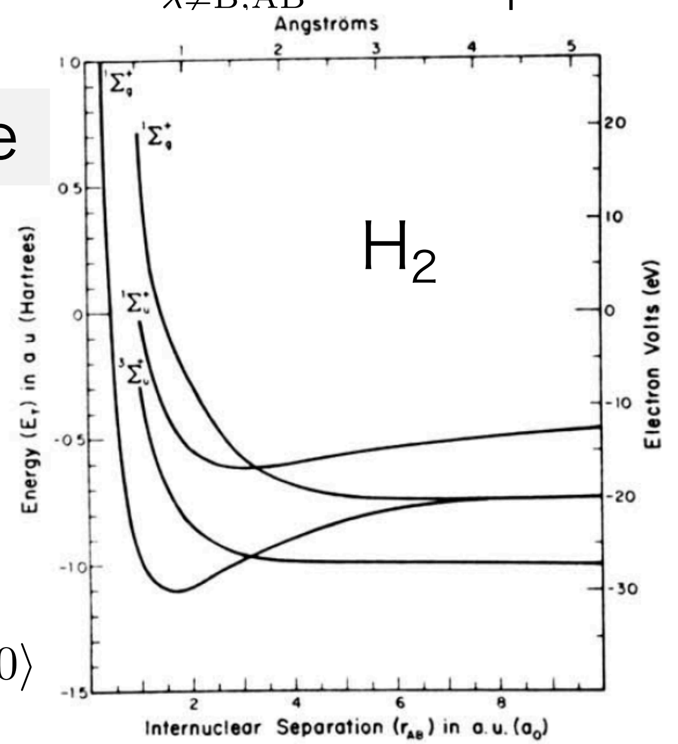
$$\phi_{\mathrm{AB}}(\vec{r}) = \frac{\phi_{1\mathrm{s}}(\vec{r}-\vec{r}_a) - \phi_{1\mathrm{s}}(\vec{r}-\vec{r}_b)}{\sqrt{2-2S_{12}}}$$

$$\phi_{1\mathrm{s}}(\vec{r}) = \frac{1}{\sqrt{\pi a_{\mathrm{B}}^3}} e^{-|\vec{r}|/a_{\mathrm{B}}} \qquad a_{\mathrm{B}} = \frac{4\pi\varepsilon_0\hbar^2}{m_{\mathrm{e}}e^2}$$

$$S_{12} = \int \phi_{1\mathrm{s}}(\vec{r}-\vec{r}_a)\phi_{1\mathrm{s}}(\vec{r}-\vec{r}_b)d^3r$$

Field operator

$$\hat{\phi}_\sigma(\vec{r}) = C\left[\phi_{\mathrm{B}}(\vec{r})\hat{c}^\dagger_{\mathrm{B}\sigma} + \phi_{\mathrm{AB}}(\vec{r})\hat{c}^\dagger_{\mathrm{AB}\sigma} + \sum_{\lambda\neq\mathrm{B,AB}} \phi_\lambda(\vec{r})\hat{c}^\dagger_{\lambda\sigma}\right]$$

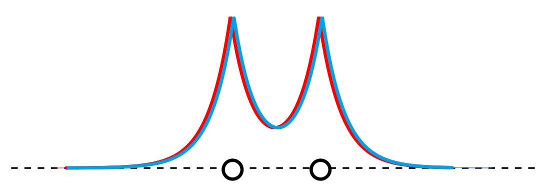


Failure of LCAO: Triplet ground state

M. J. S. Dewar and J. Keleman,
J. Chem. Education 48, 494 (1971)

Singlet S=0:

$$|{}^1\Sigma_g^+\rangle = \hat{c}^\dagger_{\mathrm{B}\uparrow}\hat{c}^\dagger_{\mathrm{B}\downarrow}|0\rangle$$



Triplet S=1 (one of three states):

$$|{}^3\Sigma_u^+\rangle = \frac{1}{\sqrt{2}}(\hat{c}^\dagger_{\mathrm{B}\uparrow} - \hat{c}^\dagger_{\mathrm{AB}\uparrow})\frac{1}{\sqrt{2}}(\hat{c}^\dagger_{\mathrm{B}\uparrow} + \hat{c}^\dagger_{\mathrm{AB}\uparrow})|0\rangle = \hat{c}^\dagger_{\mathrm{AB}\uparrow}\hat{c}^\dagger_{\mathrm{B}\uparrow}|0\rangle$$

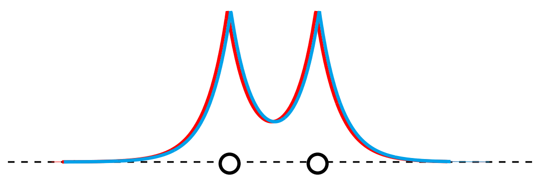
Problems in LCAO

Failure of LCAO: Triplet ground state

M. J. S. Dewar and J. Keleman,
J. Chem. Education 48, 494 (1971)

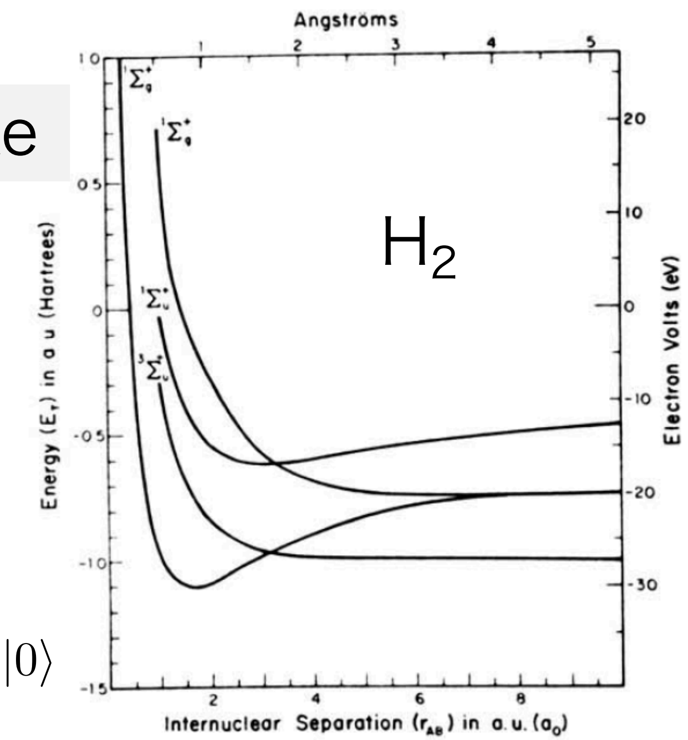
Singlet S=0:

$$|^1\Sigma_g^+\rangle = \hat{c}^\dagger_{\mathrm{B}\uparrow}\hat{c}^\dagger_{\mathrm{B}\downarrow}|0\rangle$$



Triplet S=1 (one of three states):

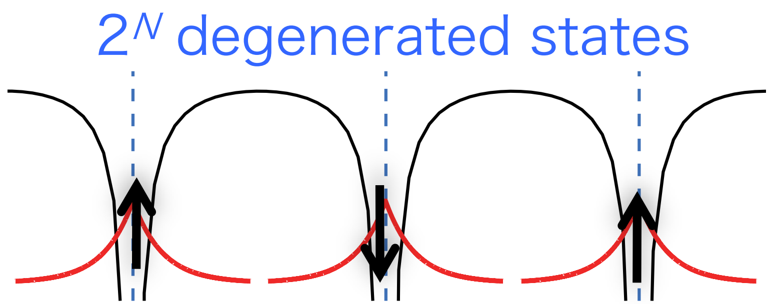
$$|^3\Sigma_u^+\rangle = \frac{1}{\sqrt{2}}(\hat{c}^\dagger_{\mathrm{B}\uparrow} - \hat{c}^\dagger_{\mathrm{AB}\uparrow})\frac{1}{\sqrt{2}}(\hat{c}^\dagger_{\mathrm{B}\uparrow} + \hat{c}^\dagger_{\mathrm{AB}\uparrow})|0\rangle = \hat{c}^\dagger_{\mathrm{AB}\uparrow}\hat{c}^\dagger_{\mathrm{B}\uparrow}|0\rangle$$



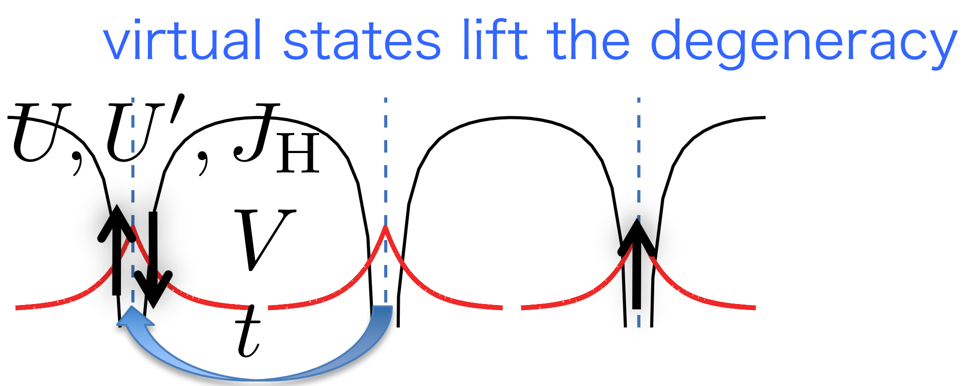
Overestimation of intra-atomic Coulomb repulsion!

Heisenberg (Spin) Hamiltonian from Strong Coupling Expansion

Unperturbed atomic Hamiltonian



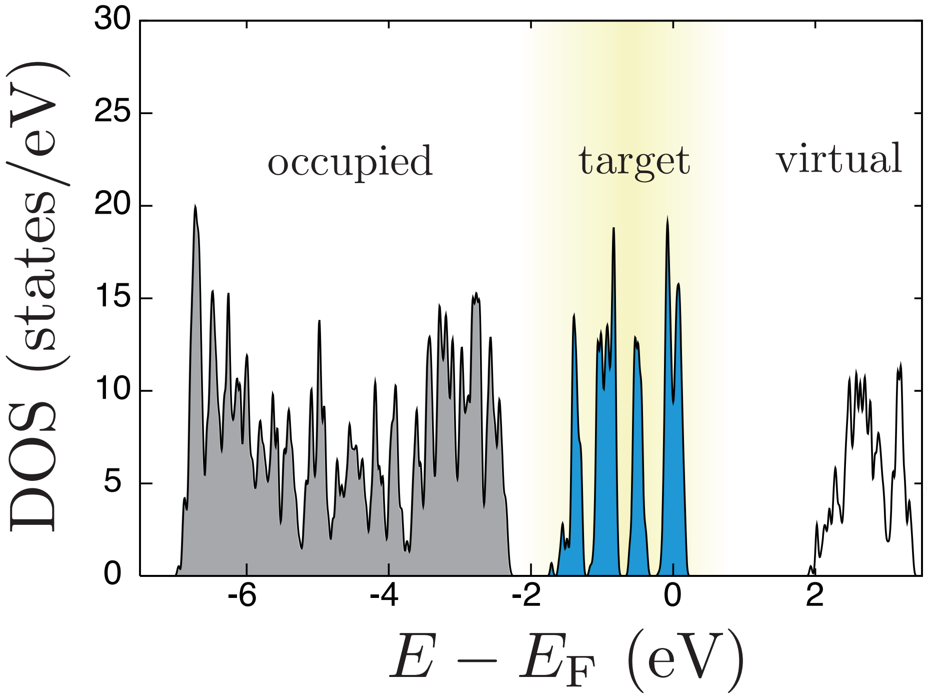
Perturbation: Tunneling



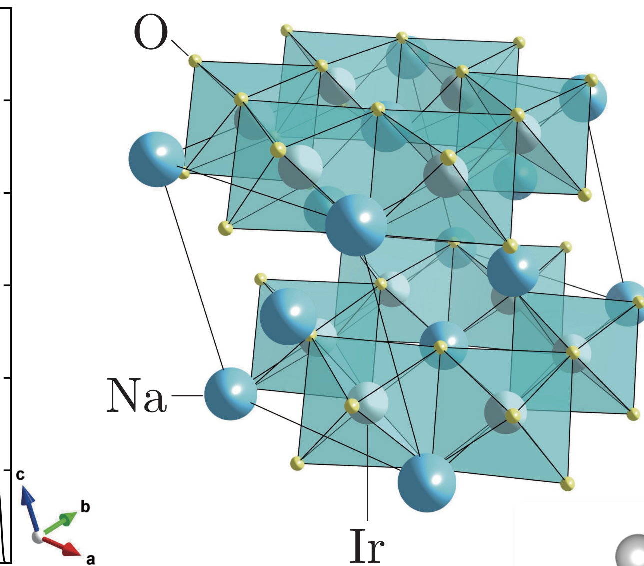
Construction of Effective Hamiltonians: An Example

- Target Hilbert space expanded by localized Wannier orbitals

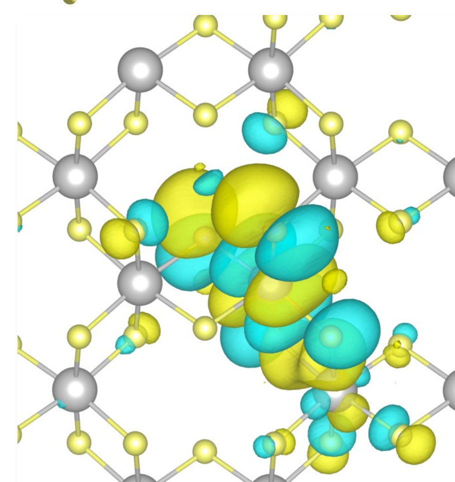
DFT result for energy spectrum



Souza-Marzari-Vanderbilt



Na_2IrO_3



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

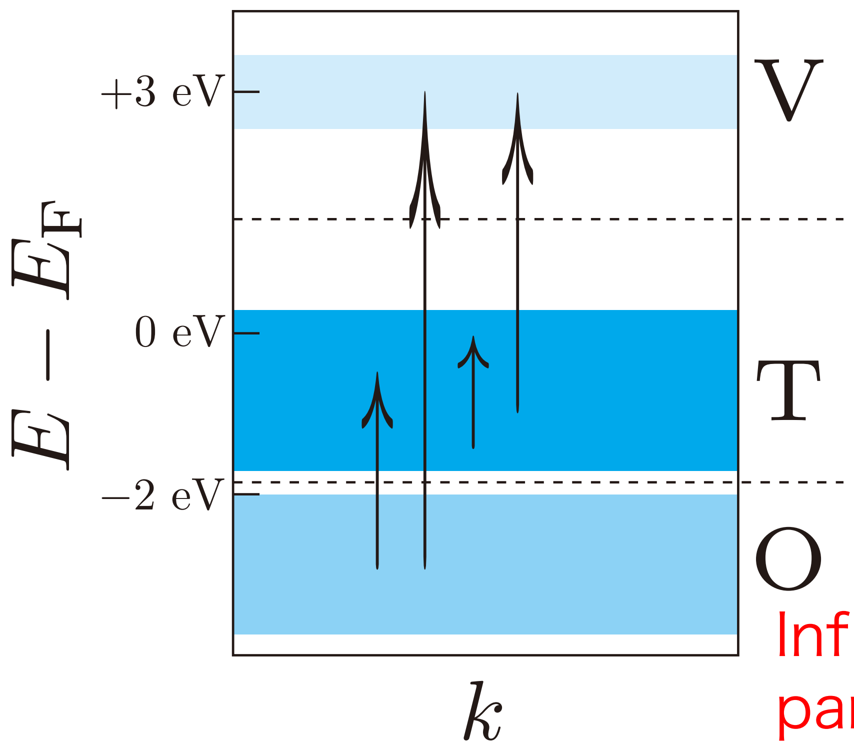
Imada & Miyake, J. Phys. Soc. Jpn. **79**, 112001 (2010)

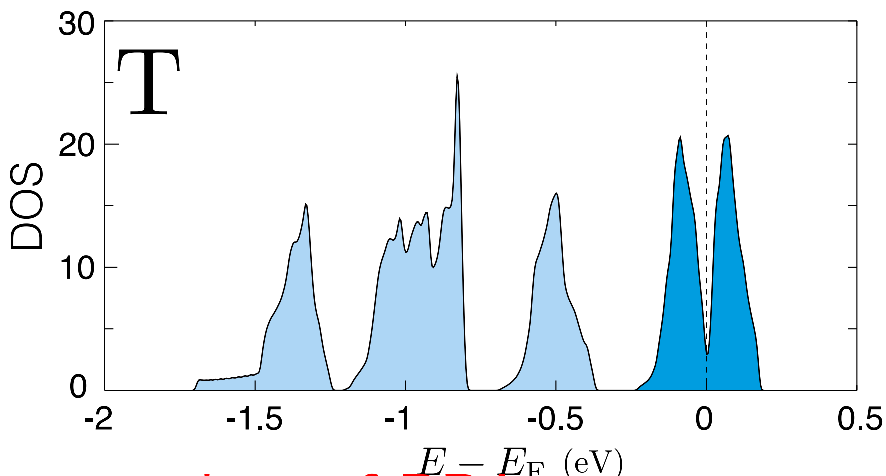
Constrained RPA Estimate on Coulomb Interaction of t_{2g}-Hubbard

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

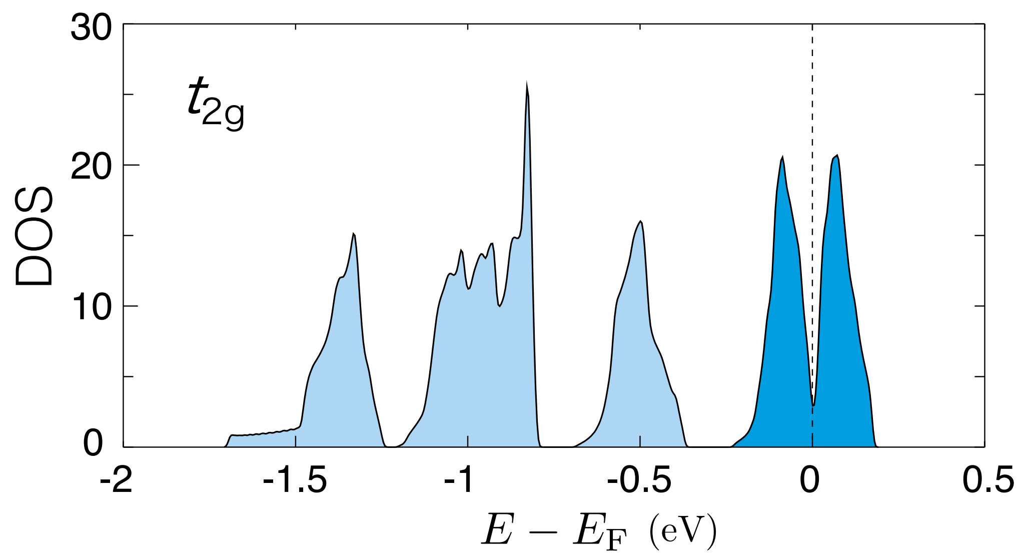
$$\hat{H}_{\text{SOC}} = \frac{\zeta_{\text{so}}}{2}\sum_\ell \vec{\hat{c}}^\dagger_\ell \begin{bmatrix} 0 & +i\hat{\sigma}_z & -i\hat{\sigma}_y \\ -i\hat{\sigma}_z & 0 & +i\hat{\sigma}_x \\ +i\hat{\sigma}_y & -i\hat{\sigma}_x & 0 \end{bmatrix}\vec{\hat{c}}_\ell$$

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

Coulomb

$$\hat{H}_U = U\sum_\ell\sum_{a=yz,zx,xy}\hat{n}_{\ell a\uparrow}\hat{n}_{\ell a\downarrow}$$
$$+\sum_{\ell\neq m}\sum_{a,b}\frac{V_{\ell,m}}{2}(\hat{n}_{\ell a\uparrow}+\hat{n}_{\ell a\downarrow})(\hat{n}_{mb\uparrow}+\hat{n}_{mb\downarrow})$$
$$+\sum_\ell\sum_{a<b}\sum_\sigma[U'\hat{n}_{\ell a\sigma}\hat{n}_{\ell b\bar{\sigma}} + (U'-J_{\text{H}})\hat{n}_{\ell a\sigma}\hat{n}_{\ell b\sigma}]$$
$$+J_{\text{H}}\sum_\ell\sum_{a\neq b}\left[\hat{c}^\dagger_{\ell a\uparrow}\hat{c}^\dagger_{\ell b\downarrow}\hat{c}_{\ell a\downarrow}\hat{c}_{\ell b\uparrow} + \hat{c}^\dagger_{\ell a\uparrow}\hat{c}^\dagger_{\ell a\downarrow}\hat{c}_{\ell b\downarrow}\hat{c}_{\ell b\uparrow}\right]$$

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

Lecture Schedule

Classical

Quantum

#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

Next Lecture (6/7)

6/7 8th Quantum Monte Carlo (MC) methods

-McMillan, Phys. Rev. 138, A442 (1965).
 variational MC for Liquid helium 4
-Ceperley-Chester-Kalos, Phys. Rev. B 16, 3081 (1977).
 variational MC for Liquid helium 3
-(Electron gas & LDA)
-Blankenbecler-Scalapino-Sugar, auxiliary field MC (1981)
-(World line MC)