ManyBody theory

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Chapter 1

General Remarks and Conventions

The problem we want to solve is to find the solution of many-body Hamiltonian[1]

$$\hat{H} = \sum_{i=1}^{A} \hat{T}_i + \frac{1}{2}\sum_{ij} V_{ij} + \frac{1}{6}\sum_{ijk} V_{ijk} + \cdots \tag{1.1}$$

such that

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle \tag{1.2}$$

where, E_n is an eigen-energy value of A-body system and $|\Psi_n\rangle$ is eigen-state A-body wave function. If we can find such eigen values and wave functions for all possible states of A-nucleon system, we would be able to get any physical observables. Note that the coordinates and quantum numbers are implied in above expressions.

However, in general, it is very difficult to get such solutions, even in few-body case with only two-body interactions. Thus, in many case, the many-body theory is to find better approximation to the problem.

Also note that the SChrodinger equation is actually equivalent to the variational minimization of[2]

$$E[\psi] = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{1.5}$$

1.1 Mass Formula

- **Mass excess**, $\Delta M(N,Z)$, is defined from the atomic mass $M(N,Z)$ and u,

$$\Delta M(N,Z) = M(N,Z) - uA, \quad u = M(^{12}C)/12 = 931.49386 MeV/c^2. \tag{1.6}$$

- nucleon mass

$$\begin{aligned} m_p &= 938.272 MeV/c^2 = 1.007276u \\ m_n &= 939.565 MeV/c^2 = 1.00866u \end{aligned} \tag{1.7}$$

[1] Be careful that $\sum_{i<j} V_{ij} = \frac{1}{2}\sum_{ij} V_{ij}$ and $\sum_{i<j<k} V_{ijk} = \frac{1}{6}\sum_{ijk} V_{ijk}$.

[2]

$$\delta E[\psi] = 0 \to \frac{1}{\langle\psi|\psi\rangle}\left(\hat{H}|\psi\rangle - \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}|\psi\rangle\right) = \frac{1}{\langle\psi|\psi\rangle}\Big(\hat{H}|\psi\rangle - E[\psi]|\psi\rangle\Big) = 0. \tag{1.3}$$

Or, with Lagrange multiplier $\lambda = E$,

$$\delta\Big(\langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle\Big) = 0 \to \hat{H}|\psi\rangle - \lambda|\psi\rangle = 0. \tag{1.4}$$

- **Binding Energy**, $BE(N,Z)$, is defined as

$$\begin{aligned} BE(N,Z) &= ZM_Hc^2 + Nm_nc^2 - M(N,Z)c^2, \\ &= Z\Delta_Hc^2 + N\Delta_nc^2 - \Delta(N,Z)c^2 \end{aligned} \tag{1.8}$$

  where M_H is the mass of hydrogen atom (not proton mass) and $\Delta_Hc^2 = 7.2890$ MeV and $\Delta_nc^2 = 8.0713$ MeV.

- **Liquid drop model**

$$BE(N,Z) = a_1A - a_2A^{2/3} - a_3\frac{Z^2}{A^{1/3}} - a_4\frac{(N-Z)^2}{A} \tag{1.9}$$

  $a_1 = 15.49$ MeV, $a_2 = 17.23$ MeV, $a_3 = 0.697$ MeV, $a_4 = 22.6$ MeV.

  Surface energy term is negative because nucleons at the surface will have less interactions and thus reduce binding energy for whole volume average. Coulomb term is negative because the coulomb repulsion would reduce the binding. Asymmetry implies that the binding becomes weaker as asymmetry becomes larger.

- **Q-value**

- **Separation energy** : Staggering of separation energy indicate pairing interaction.

- **energy gap** : energy gap for neutrons or protons are can be defined as (difference of single nucleon separation energy between nearby nucleus. This corresponds to the difference between two single particle levels.)

$$\begin{aligned} \Delta S_n &= BE(N,Z) - BE(N-1,Z) - (BE(N+1,Z) - BE(N,Z)) \\ &= 2BE(N,Z) - BE(N-1,Z) - BE(N+1,Z) \end{aligned} \tag{1.10}$$

$$\Delta S_p = 2BE(N,Z) - BE(N,Z-1) - BE(N,Z+1) \tag{1.11}$$

1.2 Short description of various models

Ground state description

- Shell model : independent particle model, residual interaction
- Hartree-Fock method
- HF-BCS method
- HFB

Excited state

- independent particle approximation
- Tamm-Dancoff approximation (TDA) : HF 바닥상태+ 들뜬 상태를 구하는데만 잔류 상호 작용 고려하는 근사법.
- RPA

Ab-initio methods

- Faddeev-Yakubowski (FY) method

  - configuration space : FY method
  - momentum space : AGS equations

- Based on variational theorem(Diagonalization method): wave function or model space ansatz
  - Hartree-Fock method : trial w.f is a Slater determinant
  - Resonating Group method : trial w.f. reflect cluster picture
  - variational Monte Carlo : trial w.f. reflect potential form
  - Hyperspherical Harmonics(HH) method : trial w.f. in HH basis. Extenstion to CHH (correlatiob by Jastrow operator) and EIHH methods.
  - stochastic variational method (SVM) : variation by trial and error
  - No core shell model(NCSM)

- Based on similarity transformation
  - Coupled Cluster : Similarity transformation (non-Unitary)
  - Similarity Renormalization for effective interaction

- Quantum Monte Carlo method
  - Green's Function MC(GFMC)
  - Diffusion MC (DMC)
  - Auxiliary Field Diffusion MC (AFDMC)
  - NLEFT
  - VMC

1.3 Independent Particle Model. Slater determinant Wave function.

Because of Pauli principle, many-nucleon wave function have to be anti-symmetric for any exchange of nucleon.

The simplest case is a collection of A-independent particles.

$$H = \sum_{j=1}^{A} h_j, \quad h_j \phi_k(\boldsymbol{r}_j) = \epsilon_k \phi_k(\boldsymbol{r}_j), \tag{1.12}$$

Then, the many-body wave function simply becomes a slater determinant,

$$\begin{aligned} H\Phi &= E\Phi, \quad E = \sum_i \epsilon_i, \\ \Phi(\boldsymbol{r}_{j=1,A}) &= \frac{1}{\sqrt{A!}} \det(\phi_i(\boldsymbol{r}_j)), \end{aligned} \tag{1.13}$$

where $j = 1, A$ is a particle index and i is a state index for A single particle states. In this case, the ground state would corresponds to the case A-lowest energy level ϵ_k is occupied. In similar way, excited states will have different combination of single particle states.

여기서, Slater determinant Φ 과 Hartree wave function Φ_H 와 anti-symmetrization operator 를 도입하자.

$$\Phi(r_{1\ldots A}; \mu_{1\ldots A}) = \frac{1}{\sqrt{A!}} \det(\phi_{\mu_i}(\boldsymbol{r}_j)) = \sqrt{A!}\hat{A}\Phi_H(r_{1\ldots A}; \mu_{1\ldots A}) \tag{1.14}$$

여기서, Φ_H 는 simple product of sp wave functions 이고, anti-symmetrization operator 는 모든 가능한 permutation 을 포함한다. (위식에서 $\sqrt{A!}$은 Φ_{HF} 의 normalization을 맞춰주기 위함.)

$$\hat{A} = \frac{1}{A!}\sum_P (-1)^P \hat{P} \tag{1.15}$$

Note that anti-symmetrization operator commutes with Hamiltonian even when it have two-body interactions

$$[\hat{H}_0, \hat{A}] = [\hat{H}_I, \hat{A}] = 0 \tag{1.16}$$

with $\hat{H} = \hat{H}_0 + \hat{H}_I$. And also $\hat{A}^2 = \hat{A}$.

The Hamiltonian of simple shell model for a single nucleon have only a central potential which may be originate from mean field of other nucleons.

$$h(\boldsymbol{r}_i) = T(\boldsymbol{r}_i) + U(\boldsymbol{r}_i) \tag{1.17}$$

Then the complete eigen-states $\phi_k(\boldsymbol{r})$ and energies ϵ_k can be easily obtained for given single particle potential $U(\boldsymbol{r})$.

We can easily see that the expectation value of $\hat{H}_0$ for Slater determinant wave function

$$\begin{aligned}
\langle\Phi|\hat{H}_0|\Phi\rangle &= A!\int \Phi_H^* \hat{A}\hat{H}_0\hat{A}\Phi_H d\tau, \\
&= A!\int \Phi_H^* \hat{H}_0\hat{A}\Phi_H d\tau, \\
&= \int \Phi_H^* \hat{H}_0 \sum_P (-1)^P \hat{P}\Phi_H d\tau
\end{aligned} \tag{1.18}$$

Integral vanishes when permutation is non-trivial because of orthogonality of sp. wf. Thus, only trivial permutation(identity) gives non-zero results, and we get

$$\begin{aligned}
\langle\Phi|\hat{H}_0|\Phi\rangle &= \sum_{i=1}^{A}\int \Phi_H^* \hat{h}_0\Phi_H d\tau \\
&= \sum_{\mu=1}^{A}\langle\mu|\hat{h}_0|\mu\rangle = \sum_{\mu=1}^{A}\epsilon_\mu.
\end{aligned} \tag{1.19}$$

as expected.

For a expectation value of the two-body part of the Hamiltonian can be done in similar way,

$$\begin{aligned}
\langle\Phi|\hat{H}_I|\Phi\rangle &= A!\int \Phi_H^* \hat{A}\hat{H}_I\hat{A}\Phi_H d\tau, \\
&= \sum_{i\le j=1}^{A}\sum_P (-1)^P \int \Phi_H^* \hat{v}(r_{ij})\hat{P}\Phi_H d\tau, \\
&= \sum_{i\le j=1}^{A}\int \Phi_H^* \hat{v}(r_{ij})(1-P_{ij})\Phi_H d\tau, \\
&= \frac{1}{2}\sum_{\mu,\nu=1}^{A}[(\mu\nu|\hat{v}|\mu\nu) - (\mu\nu|\hat{v}|\nu\mu)]
\end{aligned} \tag{1.20}$$

where, the integral does not vanish only for trivial or when two-states are permuted in Φ_H.

1.4 second quantization

For one given single particle basis, regardless whether harmonic oscillators or plane waves, if it is complete, the Hamiltonian can be expressed in terms of matrix elements in that basis. Similarly, the wave function and any physical quantities also can be expressed in terms of such basis.

Let us define particle creation and annihilation operators in state n as $c_n^\dagger$ and c_n, satisfying following properties,

$$\begin{aligned} c_n|-\rangle &= 0, \\ \{c_n, c_{n'}^\dagger\} &= c_n c_{n'}^\dagger + c_{n'}^\dagger c_n = \delta_{nn'}, \\ \{c_n, c_{n'}\} &= \{c_n^\dagger, c_{n'}^\dagger\} = 0, \end{aligned} \tag{1.21}$$

where $|-\rangle$ is the vacuum state without any particles.

주의: $|ab\rangle$ 와 $|ab)$ 를 항상 구분할 것! $|ab) = |a)\otimes|b)$ 는 simple product of states 인 반면, $|ab\rangle$ 는 anti-symmetrized states, 즉 $|ab\rangle \sim |ab) - |ba)$이다. $|ab)$의 경우에는 순서를 바꿀 수 없지만 ($|ab) \neq -|ba)$!) , $|ab\rangle$ 는 순서가 특별한 의미가 있는 것은 아니다. ($|ab\rangle = -|ba\rangle$)

또한, 특별한 말이 없는 한 normalized state로 생각한다.

However, note that $|s1, s2\ldots\rangle$ created from creation operators on vacuum is always anti-symmetric states. 즉, $a_a^\dagger a_b^\dagger|0>=|ba>$ 는 anti-symmetrized state 이지, $|ab)$ 가 아님.

$|\phi_{s1}(1)\phi_{s2}(2)\ldots)$ which is a simple product of wave functions is not anti-symmetric. **To distinguish two cases let us use $|\phi_1\phi_2\rangle_{AS}$ as a anti-symmetric one or $|\phi_1\phi_2)$ as a simple product.**

Be careful that creation and annihilation operator and Ground state and Excited states are all correlated and have to be defined together. For example, one may consider a specific ground state in shell model as $|\Phi_A\rangle$ and define creation and annihilation operators to describe the excitations from such states so that $\alpha_n|\Phi_A\rangle = 0$.

1.5 Matrix elements of operators

1.5.1 1-Body operator

General one-body operator can be written as

$$\hat{F} = \sum_{\alpha\beta}\langle\alpha|\hat{f}|\beta\rangle a_\alpha^\dagger a_\beta \tag{1.22}$$

The matrix elements of 1-body operator for one-body, two-body states,

$$\begin{aligned} \langle\alpha_1|\hat{F}|\alpha_2\rangle &= \langle\alpha_1|\hat{f}|\alpha_2\rangle \\ \langle\alpha_1\alpha_2|\hat{F}|\alpha_3\alpha_4\rangle &= \delta_{\alpha_1\alpha_3}\langle\alpha_2|\hat{f}|\alpha_4\rangle - \delta_{\alpha_1\alpha_4}\langle\alpha_2|\hat{f}|\alpha_3\rangle \\ &\quad -\delta_{\alpha_2\alpha_3}\langle\alpha_1|\hat{f}|\alpha_4\rangle + \delta_{\alpha_2\alpha_4}\langle\alpha_1|\hat{f}|\alpha_3\rangle. \end{aligned} \tag{1.23}$$

For energy calculation, where initial and final state is the same,

$$\langle\alpha_1\alpha_2|\hat{F}|\alpha_1\alpha_2\rangle = \langle\alpha_1|\hat{f}|\alpha_1\rangle + \langle\alpha_2|\hat{f}|\alpha_2\rangle. \tag{1.24}$$

Similar expression can be obtained for many-body anti-symmetric Slater-determinant. (Basically, only one state in left and right can be different and one can consider different combinations.)

$$\langle\Phi|\hat{F}|\Phi\rangle = \sum_{\mu=1}^{A}\langle\mu|\hat{f}|\mu\rangle \tag{1.25}$$

1.5.2 2-Body operator

General two-body operator can be written as

$$\begin{aligned}\hat{G} &= \frac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|\hat{g}|\gamma\delta)a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \\ &= \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{g}|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \end{aligned} \tag{1.26}$$

Matrix elements for two-body states is

$$\langle\alpha_1\alpha_2|\hat{G}|\alpha_3\alpha_4\rangle = \langle\alpha_1\alpha_2|\hat{g}|\alpha_3\alpha_4\rangle \tag{1.27}$$

For energy calculation, matrix element becomes [3]

$$\langle\alpha_1\alpha_2|\hat{G}|\alpha_1\alpha_2\rangle = \langle\alpha_1\alpha_2|\hat{g}|\alpha_1\alpha_2\rangle = (\alpha_1\alpha_2|\hat{g}|\alpha_1\alpha_2 - \alpha_2\alpha_1) \tag{1.28}$$

We can do similar calculations for three-body states $|\alpha_1\alpha_2\alpha_3\rangle$ which will leave at least one nucleon to be a spectator. Then, energy calculation gives

$$\begin{aligned}\langle\alpha_1\alpha_2\alpha_3|\hat{G}|\alpha_1\alpha_2\alpha_3\rangle &= \langle\alpha_2\alpha_3|\hat{g}|\alpha_2\alpha_3\rangle + \langle\alpha_1\alpha_3|\hat{g}|\alpha_1\alpha_3\rangle + \langle\alpha_1\alpha_2|\hat{g}|\alpha_1\alpha_2\rangle \\ &= \frac{1}{2}\sum_{\mu\nu}\langle\mu\nu|\hat{g}|\mu\nu\rangle \end{aligned} \tag{1.29}$$

In actual construction of Hamiltonian for A-body, we need matrix elements for A-body Slater determinant states. But these can be reduced into sum of one-body and two-body matrix elements.

$$\langle\Phi|\hat{G}|\Phi\rangle = \frac{1}{2}\sum_{\mu\nu}\langle\mu\nu|\hat{g}|\mu\nu\rangle \tag{1.30}$$

1.5.3 three-body operator

$$\hat{V}_3 = \frac{1}{36}\sum_{pqrstu}\langle pqr|\hat{v}_3|stu\rangle_{AS}a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s \tag{1.31}$$

where anti-symmetrized matrix element

$$\langle pqr|\hat{v}_3|stu\rangle_{AS} = (pqr|\hat{v}_3|stu) + (pqr|\hat{v}_3|tus) + (pqr|\hat{v}_3|ust) - (pqr|\hat{v}_3|sut) - (pqr|\hat{v}_3|tsu) - (pqr|\hat{v}_3|uts) \tag{1.32}$$

This will gives matrix element for 3-body state

$$\langle\alpha_1\alpha_2\alpha_3|\hat{V}_3|\alpha_1\alpha_2\alpha_3\rangle = \langle\alpha_1\alpha_2\alpha_3|\hat{v}_3|\alpha_1\alpha_2\alpha_3\rangle \tag{1.33}$$

For many-body SD state,

$$\langle\Phi|\hat{V}_3|\Phi\rangle = \frac{1}{6}\sum_{ijk}\langle ijk|\hat{v}_3|ijk\rangle \tag{1.34}$$

Note that we only considered matrix elements for reference state, $\langle\Phi|H|\Phi\rangle$, here. However, in general, we need Hamiltonian $\hat{H}$ matrix element $\langle\Phi^{P_H}|\hat{H}|\Phi^{P'}_{H'}\rangle$.

[3] Relation between upper line and lower line in above equation

1.6 Hamiltonian in second quantization

Usual Hamiltonian atually contains C.M. energy,

$$\begin{aligned}\hat{H} &= \hat{T}_{rel} + \hat{V}_{rel} + \hat{T}_{cm} \\ &= \sum_{pq}\langle p|\hat{t}|q\rangle a_p^\dagger a_q + \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r \end{aligned} \tag{1.35}$$

One may add and subtract one-body potential,

$$\begin{aligned}\hat{H} &= \sum_{\alpha\beta}\langle\alpha|\hat{t}+\hat{u}_{ext}|\beta\rangle a_\alpha^\dagger a_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma - \sum_{\alpha\beta}\langle\alpha|\hat{u}_{ext}|\beta\rangle a_\alpha^\dagger a_\beta \\ &= \sum_{\alpha\beta}\langle\alpha|\hat{t}+\hat{u}_{ext}|\beta\rangle a_\alpha^\dagger a_\beta + \frac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|\hat{v}|\gamma\delta) a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma - \sum_{\alpha\beta}\langle\alpha|\hat{u}_{ext}|\beta\rangle a_\alpha^\dagger a_\beta \end{aligned} \tag{1.36}$$

where, $\langle\alpha\beta|\hat{v}|\gamma\delta\rangle = \bar{v}_{\alpha\beta\gamma\delta} = (\alpha\beta|v|\gamma\delta - \delta\gamma) = \langle\alpha\beta|\hat{H}_I|\gamma\delta\rangle$.

Introduce a reference state in one basis $|\Phi\rangle = \prod_{\alpha<=A} a_\alpha^\dagger|0\rangle$. Then, reference energy becomes

$$E_{ref}[\Phi] = \langle\Phi|\hat{H}|\Phi\rangle = \sum_{\alpha<=A}\langle\alpha|\hat{t}|\alpha\rangle + \frac{1}{2}\sum_{\alpha\beta<=A}\langle\alpha\beta|v|\alpha\beta\rangle \tag{1.37}$$

Note that this is correct even when $\hat{t}$ is not diagonal in the basis.

If one use different basis and reference state such that

$$\begin{aligned}|i\rangle &= \sum_\alpha C_{i\alpha}|\alpha\rangle, \\ |\Psi\rangle &= \prod_{i<=A} a_i^\dagger|i\rangle \end{aligned} \tag{1.38}$$

In other words, in basis functions,

$$\psi_p(x) = \sum_\lambda C_{p\lambda}\phi_\lambda(x), \tag{1.39}$$

$$\Psi_{new} = \frac{1}{\sqrt{A!}}\det(\psi_p(x_q)) = \frac{1}{\sqrt{A!}}\det(C)\det(\Phi) \tag{1.40}$$

where $det(\Phi)$ is determinant given by the basis functions $\phi_\lambda(x)$.

The new reference energy is

$$\begin{aligned}E_{ref}[\Psi] &= \langle\Psi|\hat{H}|\Psi\rangle \\ &= \sum_{i<=A}\langle i|\hat{t}|i\rangle + \frac{1}{2}\sum_{ij<=A}\langle ij|v|ij\rangle \\ &= \sum_{i=1}^{A}\sum_{\alpha\beta} C_{i\alpha}^* C_{i\beta}\langle\alpha|\hat{t}|\beta\rangle + \frac{1}{2}\sum_{ij=1}^{A}\sum_{\alpha\beta\gamma\delta} C_{i\alpha}^* C_{j\beta}^* C_{i\gamma} C_{j\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle \\ &= \sum_{\alpha\beta}\left(\sum_{i=1}^{A} C_{i\alpha}^* C_{i\beta}\right)\langle\alpha|\hat{t}|\beta\rangle + \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\left(\sum_{ij=1}^{A} C_{i\alpha}^* C_{j\beta}^* C_{i\gamma} C_{j\delta}\right)\langle\alpha\beta|\hat{v}|\gamma\delta\rangle \\ &= \sum_{\alpha\beta}\rho_{\alpha\beta}\langle\alpha|\hat{t}|\beta\rangle + \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\rho_{\alpha\gamma}\rho_{\beta\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle \end{aligned} \tag{1.41}$$

where the second line is a relation between new reference energy in terms of matrix elements in old basis.

With reference energy, one can define correlation energy for exact solution in terms of normal ordered operators,

$$\Delta E = E - E_{ref} = \langle \Psi^{exact} | \hat{H}_N | \Psi^{exact} \rangle \tag{1.42}$$

later we will see that $\hat{H}_N = \hat{F}_N + \hat{V}_N$ and one-body $\hat{F}_N$ contains a contribution from two-body interactions. HF method is to choose basis such that matrix elements of $\hat{F}$ becomes diagonal.

1.7 Particle-hole formalism

Suppose a many-body Slater determinant $|c\rangle$ as a reference state.

$$|c\rangle = |\alpha_1 \dots \alpha_n\rangle = a^\dagger_{\alpha_1} \cdots a^\dagger_{\alpha_n} |0\rangle \tag{1.43}$$

One additional particle state or hole state can be expressed as

$$\begin{aligned} |\alpha_1 \dots \alpha_{n-1} \alpha_n \alpha_{n+1}\rangle &= (-1)^n a^\dagger_{\alpha_{n+1}} |c\rangle = (-1)^n |\alpha_{n+1}\rangle_c, \\ |\alpha_1 \dots \alpha_{n-1}\rangle &= (-1)^{n-1} a_{\alpha_n} |c\rangle = (-1)^{n-1} |\alpha_{n-1}\rangle_c = (-1)^{n-1} |\alpha_{n+1}\rangle_c. \end{aligned} \tag{1.44}$$

Instead, one can define new (quasi-particle) operators $b^\dagger_\alpha$, b_α so that $b_\alpha |c\rangle = 0$ regardless $\alpha > F$ or $\alpha \le F$.

$$\begin{aligned} b^\dagger_\alpha |c\rangle &= a^\dagger_\alpha |c\rangle \text{ for } \alpha > F, \quad a_\alpha |c\rangle \text{ for } \alpha \le F, \\ b_\alpha |c\rangle &= a_\alpha |c\rangle \text{ for } \alpha > F, \quad a^\dagger_\alpha |c\rangle \text{ for } \alpha \le F \end{aligned} \tag{1.45}$$

Then, general particle-hole state can be written as

$$|\beta_1 \dots \beta_{n_p} \gamma_1^{-1} \dots \gamma_{n_h}^{-1}\rangle = b^\dagger_{\beta_1} \dots b^\dagger_{\beta_{n_p}} b^\dagger_{\gamma_1} \dots b^\dagger_{\gamma_{n_h}} |c\rangle, \quad \beta_{1\dots n_p} > F, \quad \gamma_{1\dots n_f} \le F. \tag{1.46}$$

Then, number operator becomes

$$\hat{N} = \sum_\alpha a^\dagger_\alpha a_\alpha = \sum_{\alpha > F} b^\dagger_\alpha b_\alpha + n_c - \sum_{\alpha \le F} b^\dagger_\alpha b_\alpha \tag{1.47}$$

which gives $n_p + n_c - n_h$, total number of particles in the states.

We may define quasi-particle number operator

$$N_{qp} = \sum_\alpha b^\dagger_\alpha b_\alpha \tag{1.48}$$

which gives $n_p + n_h$, total number of quasi-particles.

In Index convention:

$$\begin{aligned} \textbf{Holes}: &\quad i, j, k, \cdots, \\ \textbf{Particles}: &\quad a, b, c, \cdots, \\ \textbf{General}: &\quad p, q, r, \cdots, \end{aligned}$$

Hamiltonian $\hat{H}_0$ becomes

$$\begin{aligned} \hat{H}_0 &= \sum_{pq} \langle p | \hat{h} | q \rangle a^\dagger_p a_q \\ &= \sum_{ab > F} \langle a | \hat{h} | b \rangle b^\dagger_a b_b + \sum_{a > F, i < F} \Big(\langle a | \hat{h} | i \rangle b^\dagger_a b^\dagger_i + \langle i | \hat{h} | a \rangle b_i b_a \Big) \\ &\quad + \sum_{i < F} \langle i | \hat{h} | i \rangle - \sum_{ij < F} \langle j | \hat{h} | i \rangle b^\dagger_i b_j \end{aligned} \tag{1.49}$$

(Here the $\langle i|\hat{h}|i\rangle$ term comes from anti-commutator.) In a similar way, we get for two-body Hamiltonian $\hat{H}_I$ as

$$\hat{H}_I = \hat{H}_I^{(a)} + \hat{H}_I^{(b)} + \hat{H}_I^{(c)} + \hat{H}_I^{(d)} + \hat{H}_I^{(e)} \tag{1.50}$$

which is rather complicate.

One can use normal ordering convention to express the result in simple form.

$$\hat{H}_0 = \sum_{pq}\langle p|\hat{h}|q\rangle N(a_p^\dagger a_q) + \sum_{i<F}\langle i|\hat{h}|i\rangle \tag{1.51}$$

1.8 Wick's theorem

For given state $|\Psi\rangle$, we may find a decomposition of any operator such that

$$\begin{aligned}\hat{A} &= \hat{A}_0 + \hat{A}^- + \hat{A}^+, \\ \hat{A}_0 &= \langle\Psi|\hat{A}|\Psi\rangle, \quad \hat{A}^-|\Psi\rangle = 0, \quad \langle\Psi|\hat{A}^+ = 0.\end{aligned} \tag{1.52}$$

Note that $\hat{A}^\pm$ can be a linear combination of creation and annihilation operators, $a_i^\dagger$ and a_j, with respect to $|\Psi\rangle$ such that $a_j|\Psi\rangle = 0 = \langle\Psi|a_i^\dagger$. (In this case $\hat{A}_0 = 0$.) (여기서 주의할 것은 normal ordering is defined w.r.t. reference state. 예를 들어 $|\Phi\rangle = \prod_{i=1,A} a_i^\dagger|0\rangle$, $a_{i=1,A}|\Phi\rangle \neq 0$ 이므로 $a_{i=1,A}$, $a_{i>A}^\dagger$ 는 $\hat{A}^+$ 에 속하고, $a_{i>A}$ 나 $a_{i<=A}^\dagger$ 는 $\hat{A}^-$ 에 속하게 된다.)

In many body theory, we consider decomposition of operators with respect to the ground state $|0\rangle$. Let us assume commutation relations,

$$[A_i^-, A_j^-]_\pm = [A_i^+, A_j^+]_\pm = 0, \quad [A_i^-, A_j^+]_\pm = \delta_{ij} \tag{1.53}$$

On the other hand, for any n-body operator, $\hat{F}^{(n)}$, which has n $a^\dagger$ operators and n a operators, [4]

$$\sum_\alpha a_\alpha^\dagger[a_\alpha, \hat{F}^{(n)}] = n\hat{F}^{(n)} \tag{1.55}$$

Normal ordering is defined such that all $\hat{A}^+$ operators are left to all $\hat{A}^-$ operators.
For example,

$$\begin{aligned}N[A_1A_2] &= N[A_1^+A_2^+] + N[A_1^+A_2^-] + N[A_1^-A_2^-] + N[A_1^-A_2^+] \\ &= A_1^+A_2^+ + A_1^+A_2^- + A_1^-A_2^- + N[A_1^-A_2^+] = A_1A_2 - A_1^-A_2^+ + N[A_1^-A_2^+] \\ &= A_1A_2 - [A_1^-, A_2^+]_\pm.\end{aligned} \tag{1.56}$$

This implies that $\langle\Psi|N[A_1A_2]|\Psi\rangle = 0$. However, be careful that it does not necessarily mean $N[A_1A_2]|\Psi\rangle = 0$ because it can be $A_1^+A_2^+$. (즉, reference state의 경우에는 move all operators that

[4](This can be understood as follows: if one moves a_α to right-side, one gets one $\hat{F}^{(n)}$ and operators which have sign and order changed because $\sum_\alpha a_\alpha^\dagger a_\alpha a_\beta^\dagger = a_\beta^\dagger - \sum_\alpha a_\alpha^\dagger a_\beta^\dagger a_\alpha$. Then, after moving a_α to the rightmost side, one gets $n\hat{F}^{(n)} + \sum_\alpha a_\alpha^\dagger \hat{F}^{(n)} a_\alpha$.)

Using this relation, Hamiltonian with two-body interaction $\hat{H} = \hat{T} + \hat{V}$, $\hat{T} = \sum_\alpha a_\alpha^\dagger[a_\alpha, \hat{T}]$, $\hat{V} = \frac{1}{2}\sum_\alpha a_\alpha^\dagger[a_\alpha, \hat{V}]$,

$$\begin{aligned}\langle\Psi_0^A|\hat{H}|\Psi_0^A\rangle &= \langle\Psi_0^A|\frac{1}{2}\hat{T} + \frac{1}{2}\sum_\alpha a_\alpha^\dagger[a_\alpha, \hat{T}] + \frac{1}{2}\sum_\alpha a_\alpha^\dagger[a_\alpha, \hat{V}]|\Psi_0^A\rangle \\ &= \frac{1}{2}\langle\Psi_0^A|\hat{T}|\Psi_0^A\rangle + \frac{1}{2}\langle\Psi_0^A|\sum_\alpha a_\alpha^\dagger[a_\alpha, \hat{H}]|\Psi_0^A\rangle \\ &= \frac{1}{2}\langle\Psi_0^A|\hat{T}|\Psi_0^A\rangle + \frac{1}{2}\sum_\alpha\sum_\nu [E_0^N - E_\nu^{N-1}]|\langle\Psi_\nu^{N-1}|a_\alpha|\Psi_0^N\rangle|^2 (?)\end{aligned} \tag{1.54}$$

where the last line need more explanation.

annihilate the reference state to the right of those that create on the reference state. 그리고, reference state에 대한 expectation 은 zero 가 된다. $\langle\Phi|N[\hat{O}]|\Phi\rangle = 0$. 그러나, 이것이 $N[\hat{O}]|\Phi\rangle = 0$ 을 의미하지는 않는다.)

A **contraction** is defined as,

$$\begin{aligned} \overbrace{A_1 A_2} &\equiv \hat{A}_1\hat{A}_2 - N[\hat{A}_1\hat{A}_2], \\ \overbrace{A_1 A_2} &= [A_1^-, A_2^+]_\pm = \langle 0|A_1 A_2|0\rangle \end{aligned} \tag{1.57}$$

Because the contraction is a number not an operator, by normal ordering, one can reduce the operator ranks.

Normal ordering satisfies,

$$N[AB] = -N[BA], \quad < N[AB] >= 0, \quad < AB >= \overbrace{AB} \tag{1.58}$$

Extended definition of contraction is

$$\overbrace{A A_1 A_2 \cdots A_n A'} = (\pm 1)^n \overbrace{A A'} A_1 A_2 \cdots A_n, \tag{1.59}$$

where, the order in contraction have to be kept. ($\overbrace{AA'} \neq \overbrace{A'A}$ in general.)

Note in normal ordering, any permutation of operator gives (± 1) factor,

$$N[A_1 A_2 \cdots A_n] = (\pm 1)^P N[A_{P_1} A_{P_2} \cdots A_{P_n}] \tag{1.60}$$

regardless A^+ or A^-.

Wick's theorem can be proved in steps by proving lemmas. (I am not going to prove them.)

- lemma 1:

$$A_0^-[A_1^+ \cdots A_n^+] = N[A_0^- A_1^+ \cdots A_n^+] + \sum_{i=1}^{n} N[\overbrace{A_0 \cdots A_i} \cdots A_n^+]. \tag{1.61}$$

- lemma 2:

$$A_0^-[A_1 \cdots A_n] = N[A_0^- A_1 \cdots A_n] + \sum_{i=1}^{n} N[\overbrace{A_0 \cdots A_i} \cdots A_n]. \tag{1.62}$$

- lemma 3:

$$A_0[A_1 \cdots A_n] = N[A_0 A_1 \cdots A_n] + \sum_{i=1}^{n} N[\overbrace{A_0 \cdots A_i} \cdots A_n]. \tag{1.63}$$

- (Time independent) Wick's theorem: A product of operator is equivalent to the normal ordered product plus all possible normal ordering with contractions.

$$\begin{aligned} A_1 \cdots A_n &= N[A_1 \cdots A_n] + \sum_{(ij)} N[A_1 \cdots \overbrace{A_i \cdots A_j} \cdots A_n] \\ &\quad + \sum_{(ij)(rs)} N[A_1 \cdots \overbrace{A_i \cdots \overbrace{A_r \cdots A_j} \cdots A_s} \cdots A_n] + \cdots \end{aligned} \tag{1.64}$$

- **Standard (Time independent) Wick's theorem**:A general product of operators which are in normal ordered form is given by the overall normal product plus the sum of all overall

normal products with contractions between operators that were not in the same original normal product.

$$\begin{aligned} & N\{\hat{A}_1\hat{A}_2\cdots\}N\{\hat{B}_1\hat{B}_2\cdots\}N\{\hat{C}_1\hat{C}_2\cdots\} \\ = \; & N\{\hat{A}_1\hat{A}_2\cdots\hat{B}_1\hat{B}_2\cdots\hat{C}_1\hat{C}_2\cdots\} + \sum_{all\ external\ contractions} \{\hat{A}_1\hat{A}_2\cdots\hat{B}_1\hat{B}_2\cdots\hat{C}_1\hat{C}_2\cdots\} \end{aligned} \tag{1.65}$$

where 'external contraction' is a contraction between operators that were not in the same original normal product. (The summation implies one-contraction, two-contraction, and so on for all possible cases.)

For example,

$$\begin{aligned} A_1A_2A_3 &= N[A_1A_2A_3] + N[\overbrace{A_1}A_2A_3] + N[\overbrace{A_1A_2}A_3] + N[A_1\overbrace{A_2}A_3] \\ &= N[A_1A_2A_3] + \langle 12\rangle A_3 \pm \langle 13\rangle A_2 + \langle 23\rangle A_1 \end{aligned} \tag{1.66}$$

$$\begin{aligned} A_1A_2A_3A_4 &= N[1234] + \langle 12\rangle N[34] \pm \langle 13\rangle N[24] + \langle 14\rangle N[23] \\ &\quad + \langle 23\rangle N[14] \pm \langle 24\rangle N[13] \pm \langle 34\rangle N[12] \\ &\quad + \langle 12\rangle\langle 34\rangle \pm \langle 13\rangle\langle 24\rangle + \langle 14\rangle\langle 23\rangle. \end{aligned} \tag{1.67}$$

In particular,

$$\begin{aligned} c_p^\dagger c_q^\dagger c_s c_r &= N[c_p^\dagger c_q^\dagger c_s c_r] + \langle c_p^\dagger c_q^\dagger\rangle N[c_s c_r] \pm \langle c_p^\dagger c_s\rangle N[c_q^\dagger c_r] + \langle c_p^\dagger c_r\rangle N[c_q^\dagger c_s] \\ &\quad + \langle c_q^\dagger c_s\rangle N[c_p^\dagger c_r] \pm \langle c_q^\dagger c_r\rangle N[c_p^\dagger c_s] \pm \langle c_s c_r\rangle N[c_p^\dagger c_q^\dagger] \\ &\quad + \langle c_p^\dagger c_q^\dagger\rangle\langle c_s c_r\rangle \pm \langle c_p^\dagger c_s\rangle\langle c_q^\dagger c_r\rangle + \langle c_p^\dagger c_r\rangle\langle c_q^\dagger c_s\rangle \end{aligned} \tag{1.68}$$

Thus, if we take expectation value for ground state $|\Phi\rangle$, because $\langle\Phi|N[\cdots]|\Phi\rangle = 0$,

$$\langle\Phi|c_p^\dagger c_q^\dagger c_s c_r|\Phi\rangle = \langle c_p^\dagger c_q^\dagger\rangle\langle c_s c_r\rangle \pm \langle c_p^\dagger c_s\rangle\langle c_q^\dagger c_r\rangle + \langle c_p^\dagger c_r\rangle\langle c_q^\dagger c_s\rangle \tag{1.69}$$

The matrix elements depends on the ansatz of ground state(or combinations in $c^\dagger$, c).

For H-F states that the only non-zero contractions are

$$\overbrace{c_i^\dagger c_j} = \delta_{ij}, \quad \overbrace{c_a c_b^\dagger} = \delta_{ab} \tag{1.70}$$

For HFB or HF+BCS case, one can have non-zero contraction between $\overbrace{c_i^\dagger c_j^\dagger}$ and $\overbrace{c_i c_j}$

Examples of normal ordering for reference state

Index convention:

$$\begin{aligned} \textbf{Holes}: &\quad i, j, k, \cdots, \\ \textbf{Particles}: &\quad a, b, c, \cdots, \\ \textbf{General}: &\quad p, q, r, \cdots, \end{aligned}$$

Let us use index $i, j\ldots$ for states below Fermi level, $a, b\ldots$ for states above Fermi level and $p, q, \ldots$ for any states. $\langle\Phi_0|N[c_p^\dagger c_q]|\Phi_0\rangle = 0$ implies one of p or q is above Fermi level and another is below Fermi level. $N[c_p^\dagger c_q] = c_p^\dagger c_a$ or $-c_q c_i^\dagger$. 즉 여기서 normal ordering은 $a_{a>F}$ 또는 $a_{i<F}^\dagger$ operator 를 오른쪽으로 보내는 것을 의미한다. Then,

$$\begin{aligned} \sum_{pq} h_{pq} a_p^\dagger a_q &= \sum_{ab} h_{ab} a_a^\dagger a_b + \sum_{ai} h_{ai} a_a^\dagger a_i + \sum_{ia} h_{ia} a_i^\dagger a_a + \sum_{ij} h_{ij} a_i^\dagger a_j \\ &= \sum_{pq} h_{pq} N[a_p^\dagger a_q] + \sum_i h_{ii} \end{aligned} \tag{1.71}$$

Note that h_{pq} should be anti-symmetrized in normal-ordered form.

$$\begin{aligned} N[c_a^\dagger c_i]N[c_p^\dagger c_q] &= N[c_a^\dagger c_i a_p^\dagger c_q] = N[c_p^\dagger c_q c_a^\dagger c_i], \\ N[c_p^\dagger c_q]N[c_a^\dagger c_i] &= N[c_p^\dagger c_q c_a^\dagger c_i] + N[\overbrace{c_p^\dagger c_q c_a^\dagger} c_i] + N[c_p^\dagger \overbrace{c_q c_a^\dagger} c_i] + N[\overbrace{c_p^\dagger \overbrace{c_q c_a^\dagger} c_i}] \\ &= N[c_p^\dagger c_q c_a^\dagger c_i] + \delta_{qa} N[c_p^\dagger c_i] + \delta_{pi} N[c_q c_a^\dagger] + \delta_{qa}\delta_{pi} \end{aligned} \tag{1.72}$$

(즉, $N[c_p^\dagger c_q]N[c_a^\dagger c_i]$의 경우 Wick's theorem에 의해 먼저 전체 normal ordering 한 $N[c_p^\dagger c_q c_a^\dagger c_i]$에 더해서 normal ordering이되, pq와 ai 중 한쌍이 서로 contract 된 것들 더하기 두쌍이 contract된 것.)

In other words,

$$N[c_p^\dagger c_q]N[c_a^\dagger c_i] - N[c_a^\dagger c_i]N[c_p^\dagger c_q] = \delta_{qa} N[c_p^\dagger c_i] + \delta_{pi} N[c_q c_a^\dagger] + \delta_{qa}\delta_{pi} \tag{1.73}$$

즉, 두개의 normal ordered 1-body operator의 commutator는 두 operator사이에 connected term들만이 남는다.(δ를 포함한다) 특히 fully connected되지 않는 경우는 항상 normal ordered operator항을 가진다.

Thus, for usual reference state $|\Phi\rangle = \prod_i a_i^\dagger |0\rangle$,

$$\begin{aligned} c_p^\dagger c_q^\dagger c_s c_r &= N[c_p^\dagger c_q^\dagger c_s c_r] \pm \delta_{ps<F} N[c_q^\dagger c_r] + \delta_{pr<F} N[c_q^\dagger c_s] \\ &\quad + \delta_{qs<F} N[c_p^\dagger c_r] \pm \delta_{qr<F} N[c_p^\dagger c_s] \pm \delta_{ps<F}\langle c_q^\dagger c_r\rangle + \delta_{pr<F}\langle c_q^\dagger c_s\rangle \end{aligned} \tag{1.74}$$

For fermions for usual reference state $|\Phi\rangle = \prod_i a_i^\dagger |0\rangle$,

$$\begin{aligned} \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle c_p^\dagger c_q^\dagger c_s c_r &= \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle (N[c_p^\dagger c_q^\dagger c_s c_r] \\ &\quad - \delta_{ps<F} N[c_q^\dagger c_r] + \delta_{pr<F} N[c_q^\dagger c_s] + \delta_{qs<F} N[c_p^\dagger c_r] - \delta_{qr<F} N[c_p^\dagger c_s] \\ &\quad - \delta_{ps<F}\delta_{qr<F} + \delta_{pr<F}\delta_{qs<F}) \\ &= \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle N[c_p^\dagger c_q^\dagger c_s c_r] + \frac{1}{4}\sum_{pq,i<F} 4\langle pi||qi\rangle N[c_p^\dagger c_q] + \frac{1}{4}\sum_{ij<F} 2\langle ij||ij\rangle \end{aligned}$$

Need proof: Thus, commutator of **any** normal ordered operators always results in **connected** terms between two operators. (This is related with linked cluster theorem.)

1.9 Normal ordered Hamiltonian w.r.t. a reference

For example, considering simple slater determinant with Fermi level as a ground state, we get

$$\hat{H}_0 = \sum_{pq}\langle p|\hat{h}_0|q\rangle c_p^\dagger c_q = \sum_{pq}\langle p|\hat{h}_0|q\rangle N[c_p^\dagger c_q] + \sum_{i\le F}\langle i|\hat{h}_0|i\rangle \tag{1.75}$$

where $\hat{h}_0 = \hat{t} + \hat{u}_{ext}$ is a s.p. Hamiltonian. But, usually there is no u_{ext}.

$$\begin{aligned} \hat{V} &= \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle_{AS} c_p^\dagger c_q^\dagger c_s c_r \\ &= \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle_{AS} N[c_p^\dagger c_q^\dagger c_s c_r] + \sum_{pq}\sum_{i\le F}\langle pi|\hat{v}|qi\rangle_{AS} N[c_p^\dagger c_q] + \frac{1}{2}\sum_{ij\le F}\langle ij|\hat{v}|ij\rangle_{AS} \end{aligned} \tag{1.76}$$

where matrix elements are defined to be anti-symmetric, **(From now on, $\langle pq|v|rs\rangle$ is implied to be anti-symmetrized,$\langle pq|v|rs\rangle_{AS}$)**

For 3-body interaction

$$\begin{aligned}\hat{V}_3 &= \frac{1}{36}\sum_{pqrstu}\langle pqr|\hat{V}_3|stu\rangle c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s \\ &= \frac{1}{36}\sum_{pqrstu}\langle pqr|\hat{V}_3|stu\rangle N[c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s] + \sum_{pqrs}\sum_{i\le F}\langle pqi|\hat{V}_3|rsi\rangle N[c_p^\dagger c_q^\dagger c_s^\dagger c_r] \\ &\quad + \sum_{pq}\sum_{ij\le F}\langle pij|\hat{V}_3|qij\rangle N[c_p^\dagger c_q] + \frac{1}{6}\sum_{ijk\le F}\langle ijk|\hat{V}_3|ijk\rangle \end{aligned} \tag{1.77}$$

where 3-body anti-symmetrized matrix element is

$$\begin{aligned}\langle pqr|\hat{V}_3|stu\rangle_{AS} &= \langle pqr|\hat{V}_3|stu\rangle + \langle pqr|\hat{V}_3|tus\rangle + \langle pqr|\hat{V}_3|ust\rangle \\ &\quad -\langle pqr|\hat{V}_3|sut\rangle - \langle pqr|\hat{V}_3|tsu\rangle - \langle pqr|\hat{V}_3|uts\rangle.\end{aligned}$$

By combining these, we can rewrite (여기서 V_{2N} 의 N 은 nucleon이 아니라 Normal ordered 를 의미한다.)

$$\begin{aligned}\hat{H} &= \sum_{pq}\langle p|\hat{h}_0|q\rangle a_p^\dagger a_q + \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle_{AS} c_p^\dagger c_q^\dagger c_s c_r + \frac{1}{36}\sum_{pqrstu}\langle pqr|\hat{V}_3|stu\rangle c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s \\ &= E_{ref} + \hat{H}_N = E_{ref} + \hat{F}_N + \hat{V}_{2N} + \hat{V}_{3N}\end{aligned} \tag{1.78}$$

Reference Energy (여기서, F는 $|\Phi_0\rangle$에 포함된 state인가 아닌가를 나타냄.)[5]

$$E_{ref} = \langle\Phi_0|\hat{H}|\Phi_0\rangle = \sum_{i\le F}\langle i|\hat{h}_0|i\rangle + \frac{1}{2}\sum_{ij\le F}\langle ij|\hat{v}_2|ij\rangle_{AS} + \frac{1}{6}\sum_{ijk\le F}\langle ijk|\hat{v}_3|ijk\rangle. \tag{1.80}$$

Normal-ordered one-body(which include terms induced from 2-body interaction.)

$$\begin{aligned}\hat{F}_N &= \sum_{pq}\langle p|\hat{f}|q\rangle N[c_p^\dagger c_q], \\ \langle p|\hat{f}|q\rangle &= \langle p|\hat{h}_0|q\rangle + \sum_{i\le F}\langle pi|\hat{v}_2|qi\rangle_{AS} + \sum_{ij\le F}\langle pij|\hat{v}_3|qij\rangle\end{aligned} \tag{1.81}$$

In general, this matrix elements are not diagonal in usual basis. (만약 여기서, external potential이 없는 경우 $\hat{h_0} \to \hat{t}_0$가 되고, 일반적으로 $\langle p|\hat{t}_0|q\rangle$ 는 diagonal이 아님. 만약 external potential을 포함하여 basis가 eigen state 라면, $\langle p|\hat{h}_0|q\rangle$ 는 diagonal 이 된다. 한편, 만약 처음부터 external potential이 없는 경우를 생각한다면, 다시 $\langle p|\hat{u}|q\rangle$를 빼주어야 하는데, $-\langle p|\hat{u}|q\rangle + \sum_{i\le F}\langle pi|\hat{v}_2|qi\rangle_{AS} = 0$이 되도록 $\hat{u}$ 와 basis를 정한다면, H-F basis이고 $\langle p|\hat{f}|q\rangle$ 는 two-body interaction만 생각할 때 diagonal이 된다. 3-body interaction을 고려하면, HF basis에서도 diagonal이 아니다.)

Normal-ordered two-body and 3-body Hamiltonian

$$\begin{aligned}\hat{V}_{2N} &= \frac{1}{4}\sum_{pqrs}\left(\langle pq|\hat{v}_2|rs\rangle_{AS} + 4\sum_{i\le F}\langle pqi|\hat{v}_3|rsi\rangle\right) N[c_p^\dagger c_q^\dagger c_s c_r], \\ \hat{V}_{3N} &= \frac{1}{36}\sum_{pqrstu}\langle pqr|\hat{v}_3|stu\rangle N[c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s]\end{aligned} \tag{1.82}$$

[5]Multi-reference normal ordered approximation use reference state $|\Phi\rangle$ as a combination of multiple slater determinant. This can be expressed in terms of density matrix of reference state,

$$\begin{aligned}\gamma_{pq} &= \langle\Phi|c_p^\dagger c_q|\Phi\rangle, \\ \gamma_{pqrs} &= \langle\Phi|c_p^\dagger c_q^\dagger c_s c_r|\Phi\rangle, \\ \gamma_{pqrstu} &= \langle\Phi|c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s|\Phi\rangle.\end{aligned} \tag{1.79}$$

Normal order N-body approximation ia an approximation taking only operators up to normal ordered N-body operator. For example, $NO2A$ corresponds to neglecting $\hat{V}_{3N}$ but keeping induced 2-body interactions $\hat{V}_{2N}$. Also, note that c operators defined for physical vacuum, not for reference $|\Phi\rangle$. And matrix elements are all for original s.p. basis.

Using normal-ordered form, we can easily calculate the matrix elements for excited configurations. Introduce an excited configuration, $|\Phi_i^a\rangle = c_a^\dagger c_i|\Phi\rangle$ with $i \le F, a > F$, ($|\Phi_i^a\rangle$ is a slater determinant replacing s.p. state i to a in $|\Phi\rangle$.). The matrix elements of normal-ordered terms can be written as

$$\begin{aligned}
\langle\Phi|\hat{F}_N|\Phi\rangle &= \langle\Phi|\hat{V}_{2N}|\Phi\rangle = 0, \\
\langle\Phi|\hat{F}_N|\Phi_i^a\rangle &= \langle i|\hat{f}|a\rangle, \quad \langle\Phi|\hat{V}_{2N}|\Phi_i^a\rangle = 0, \\
\langle\Phi|\hat{F}_N|\Phi_{ij}^{ab}\rangle &= 0, \quad \langle\Phi|\hat{V}_{2N}|\Phi_{ij}^{ab}\rangle = \langle ij|\hat{v}|ab\rangle_{AS}, \\
\langle\Phi|\hat{F}_N|\Phi_{ijk}^{abc}\rangle &= \langle\Phi|\hat{V}_{2N}|\Phi_{ijk}^{abc}\rangle = 0.
\end{aligned} \tag{1.83}$$

Also,

$$\begin{aligned}
\langle\Phi_i^a|\hat{F}_N|\Phi\rangle &= \langle a|f|i\rangle \\
\langle\Phi_{ij}^{ab}|\hat{V}_{2N}|\Phi\rangle &= \langle ab|v|ij\rangle_{AS}
\end{aligned} \tag{1.84}$$

$$\langle\Phi_i^a|\hat{F}_N|\Phi_i^a\rangle = \langle a|f|a\rangle - \langle i|f|i\rangle \tag{1.85}$$

Details for the matrix elements of normal ordered Hamiltonian

For more detailed derivation,

$$\begin{aligned}
\langle\Phi_0|\hat{T}|\Phi_i^a\rangle &= \sum_{pq}\langle p|\hat{t}|q\rangle\langle\Phi_0|c_p^\dagger c_q|\Phi_i^a\rangle \\
&= \sum_{pq}\langle p|\hat{t}|q\rangle\langle \overbrace{c_p^\dagger c_q c_a^\dagger} c_i\rangle = \langle i|\hat{t}|a\rangle
\end{aligned} \tag{1.86}$$

$$\begin{aligned}
\langle\Phi_0|\hat{V}|\Phi_i^a\rangle &= \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle\langle\Phi_0|c_p^\dagger c_q^\dagger c_s c_r|\Phi_i^a\rangle \\
&= \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle\left(\langle \overbrace{c_p^\dagger c_q^\dagger c_s c_r c_a^\dagger} c_i\rangle + \langle \overbrace{c_p^\dagger c_q^\dagger c_s c_r c_a^\dagger} c_i\rangle + \langle \overbrace{c_p^\dagger c_q^\dagger c_s c_r c_a^\dagger} c_i\rangle + \langle \overbrace{c_p^\dagger c_q^\dagger c_s c_r c_a^\dagger} c_i\rangle\right) \\
&= \sum_{m\le F}\langle im|\hat{v}|am\rangle
\end{aligned} \tag{1.87}$$

Thus,[6]

$$\langle\Phi_0|\hat{H}|\Phi_i^a\rangle = \langle\Phi_0|\hat{H}_N|\Phi_i^a\rangle = \langle i|\hat{t}|a\rangle + \sum_{m\le F}\langle im|\hat{v}|am\rangle = \langle i|\hat{f}|a\rangle \tag{1.90}$$

[6]However, individually

$$\begin{aligned}
\langle\Phi_0|\hat{F}_N|\Phi_i^a\rangle &= \sum_{pq}\langle p|\hat{f}|q\rangle\langle\Phi_0|N[a_p^\dagger a_q]|\Phi_i^a\rangle = \sum_{pq}\langle p|\hat{f}|q\rangle\left(\langle\Phi_0|a_p^\dagger a_q|\Phi_i^a\rangle - \langle\Phi_0|\overbrace{a_p^\dagger a_q}|\Phi_i^a\rangle\right) \\
&= \langle i|\hat{f}|a\rangle \neq \langle\Phi_0|\hat{T}|\Phi_i^a\rangle.
\end{aligned} \tag{1.88}$$

While

$$\langle\Phi_0|\hat{V}_N|\Phi_i^a\rangle = \langle\Phi_0|\hat{V}|\Phi_i^a\rangle - \langle\Phi_0|V|\Phi_0\rangle\langle\Phi_0|\Phi_i^a\rangle = \sum_{m\le F}\langle im|v|am\rangle \tag{1.89}$$

For 2p-2h excitation $|\Phi_{ij}^{ab}\rangle$,

$$\begin{aligned}\langle\Phi_0|\hat{T}|\Phi_{ij}^{ab}\rangle &= 0.\\ \langle\Phi_0|\hat{V}|\Phi_{ij}^{ab}\rangle &= \langle ij|\hat{v}|ab\rangle.\end{aligned} \tag{1.91}$$

For 3p-3h excitation, $|\Phi_{ijk}^{abc}\rangle$,

$$\langle\Phi_0|\hat{T}|\Phi_{ijk}^{abc}\rangle = 0, \quad \langle\Phi_0|\hat{V}|\Phi_{ijk}^{abc}\rangle = 0. \tag{1.92}$$

Up to here, there is no assumption on the basis and their matrix elements.

For general one-body and two-body operators $\hat{F} = \sum_{ab}\langle a|\hat{f}|b\rangle a_a^\dagger a_b$, $\hat{G} = \sum_{pqrs}\langle pq|\hat{g}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$, we get for $|\Phi_0\rangle$

$$\begin{aligned}\langle\Phi_0|\hat{F}|\Phi_0\rangle &= \sum_{i\le F}\langle i|\hat{f}|i\rangle,\\ \langle\Phi_0|\hat{G}|\Phi_0\rangle &= \frac{1}{2}\sum_{ij\le F}\langle ij|\hat{g}|ij\rangle\end{aligned} \tag{1.93}$$

for 1p-1h state $|\Phi_i^a\rangle$,

$$\begin{aligned}\langle\Phi_0|\hat{F}|\Phi_i^a\rangle &= \langle i|\hat{f}|a\rangle,\\ \langle\Phi_0|\hat{G}|\Phi_i^a\rangle &= \sum_{m\le F}\langle im|\hat{g}|am\rangle\end{aligned} \tag{1.94}$$

for 2p-2h states $|\Phi_{ij}^{ab}\rangle$,

$$\begin{aligned}\langle\Phi_0|\hat{F}|\Phi_{ij}^{ab}\rangle &= 0,\\ \langle\Phi_0|\hat{G}|\Phi_{ij}^{ab}\rangle &= \langle ij|\hat{g}|ab\rangle\end{aligned} \tag{1.95}$$

for 3p-3h states $|\Phi_{ijk}^{abc}\rangle$,

$$\begin{aligned}\langle\Phi_0|\hat{F}|\Phi_{ij}^{ab}\rangle &= 0,\\ \langle\Phi_0|\hat{G}|\Phi_{ij}^{ab}\rangle &= 0.\end{aligned} \tag{1.96}$$

If we only consider two-body interaction, only matrix elements between configurations which have only up to two index are different. (For example, like $\langle\Phi_{ij}^{ab}|H|\Phi_{ij}^{a'b'}\rangle$ or $\langle\Phi_{ij}^{ab}|H|\Phi_{i'j'}^{ab}\rangle$ or $\langle\Phi_{ij}^{ab}|H|\Phi_{i'j}^{a'b}\rangle$.)

Let us consider a reference Slater determinant $|SD\rangle$. For one-body and two-body operators,

$$\begin{aligned}\langle SD|O_1|SD\rangle &= \sum_{i\in\Phi}\langle\phi_i|O_1|\phi_i\rangle,\\ \langle SD|O_2|SD\rangle &= \frac{1}{2}\sum_{(i,j)\in SD}(\phi_i\phi_j|O_2|\phi_i\phi_j) - (\phi_i\phi_j|O_2|\phi_j\phi_i),\end{aligned} \tag{1.97}$$

For Slater Determinant which is different from reference by replacing one single particle states $i \to j$,

$$\begin{aligned}\langle SD|O_1|SD_i^j\rangle &= \langle\phi_i|O_1|\phi_j\rangle,\\ \langle SD|O_2|SD_i^j\rangle &= \sum_{k\in SD}(\phi_i\phi_k|O_2|\phi_j\phi_k) - (\phi_i\phi_k|O_2|\phi_k\phi_j),\end{aligned} \tag{1.98}$$

For two determinants which differ by two s.p. states,

$$\begin{aligned}\langle SD|O_1|SD_{ik}^{jl}\rangle &= 0,\\ \langle SD|O_2|SD_{ik}^{jl}\rangle &= (\phi_i\phi_k|O_2|\phi_j\phi_l) - (\phi_i\phi_k|O_2|\phi_l\phi_j),\end{aligned} \tag{1.99}$$

In this way, we can construct full Hamiltonian matrix for all $|SD\rangle, |SD_i^j\rangle, \ldots$ states.

General solution

The object is to find a eigen-value of equation with reference state $|\Phi\rangle$

$$\begin{aligned} \hat{H}|\Psi\rangle &= E|\Psi\rangle \\ &= (\hat{H}_N + E_0)|\Psi\rangle \end{aligned} \tag{1.100}$$

where up to 2-body interaction

$$\begin{aligned} \hat{H} &= \sum_{pq} \epsilon_{pq} a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} \langle pq||rs\rangle a_p^\dagger a_q^\dagger a_s a_r \\ E_0 &= \sum_i \epsilon_{ii} + \frac{1}{2} \sum_{ij} \langle ij||ij\rangle, \quad i,j \in |\Phi\rangle \\ \hat{H}_N &= \sum_{pq} f_{pq} N\left[a_p^\dagger a_q\right] + \frac{1}{4} \sum_{pqrs} \langle pq||rs\rangle N\left[a_p^\dagger a_q^\dagger a_s a_r\right] \\ f_{pq} &= \epsilon_{pq} + \sum_{i\in|\Phi\rangle} \langle ip||iq\rangle, \\ \epsilon_{pq} &= \langle p|h_0|q\rangle \end{aligned} \tag{1.101}$$

(It looks like there is some type. One may have to remove 1/2 in f_{pq} expression.) For clarity, usually $\epsilon_{pq} = \langle p|\hat{t}|q\rangle$ which is not diagonal for s.p. basis. But, one may use eigen-value of $\hat{h}_0 = \hat{t} + \hat{u}$ which generates s.p. basis.

$$\epsilon_{pq} = \langle p|\hat{t} + \hat{u} - \hat{u}|q\rangle = \epsilon_p \delta_{pq} - \langle p|\hat{u}|q\rangle \tag{1.102}$$

HF corresponds to choosing basis such that $f_{pq} = \epsilon_p \delta_{pq}$.

Reference state is assumed to be

$$|\Phi\rangle \propto \left(\prod_i a_i^\dagger\right)|0\rangle \tag{1.103}$$

In general, (with $\hat{H}_N|\Phi\rangle = 0$)

$$\begin{aligned} \hat{H}|\Psi\rangle &= E_0 c_0|\Phi\rangle + \sum_{ia} c_1 H|\Phi_i^a\rangle + \sum_{ijab} c_2 H|\Phi_{ij}^{ab}\rangle + \cdots \\ &= E_0 c_0'|\Phi\rangle + \sum_{ia} c_1'|\Phi_i^a\rangle + \sum_{ijab} c_2'|\Phi_{ij}^{ab}\rangle + \cdots \\ &= E\left(c_0|\Phi\rangle + \sum_{ia} c_1|\Phi_i^a\rangle + \sum_{ijab} c_2|\Phi_{ij}^{ab}\rangle + \cdots\right) \end{aligned} \tag{1.104}$$

and $|\Psi\rangle$ contains various excitations from reference states.

$$|\Psi\rangle = c_0|\Phi\rangle + \sum_{ia} c_1|\Phi_i^a\rangle + \sum_{ijab} c_2|\Phi_{ij}^{ab}\rangle + \cdots \tag{1.105}$$

MBPT 의 경우는 each term 이 preturbative하다고 하고, 순서대로 coefficient c 를 결정한다. 예를 들어 왼쪽에 $\langle\Phi|$ 를 두면 맨 위와 맨 아래 식에서

(no-core) Shell model truncates the series within model space and try to find $|\Psi\rangle$ which satisfies $\hat{H}|\Psi\rangle = E|\Psi\rangle$ up to this truncation.

H-F theory one approximates $\langle\Phi|H|\Psi\rangle = E_0 + c_1\langle\Phi|H|\Phi_i^a\rangle + \cdots \simeq E_0 + \cdots$ by requiring $\langle\Phi|\hat{H}|\Phi_i^a\rangle = 0$. Then, for such reference state, we have $|\Psi\rangle \simeq |\Phi\rangle$. HF-BCS theory theory or HF-Bogoliubov theory makes additional assumptions on $|\Phi\rangle$ and thus gives another constraints on truncation.

Coupled Cluster theory changes the problem to find a transformation $\bar{H} = e^{-T} H e^T$ such that the series $\bar{H}|\Phi\rangle = |\Phi\rangle + \sum|\Phi_i^a\rangle + \cdots$ is truncated, $\langle\Phi_i^a|\bar{H}|\Phi\rangle = 0$ and so on. (Note that this truncation does not imply 1p-1h truncation in $|\Psi\rangle$ because of e^T generates infinite series of excitations.)

Simple Shell model

One can choose basis by introducing s.p. potential $\hat{u}$ such that $\hat{h} = \hat{h}_0 + \hat{u}$,

$$\hat{h}|i\rangle = (\hat{t} + \hat{u})|i\rangle = \epsilon_i|i\rangle. \tag{1.106}$$

Here, the s.p. potential is arbitrary.

Then,

$$\begin{aligned} E_{ref} &= \langle\Phi_0|\hat{H}|\Phi_0\rangle = \sum_{i\leq F}\langle i|\hat{h}_0 + \hat{u}|i\rangle + \frac{1}{2}\sum_{ij\leq F}\langle ij|\hat{v}|ij\rangle_{AS} - \sum_{i\leq F}\langle i|\hat{u}|i\rangle \\ &= \sum_{i\leq F}\epsilon_i + \frac{1}{2}\sum_{ij\leq F}\langle ij|\hat{v}|ij\rangle_{AS} - \sum_{i\leq F}\langle i|\hat{u}|i\rangle \end{aligned} \tag{1.107}$$

$$\begin{aligned} \hat{H} &= E_{ref} + \hat{H}_N, \quad \hat{H}_N = \hat{F}_N + \hat{V}_N, \\ \hat{F}_N &= \sum_{pq}\langle p|\hat{t} + \hat{u}|q\rangle N[a_p^\dagger a_q] + \sum_{pq}\left(-\langle p|\hat{u}|q\rangle + \sum_{i\leq F}\langle pi|\hat{v}|qi\rangle\right)N[a_p^\dagger a_q] \\ &= \sum_{p}\epsilon_p N[a_p^\dagger a_p] + \sum_{pq}\left(-\langle p|\hat{u}|q\rangle + \sum_{i\leq F}\langle pi|\hat{v}|qi\rangle\right)N[a_p^\dagger a_q] \\ &= \sum_{pq}\langle p|f|q\rangle N[a_p^\dagger a_q] \end{aligned} \tag{1.108}$$

Here,

$$\langle p|f|q\rangle = \epsilon_p\delta_{pq} - \langle p|\hat{u}|q\rangle + \sum_{i\leq F}\langle pi|\hat{v}|qi\rangle \tag{1.109}$$

and the second and third terms are not diagonal in general.

In a simple shell model, a core is assumed and a many-body state consists of additional model space with core $|\Phi\rangle = |core\rangle \otimes |\Phi'\rangle$.

No core shell model is basically the same as shell model except that it does not introduce single particle potential and core.

HF theory

In a H.F theory, there is no external potential $\hat{u}_{ext}$. But, one may add and subtract $\hat{u}_{HF}$ such that the Slater determinant state made from the eigen states of $\hat{t} + \hat{u}_{HF}$, $|\Phi_{HF}\rangle = |c\rangle = a_i^\dagger \dots a_l^\dagger|0\rangle$ gives a variational minimum of $\langle c|\hat{H}|c\rangle$. HF equation determines such $\hat{u}_{HF}$. HF theory choose basis of $|\Phi_0\rangle$ and $\hat{u}$ such that

$$\langle p|\hat{u}_{HF}|q\rangle = \sum_{i\leq F}\langle pi|\hat{v}|qi\rangle. \tag{1.110}$$

and the Fock matrix (matrix elements of $\hat{F}_N$) becomes diagonal in HF basis. Hopefully, there is a clear gap in the single-particle spectrum at the Fermi surface, i.e. after A orbitals are filled. Thus, HF state can be a good reference for many-body calculation.

This makes the HF energy,

$$\begin{aligned} E_{HF} &= \langle\Phi^{HF}|\hat{H}|\Phi^{HF}\rangle = \sum_{i\leq F}\epsilon_i^{HF} + \frac{1}{2}\sum_{ij\leq F}\langle ij|\hat{v}|ij\rangle_{AS} - \sum_{i\leq F}\langle i|\hat{u}_{HF}|i\rangle \\ &= \sum_{i\leq F}\epsilon_i^{HF} - \frac{1}{2}\sum_{ij\leq F}\langle ij|\hat{v}|ij\rangle_{AS} \end{aligned} \tag{1.111}$$

and Hamiltonian

$$\begin{aligned}
\hat{H} &= E_{HF} + \hat{F}_N^{HF} + \hat{V}_N, \\
\hat{F}_N^{HF} &= \sum_p \epsilon_p^{HF} N[c_p^\dagger c_p] + \sum_{pq} \left(-\langle p|\hat{u}_{HF}|q\rangle + \sum_{i\leq F} \langle pi|\hat{v}|qi\rangle \right) N[c_p^\dagger c_q] \\
&= \sum_p \epsilon_p^{HF} N[c_p^\dagger c_p], \\
\hat{V}_N &= \frac{1}{4} \sum_{pqrs} \langle pq|\hat{v}|rs\rangle_{AS} N[c_p^\dagger c_q^\dagger c_s c_r]
\end{aligned} \tag{1.112}$$

Actual basis of H.F. have to be found from the self consistency relation,

$$\hat{h}_{HF}|i\rangle = (\hat{t} + \hat{u}_{HF})|i\rangle = \epsilon_i^{HF}|i\rangle \tag{1.113}$$

and

$$\langle p|\hat{u}_{HF}|q\rangle = \sum_{i\leq F} \langle pi|\hat{v}|qi\rangle. \tag{1.114}$$

One can see that $\langle\Phi|\hat{H}_N|\Phi\rangle = 0$. HF basis implies , for 1p-1h excitation ,

$$\langle\Phi_0|\hat{H}|\Phi_i^a\rangle = \langle\Phi_0|\hat{H}_N|\Phi_i^a\rangle = \langle i|\hat{t}|a\rangle + \sum_{m\leq F} \langle im|\hat{v}|am\rangle = \langle i|\hat{f}|a\rangle = \langle i|\hat{h}_{HF}|a\rangle = 0. \tag{1.115}$$

This is Brillouin's theorem. Equivalently, solving the HF equation is the same as ensuring that the HF vacuum does not mix with singly-excited determinants. Note that Brilloun's theorem prevents the HF vacuum from direct mixing with singly-excited determinants. This does not mean that there are no singly-excited states in the exact ground-state wave function. Mixing can still appear indirectly via matrix elements of the type $\langle\Phi_i^a|\hat{H}|\Phi_{ij}^{ab}\rangle$. The above statement has several important consequences—in particular for many-body perturbation theory. For example it follows that, when using Hartree-Fock single-particle states, there are no diagrams containing one-body vertices in Hartree-Fock many-body perturbation theory. This significantly reduces the number of diagrams and the implementational effort decreases considerably.

1.10 HF method

In HF method, one try to find a new basis which makes the single slater determinant $|\Psi_0\rangle$ becomes a variational minimum of $\langle\Psi|H|\Psi\rangle$. There are many ways to derive HF equation.

- Derivation in coordinate space from Variation of wave function $\delta\phi_\alpha(x)$
- Derivation in coordinate space from Variation of coefficients of wave function expansion, $\delta\psi(x) = \sum_\lambda \delta C_{p\lambda}\phi_\lambda$
- Derivation in second quantization by normal ordered Hamiltonian.

1.10.1 Derivation of HF equation: 1st

In fact, previous formalism of HF basis would be equivalent to minimizing the variational energy expectation value up to variation of 1p-1h excitation. Consider following variation,

$$\begin{aligned}
|\Phi_0\rangle &\rightarrow \exp\left(i\sum_{a>F,i\le F} t_i^a a_a^\dagger a_i\right)|\Phi_0\rangle, \quad (t_i^a)^* = t_i^a, \\
&\rightarrow (1+i\sum_{ai} t_i^a a_a^\dagger a_i)|\Phi_0\rangle = |\Phi_0\rangle + i\sum_{a>F,i\le F} t_{ai}|\Phi_i^a\rangle \\
\langle\Phi_0| &\rightarrow \langle\Phi_0| - i\sum_{ai} t_{ai}\langle\Phi_i^a|. \qquad (1.116)
\end{aligned}$$

Thus, the variational minimum condition is the same as $\langle\Phi_0|\hat{H}|\Phi_i^a\rangle = 0$. This implies that

$$\langle\Phi_0|\hat{H}|\Phi_i^a\rangle = 0 \;\leftrightarrow\; \langle i|\hat{h}_{HF}|a\rangle = 0 \;\leftrightarrow\; \hat{h}_{HF}|i\rangle = \epsilon_i|i\rangle. \qquad (1.117)$$

Note that, in fact, the same condition can be satisfied even when $\hat{h}_{HF}|a\rangle \neq \epsilon_a|a\rangle$, as long as $\langle i|a\rangle = 0$. In other words, single particle potential above Fermi level $\langle a|\hat{u}_{HF}|a\rangle$ can be different from $\sum_{i\le F}\langle ai|\hat{v}|ai\rangle$.

In BCS theory, the $|\Phi^{BCS}\rangle$ is allowed to have matrix element $\langle a_i a_{-i}\rangle$. In HF-Bogoliubov theory, the $|\Phi^{HFB}\rangle$ is allowed to have matrix element $\langle a_p a_q\rangle$ or $\langle a_p^\dagger a_q^\dagger\rangle$.

1.10.2 Another derivation of HF equation

Suppose we have new basis ψ from old basis ϕ,

$$\psi_i = \sum_\alpha C_{i\alpha}\phi_\alpha. \qquad (1.118)$$

This makes the Hamiltonian to be rewritten in terms of $a_i^\dagger$, a_i which is defined w.r.t. $|\Psi_0^{HF}\rangle$. (In other words, i,j corresponds to a HF s.p. wave function while $\alpha\beta$ corresponds to original s.p. basis function.) Thus, the new reference energy becomes

$$\begin{aligned}
\langle\Psi_0^{HF}|\hat{H}|\Psi_0^{HF}\rangle &= \sum_{i\le F}\langle i|\hat{h}_0|i\rangle + \frac{1}{2}\sum_{ij\le F}\langle ij|\hat{v}|ij\rangle_{AS} \\
&= \sum_{i\le F}\sum_{\alpha\beta} C_{i\alpha}^* C_{i\beta}\langle\alpha|\hat{h}_0|\beta\rangle + \frac{1}{2}\sum_{ij\le F}\sum_{\alpha\beta\gamma\delta} C_{i\alpha}^* C_{j\beta}^* C_{i\gamma} C_{j\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle_{AS} \qquad (1.119)
\end{aligned}$$

where C coefficients are not known yet. We want to find C which minimize $\langle\Psi_0^{HF}|\hat{H}|\Psi_0^{HF}\rangle$ under the constraints $\sum_\alpha C_{i\alpha}^* C_{j\alpha} = \delta_{ij}$. Thus, by introducing Lagrange multiplier ϵ_i, we minimize

$$\frac{\delta}{\delta C_{i\alpha}^*}\left[\langle\Psi_0^{HF}|\hat{H}|\Psi_0^{HF}\rangle - \sum_j \epsilon_j \sum_\alpha C_{j\alpha}^* C_{j\alpha}^*\right] = 0. \qquad (1.120)$$

This gives H-F equations for any i,

$$\begin{aligned}
&\sum_\beta C_{i\beta}\langle\alpha|h_0|\beta\rangle + \sum_{j\le F}\sum_{\beta\gamma\delta} C_{j\beta}^* C_{i\gamma} C_{j\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle_{AS} = \epsilon_i^{HF} C_{i\alpha}, \\
\Rightarrow\quad &\sum_\beta h_{\alpha\beta}^{HF} C_{i\beta} = \epsilon_i^{HF} C_{i\alpha}, \quad h_{\alpha\beta}^{HF} = \langle\alpha|\hat{h}_0|\beta\rangle + \sum_{j\le F}\sum_{\gamma\delta} C_{j\gamma}^* C_{j\delta}\langle\alpha\gamma|\hat{v}|\beta\delta\rangle_{AS} \qquad (1.121)
\end{aligned}$$

This is suitable for numerical calculation. One needs to tabulate the matrix elements and obtain $C_{i\beta}$ by iteration and tabulate $h_{\alpha\beta}^{HF}$ each time from previous C's .

- start with initial guess $C^{(0)}_{i\alpha} = \delta_{i\alpha}$
- Construct HF matrix $h^{HF}_{\alpha\beta}$ with $C^{(0)}_{i\alpha}$. (using above equation)
- Solve HF eigenvalue problem and get new eigenvectors $C^{(1)}_{i\alpha}$ and eigenvalues $\epsilon^{HF(1)}_i$.
- repeat by updating C's in each iteration. Updated C corresponds to updating density matrix $\rho_{\alpha\beta} = \sum_{i\leq F} C^*_{i\alpha} C_{i\beta}$ and re-calculate HF matrix $h^{HF}_{\alpha\beta}$.
- Stops when

$$\frac{1}{m}\sum_{p=1}^{m} |\epsilon^{(n)}_p - \epsilon^{(n-1)}_p| \leq \lambda \simeq 10^{-8} \tag{1.122}$$

  Here p runs over all calculated single particle energies and m is the number of single-particle states.

Note: Considering the new basis ψ_i as an expansion from given basis ϕ_α, index i or α is not necessary to be less than total number of nucleon A. (It is related with model space, not with many-body system). Thus, when initialize $C^{(0)}_{i\alpha} = \delta_{i\alpha}$, the matrix $\boldsymbol{C}$ is **not** a $A \times A$ matrix , but $m_{new} \times m_{old}$ matrix. (It is not necessary $m_{new} = m_{old}$, but usually is chosen as such.) It is also true to the HF eigen value equation. Index i of ϵ^{HF}_i can be larger than A. However, one have to use number of nucleons A to compute HF energy of the system.

We can introduce density matrix

$$\rho_{\gamma\delta} = \sum_{j\leq F} C^*_{j\gamma} C_{j\delta} \tag{1.123}$$

Then, the HF energy can be written as

$$\langle \Psi^{HF}_0 | \hat{H} | \Psi^{HF}_0 \rangle = \sum_{\alpha\beta} \rho_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \rho_{\alpha\gamma}\rho_{\beta\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle_{AS} \tag{1.124}$$

This form means HF energy is a functional of one-body density, $E_{HF}[\rho]$.

Originally $\hat{h}_0$ should be a free kinetic energy. But, to get binding energy one have to subtract kinetic energy of CM.

On the other hand, if there is a external H.O. trap. one can use $\hat{h}_0$ as a H.O. Hamiltonian.

1.11 Energy density functional

The HF energy for Hamiltonian can be expressed as

$$\begin{aligned} E_{HF} &= \langle HF | \hat{H} | HF \rangle \\ &= \sum_{pq} t_{pq} \langle HF | \hat{c}^\dagger_p \hat{c}_q | HF \rangle + \frac{1}{4} \sum_{pq,p'q'} v_{pq,p'q'} \langle HF | \hat{c}^\dagger_p \hat{c}^\dagger_q \hat{c}_{q'} \hat{c}_{p'} | HF \rangle + \frac{1}{36} \sum_{pqr,p'q'r'} v^{3N}_{pqr,p'q'r'} \langle HF | \hat{c}^\dagger_p \hat{c}^\dagger_q \hat{c}_r \hat{c}_{r'} \hat{c}_{q'} \hat{c}_{p'} | HF \rangle \end{aligned} \tag{1.125}$$

Let us define density matrices,

$$\begin{aligned} \rho_{p'p} &= \langle HF | \hat{c}^\dagger_p \hat{c}_{p'} | HF \rangle \\ \rho_{p'q',pq} &= \langle HF | \hat{c}^\dagger_p \hat{c}^\dagger_q \hat{c}_{q'} \hat{c}_{p'} | HF \rangle \\ \rho_{p'q'r',pqr} &= \langle HF | \hat{c}^\dagger_p \hat{c}^\dagger_q \hat{c}^\dagger_r \hat{c}_{r'} \hat{c}_{q'} \hat{c}_{p'} | HF \rangle \end{aligned} \tag{1.126}$$

Then, HF energy can be expressed as a functional of density matrices,

$$E_{HF}[\rho^{1B},\rho^{2B},\rho^{3B}] = \sum_{pp'} t_{pp'}\rho_{p'p} + \frac{1}{4}\sum_{pq,p'q'} v_{pq,p'q'}\rho_{p'q',pq} + \frac{1}{36}\sum_{pqr,p'q'r'} v^{3N}_{pqr,p'q'r'}\rho_{p'q'r',pqr} \quad (1.127)$$

Because HF states are simple Slater-Determinant, one can reduce the density matrices as a product of 1B density matrices (now index is only for occupied states),

$$\sum_{ij,i'j'} v_{ij,i'j'}\rho_{i'j',ij} = \sum_{ij,i'j'} v_{ij,i'j'}(\rho_{j',j}\rho_{i',i} - \rho_{j',i}\rho_{i',j}) = 2\sum_{ij,i'j'} v_{ij,i'j'}\rho_{j',j}\rho_{i',i} \quad (1.128)$$

$$\sum_{ijk,i'j'k'} v^{3N}_{ijk,i'j'k'}\rho_{i'j'k',ijk} = 6\sum_{ijk,i'j'k'} v^{3N}_{ijk,i'j'k'}\rho_{k',k}\rho_{i',i}\rho_{j',j} \quad (1.129)$$

Thus, practically, Energy becomes a functional of 1B density matrices, $E[\rho]$. (This reduction to one-body density is only possible because of reference is HF S.D. In general, the many-body density can not be reduced into one-body density.) In this way, one can derive the H.F. equation from $\delta E[\rho] = 0$, which becomes

$$\begin{aligned} \delta E[\rho] &= \sum_{i,i'} h_{i,i'}[\rho]\delta\rho_{i',i} \\ h_{i,i'}[\rho] &= t_{i,i'} + \sum_{j,j'} v_{ij,i'j'}\rho_{j',j} + \frac{1}{2}\sum_{jk,j'k'} v^{3N}_{ijk,i'j'k'}\rho_{j',j}\rho_{k',k} \end{aligned} \quad (1.130)$$

Thus, if one have solution of $\hat{h}[\rho]|i\rangle = \epsilon_i|i\rangle$, it is equivalent to solve $\delta E[\rho] = 0$. In terms of HF basis states,

$$E_{HF} = \sum_{i}^{occ}\epsilon_i - \frac{1}{2}\sum_{ij}^{occ} v_{ij,ij} - \frac{1}{3}\sum_{ijk}^{occ} v^{3N}_{ijk,ijk} \quad (1.131)$$

where density matrix $\rho_{i,j} = \delta_{i,j}\theta(\epsilon_i - \epsilon_F)$ (즉, 1 for occupied HF states). This can also be expressed as $\rho_{i,j} = \sum_{\alpha\beta} C^*_{i\alpha}C_{j\beta}$ with $|i\rangle = \sum_\alpha C_{i\alpha}|\alpha\rangle$ for H.O. basis $|\alpha\rangle$.

If matrix elements were written in other basis like H.O., $h_{\alpha,\beta}$ (i,j is H.F. basis index and α,β for H.O. basis), one have to transform these as such,

$$h_{i,j} = \langle i|\hat{h}|j\rangle = \sum_{\alpha,\beta}\langle i|\alpha\rangle h_{\alpha,\beta}\langle\beta|j\rangle = \sum_{\alpha,\beta} C^*_{i\alpha}h_{\alpha\beta}C_{j\beta} \quad (1.132)$$

Thus, HF equation in terms of matrix elements in basis α is to find $C_{i\alpha}$ such that

$$h_{\alpha\beta}C_{i\beta} = \epsilon_i C_{i\alpha}, \quad \delta_{ij} = \sum_\alpha C^*_{i\alpha}C_{i\alpha} \quad (1.133)$$

where

$$h_{\alpha\beta} = \langle\alpha|\hat{t}|\beta\rangle + \sum_{j\in F}\sum_{\gamma\delta} C^*_{j\gamma}C_{j\delta}\langle\alpha\gamma|v|\beta\delta\rangle \quad (1.134)$$

1.12 Full Configuration interaction

Suppose we have full configurations of s.p. slater determinants. (In fact, this is almost impossible because too large number of possible configurations) Exact eigen-state of Hamiltonian may be expanded with configurations,

$$|\Psi_0\rangle = C_0|\Phi_0\rangle + \sum_{ai} C^a_i|\Phi^a_i\rangle + \sum_{abij} C^{ab}_{ij}|\Phi^{ab}_{ij}\rangle + \cdots = (C_0 + \hat{C})|\Phi_0\rangle \quad (1.135)$$

where particle-hole excited configurations are

$$|\Phi^{abc\cdots}_{ijk\cdots}\rangle = \hat{a}^\dagger_a \hat{a}^\dagger_b \cdots \hat{a}_j \hat{a}_i |\Phi_0\rangle. \tag{1.136}$$

In a compact form,

$$|\Psi_0\rangle = \sum_{PH} C^P_H |\Phi^P_H\rangle = \left(\sum_{PH} C^P_H \hat{A}^P_H\right)|\Phi_0\rangle. \tag{1.137}$$

We require normalization condition

$$\langle\Psi_0|\Psi_0\rangle = \sum_{PH} |C^P_H|^2 = 1 \tag{1.138}$$

Then, energy expectation value becomes

$$\langle\Psi_0|H|\Psi_0\rangle = \sum_{PP'HH'} C^{*P}_H \langle\Phi^P_H|H|\Phi^{P'}_{H'}\rangle C^{P'}_{H'} \tag{1.139}$$

Variational minimization under constraint gives for any P, H,

$$\begin{aligned} & \frac{\delta}{\delta C^{*P}_H}[\langle\Psi_0|\hat{H}|\Psi_0\rangle - \lambda\langle\Psi_0|\Psi_0\rangle] = 0, \\ \Rightarrow \quad & \sum_{P'H'} \langle\Phi^P_H|\hat{H}|\Phi^{P'}_{H'}\rangle C^{P'}_{H'} - \lambda C^P_H = 0 \end{aligned} \tag{1.140}$$

Equivalently, we have equation for C^P_H, (renaming $\lambda \to E$)

$$\sum_{P'H'} \langle\Phi^P_H|\hat{H} - E|\Phi^{P'}_{H'}\rangle C^{P'}_{H'} = 0. \tag{1.141}$$

If we choose canonical HF basis, we have $\langle 0p-0h|H|1p-1h\rangle = \langle\Phi_0|H|\Phi^a_i\rangle = 0$.

Several Approximations to reduce the dimension of configurations. In shell-model, one defines **core** and effective Hilbert space and effective Hamiltonian with respect to the core and consider possible configurations which is reduced from the full configurations.

In **configuration interaction model**, one limit possible configurations up to 1p-1h and 2p-2h excitations.(CISD: configuration interaction single double) However, be careful that truncation up to 3p-3h makes the wrong results.

In **no-core-shell model**, the truncation is done for possible excitation energy.

1.13 Correlation Energy

Assuming two-body operators at most, previous equation becomes for $\langle\Phi_0|$,

$$\begin{aligned} & \sum_{P'H'} \langle\Phi_0|\hat{H} - E|\Phi^{P'}_{H'}\rangle C^{P'}_{H'} = 0, \\ \to \quad & \langle\Phi_0|\hat{H} - E|\Phi_0\rangle + \sum_{ai}\langle\Phi_0|\hat{H} - E|\Phi^a_i\rangle C^a_i + \sum_{abij}\langle\Phi_0|\hat{H} - E|\Phi^{ab}_{ij}\rangle C^{ab}_{ij} = 0. \end{aligned} \tag{1.142}$$

Because there are two-body operators at most, we don't need to consider higher excitations. We can define correlation energy ΔE as

$$\begin{aligned} E - E_{ref} &= \Delta E = \sum_{ai}\langle\Phi_0|\hat{H}|\Phi^a_i\rangle C^a_i + \sum_{abij}\langle\Phi_0|\hat{H}|\Phi^{ab}_{ij}\rangle C^{ab}_{ij} \\ &= \sum_{ai}\langle i|\hat{f}|a\rangle C^a_i + \sum_{abij}\langle ij|\hat{v}|ab\rangle C^{ab}_{ij}. \end{aligned} \tag{1.143}$$

(In HF basis, there is no C_i^a term. E_{ref} can be from HF calculation or just the eigenstates of the non-interacting part of the Hamiltonian.) However, only with this equation, one can not determine C coefficients.

Now consider next equation with $\langle\Phi_i^a|$,

$$\begin{aligned}
&\sum_{P'H'}\langle\Phi_i^a|\hat{H}-E|\Phi_{H'}^{P'}\rangle C_{H'}^{P'}=0,\\
\Rightarrow\quad &\langle\Phi_i^a|\hat{H}-E|\Phi_0\rangle+\sum_{bj}\langle\Phi_i^a|\hat{H}-E|\Phi_j^b\rangle C_j^b+\sum_{bcjk}\langle\Phi_i^a|\hat{H}-E|\Phi_{jk}^{bc}\rangle C_{jk}^{bc}+\sum_{bcdjkl}\langle\Phi_i^a|\hat{H}-E|\Phi_{jkl}^{bcd}\rangle C_{jkl}^{bcd}=0,\\
\Rightarrow\quad &\langle i|\hat{f}|a\rangle+\langle\Phi_i^a|\hat{H}|\Phi_i^a\rangle C_i^a+\sum_{bj\neq ai}\langle\Phi_i^a|\hat{H}|\Phi_j^b\rangle C_j^b+\sum_{bcjk}\langle\Phi_i^a|\hat{H}|\Phi_{jk}^{bc}\rangle C_{jk}^{bc}+\sum_{bcdjkl}\langle\Phi_i^a|\hat{H}|\Phi_{jkl}^{bcd}\rangle C_{jkl}^{bcd}=EC_i^a
\end{aligned}$$

[7] Also for 2p2h,

$$\begin{aligned}
0\quad=\quad &\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_0\rangle+\sum_{kc}\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_k^c\rangle C_k^c\\
&+\sum_{cdkl}\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_{kl}^{cd}\rangle C_{kl}^{cd}+\sum_{cdeklm}\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_{klm}^{cde}\rangle C_{klm}^{cde}+\sum_{cdefklmn}\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_{klmn}^{cdef}\rangle C_{klmn}^{cdef},
\end{aligned}$$

In this way, one can introduce as many equations to solve C by iteration. One may start from **perturbation theory** for initial guess of C. For example, lowest order in interaction gives

$$C_i^a=\frac{\langle i|\hat{f}|a\rangle}{\epsilon_i-\epsilon_a} \tag{1.145}$$

and

$$C_{ij}^{ab}=\frac{\langle ij|\hat{v}|ab\rangle}{\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b} \tag{1.146}$$

However, this would be inefficient way to solve many-body problem. We need a method to include infinite order of perturbation series in some class.

Popular methods are

- many-body perturbation theory (in essence a Taylor expansion)
- Coupled cluster theory (coupled non-linear equations)
- Green's function approaches (matrix inversion)
- Similarity group transformation methods (coupled ordinary differential equations)[8]
- All this usually start from HF basis.

Possible truncation of many-body states,

[7] For very weak interaction, we may approximate above expression as

$$\langle i|\hat{f}|a\rangle+\langle\Phi_i^a|H|\Phi_i^a\rangle C_i^a\simeq\langle i|\hat{f}|a\rangle+(E_0+\epsilon_a-\epsilon_i)C_i^a\simeq EC_i^a \tag{1.144}$$

This gives perturbative expression of C_i^a.

[8] Similarity transform of a matrix is when

$$\boldsymbol{B}=\boldsymbol{S}^T\boldsymbol{A}\boldsymbol{S},\quad \boldsymbol{S}^T\boldsymbol{S}=\boldsymbol{S}^{-1}\boldsymbol{S}=\boldsymbol{I}. \tag{1.147}$$

Note that Similarity transformed matrix have the same eigenvalues but can have different eigen-vectors.

$$\boldsymbol{A}\boldsymbol{x}\quad=\quad\lambda\boldsymbol{x},\quad \boldsymbol{B}(\boldsymbol{S}^T\boldsymbol{x})=\lambda(\boldsymbol{S}^T\boldsymbol{x}). \tag{1.148}$$

If one can do similarity transform $\boldsymbol{A}$ to $\boldsymbol{B}$ becomes tridiagonal(Householder) or upper/lower trangular(QR method) one can use numerical techniques like power methods, iterative methods(Krylov,Lanczos,Arnold).

- Count excitation from 'filled' orbits like 1p-1h, 2p-2h excitations
- Stat Maximal orbit and allow all possible configurations. (Full configuration)
- Energy truncation called $N\hbar\Omega$ or N_{max} truncation. Any configuration(many-body) are assigned with non-interacting energy(sum of s.p. H.o. energies) ignoring spin-orbits. Excited states are labeled relative to the lowest configuration by the number of H.O. quanta. This truncation is useful because if one includes all configuration up to some N_{max}, and has a translationally invariant interaction, then the intrinsic motion and the center-of-mass motion factor. In other words, we can know exactly the center-of-mass wavefunction.
- Coupled cluster case, instead of truncate series in excitations of reference state $|\Phi$, truncate operator series $T = T_1 + T_2 + \dots$ which create many-body wave function via $e^T|\Phi\rangle$.

Usually, many-body basis states are constructed by using the conservation of $\hat{J}^2, \hat{J}_z$ (to reduce model space).

- M-scheme: construct a many-body basis which has fixed M
- J-scheme: construct a many-body basis which has fixed J
- Usually, it is not easy to construct to have both fixed J and M. Usually, J-scheme has smaller dimensions but Matrix elements are more complicate. But, M-scheme is easier to construct with Slater determinants because M is additive $M = m_i + m_j + \cdots$ for Slater determinant of s.p. states. However, each fixed M-scheme basis usually do not have good total J.

1.14 Many-body perturbation theory

For a perturbative expansion, we need to separate the Hamiltonian into unperturbed part and perturbed part.

$$H = \hat{H}_0 + \hat{H}_I = \left(\hat{T} + \hat{U}\right) + \left(\hat{V} - \hat{U}\right), \tag{1.149}$$

where non-perturbed Hamiltonian $\hat{H}_0$ have eigen states

$$\hat{H}_0|\Phi_0\rangle = W_0|\Phi_0\rangle, \quad W_0 = \sum_{i\le F} \epsilon_i \tag{1.150}$$

Let us consider the perturbavive expansion of ground state energy

$$\hat{H}|\Psi_0\rangle = E|\Psi_0\rangle, \quad |\Psi_0\rangle = |\Phi_0\rangle + \sum_{m=1}^{\infty} C_m|\Phi_m\rangle. \tag{1.151}$$

Be careful that this is not the same as previous expansion over configurations. In previous case, $\hat{H}_0$ is only from $\hat{t} + \hat{u}_{ext}$. However, here $\hat{H}_0$ contains single particle potential, $\hat{H}_0 = \hat{t} + \hat{u}_{ext} + \hat{u}$ and $\hat{H}_I = \hat{V} - \hat{u}$. One can choose $\hat{u}$ as a HF interaction $\hat{u}_{HF}$. Also reference $|\Phi_0\rangle$ was a Slater determinant of a given basis. Here $|\Phi_0\rangle$ is a Slater determinant of basis of non-perturbed Hamiltonian $\hat{H}_0$.

Here the expansion is done in power of $\hat{H}_I$. If we use intermediate normalization such that $\langle\Phi_0|\Psi_0\rangle = 1$,(this means Ψ_0 is not properly normalized yet.), we get

$$E - W_0 = \langle\Phi_0|\hat{H}_I|\Psi_0\rangle \tag{1.152}$$

For example, we may express at lowest order,

$$\langle\Phi_0|\hat{H}_I|\Phi_0\rangle = \langle\Phi_0|\hat{H}|\Phi_0\rangle - W_0 = \frac{1}{2}\sum_{ij\le F}\langle ij|\hat{v}|ij\rangle - \sum_{i\le F}\langle i|\hat{u}|i\rangle. \tag{1.153}$$

주의! MBPT 에서의 $\hat{H}_I = \hat{V} - \hat{U}$ 이다.

We can rewrite the Schrodinger equation by introducing parameter ω, [9]

$$|\Psi_0\rangle = \frac{1}{\omega - \hat{H}_0}(\omega - E + \hat{H}_I)|\Psi_0\rangle. \tag{1.154}$$

Let us introduce operator

$$\hat{P} = |\Phi_0\rangle\langle\Phi_0|, \quad \hat{Q} = \sum_{m=1}^{\infty} |\Phi_m\rangle\langle\Phi_m|. \tag{1.155}$$

Then, (note normalization $\langle\Phi_0|\Psi_0\rangle = 1$. add and subtract $\omega|\Psi_0\rangle$.)

$$\begin{aligned} |\Psi_0\rangle &= (\hat{P} + \hat{Q})|\Psi_0\rangle = |\Phi_0\rangle + \hat{Q}|\Psi_0\rangle, \\ \hat{Q}|\Psi_0\rangle &= \frac{\hat{Q}}{\omega - \hat{H}_0}(\omega - E + \hat{H}_I)|\Psi_0\rangle, \\ \Rightarrow \quad |\Psi_0\rangle &= |\Phi_0\rangle + \frac{\hat{Q}}{\omega - \hat{H}_0}(\omega - E + \hat{H}_I)|\Psi_0\rangle \end{aligned} \tag{1.156}$$

This allows one to express perturbative series,

$$\begin{aligned} |\Psi_0\rangle &= \sum_{i=0}^{\infty} \left(\frac{\hat{Q}}{\omega - \hat{H}_0}(\omega - E + \hat{H}_I) \right)^i |\Phi_0\rangle, \\ E - W_0 &= \Delta E = \sum_{i=0}^{\infty} \langle\Phi_0|\hat{H}_I \left(\frac{\hat{Q}}{\omega - \hat{H}_0}(\omega - E + \hat{H}_I) \right)^i |\Phi_0\rangle \end{aligned} \tag{1.157}$$

In the right hand side, there is a still exact energy E which is unknown. Also, there are all $|\Phi_i\rangle$ which are solution of unperturbed Hamiltonian. Thus, equation is not practical.

Though this is an expansion over interaction, it includes all s.p. configurations by $\hat{Q}$.

In Brilluion-Wigner perturbation theory, we set $\omega = E$. In Rayleigh-Schrodinger perturbation theory, we set $\omega = W_0$.

$$\begin{aligned} \Delta E &= \sum_{i=0}^{\infty} \langle\Phi_0|\hat{H}_I \left(\frac{\hat{Q}}{W_0 - \hat{H}_0}(-\Delta E + \hat{H}_I) \right)^i |\Phi_0\rangle \\ &= \langle\Phi_0| \left(\hat{H}_I + \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I + \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} (\hat{H}_I - \Delta E) \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I + \cdots \right) |\Phi_0\rangle \end{aligned} \tag{1.158}$$

Assume perturbation of interaction,

$$\Delta E = \sum_{i=1}^{\infty} \Delta E^{(i)} \tag{1.159}$$

$$\begin{aligned} \Delta E^{(1)} &= \langle\Phi_0|\hat{H}_I|\Phi_0\rangle, \\ \Delta E^{(2)} &= \langle\Phi_0|\hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I|\Phi_0\rangle, \\ \Delta E^{(3)} &= \langle\Phi_0|\hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I|\Phi_0\rangle - \langle\Phi_0|\hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \langle\Phi_0|\hat{H}_I|\Phi_0\rangle \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I|\Phi_0\rangle \end{aligned} \tag{1.160}$$

[9] Why introduce ω? To make a perturbation theory?

For example, we have

$$\langle\Phi_0|H_0|\Phi_0\rangle = W_0, \quad \langle\Phi_0|\hat{H}_I|\Phi_0\rangle = \frac{1}{2}\sum_{ij\leq F}\langle ij|\hat{v}|ij\rangle - \sum_{i\leq F}\langle i|\hat{u}|i\rangle. \tag{1.161}$$

$$\begin{aligned}
\langle\Phi_0|\hat{H}_0|\Phi_i^a\rangle &= 0, \\
\langle\Phi_0|\hat{H}_I|\Phi_i^a\rangle &= \langle\Phi_0|\hat{H}|\Phi_i^a\rangle = \langle i|\hat{t}|a\rangle + \sum_{m\leq F}\langle im|\hat{v}|am\rangle \\
&= \sum_{m\leq F}\langle im|\hat{v}|am\rangle - \langle i|\hat{u}|a\rangle.
\end{aligned} \tag{1.162}$$

This implies that $\langle\Phi_0|\hat{H}_I|\Phi_i^a\rangle = 0$ for HF basis.

$$\begin{aligned}
\langle\Phi_0|\hat{H}_0|\Phi_{ij}^{ab}\rangle &= 0, \\
\langle\Phi_0|\hat{H}_I|\Phi_{ij}^{ab}\rangle &= \langle\Phi_0|\hat{H}|\Phi_{ij}^{ab}\rangle = \langle ij|\hat{v}|ab\rangle.
\end{aligned} \tag{1.163}$$

By explicitly inserting $\hat{Q}$ operator for various excitations will corresponds to the Diagramatic expression of $\Delta E^{(2)}$ and $\Delta E^{(3)}$ is given in figure. Note that only linked diagrams contribute in $\Delta E^{(3)}$. Also, diagrams with tadpole like attachment gives zero for HF basis. (**It seems we can understand the sign and symmetry factor of MBPT diagrams in the same way as Coupled Cluster diagrams. See later.**)

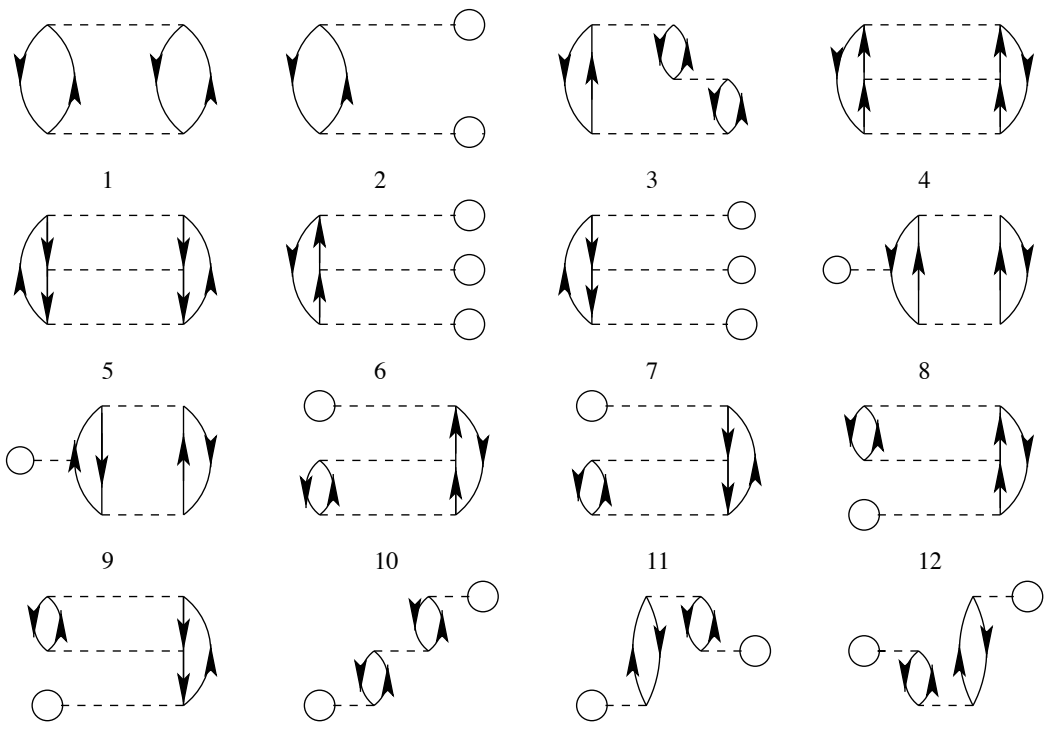

Figure 1.1: MBPT upto 3rd order. Diagram (1-2) corresponds to $\Delta E^{(2)}$ and others to $\Delta E^{(3)}$.

The explicit expressions for each diagrams are as follows: for $\Delta E^{(2)}$,(including 2p-2h intermediate

states)

$$(1) = \frac{1}{2^2} \sum_{ij \le F} \sum_{ab > F} \frac{\langle ij|\hat{v}|ab\rangle\langle ab|\hat{v}|ij\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}. \tag{1.164}$$

This is similar to FCI case with only considering 2p-2h.

$$E - W_0 = \Delta E = \sum_{abij} \langle ij|v|ab\rangle C_{ij}^{ab} \tag{1.165}$$

But, FCI includes such 2p-2h correlations to infinite order. (In other words, MBPT C_{ij}^{ab} is proportional to v. However, in FCI, C_{ij}^{ab} is non-linear to v.)

for $\Delta E^{(3)}$,

$$\begin{aligned}
(3) &= \sum_{ijk \le F} \sum_{abc > F} \frac{\langle ij|\hat{v}|ab\rangle\langle bk|\hat{v}|ic\rangle\langle ac|\hat{v}|ik\rangle}{(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)(\epsilon_i + \epsilon_k - \epsilon_a - \epsilon_c)}, \\
(4) &= \frac{1}{2^3} \sum_{ij \le F} \sum_{abcd > F} \frac{\langle ij|\hat{v}|cd\rangle\langle cd|\hat{v}|ab\rangle\langle ab|\hat{v}|ij\rangle}{(\epsilon_i + \epsilon_j - \epsilon_c - \epsilon_d)(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)}, \\
(5) &= \frac{1}{2^3} \sum_{ijkl \le F} \sum_{ab > F} \frac{\langle ab|\hat{v}|kl\rangle\langle kl|\hat{v}|ij\rangle\langle ij|\hat{v}|ab\rangle}{(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)(\epsilon_k + \epsilon_l - \epsilon_a - \epsilon_b)}.
\end{aligned} \tag{1.166}$$

All other diagrams are zero for infinite matter or in HF basis.

Note: One possible way to understand symmetry factors are to see that sum $\sum_m$ includes unique $|\Phi_{ij\cdots}^{ab\cdots}\rangle$ while the sum $\sum_{ij \le F} \sum_{ab > F}$ includes $|\Phi_{ij\cdots}^{ab\cdots}\rangle$, $|\Phi_{ij\cdots}^{ba\cdots}\rangle$, $|\Phi_{ji\cdots}^{ab\cdots}\rangle$, $|\Phi_{ji\cdots}^{ba\cdots}\rangle$. Thus there are additional 2×2 over-counting. (For example, for given ij and ab, the exchanged one ji or ba gives the same contribution in (1),(4),(5). However, (3) does not have such symmetry for exchange of ijk and abc.)

Thus, by using MBPT, we can compute ground state energy correction or correlation energy ΔE up to certain order by just doing straightforward calculation. It can be done in principle also for infinite nuclear matter by using plain wave basis and s.p. energies. However, in case of hard-core potential, the matrix elements $\langle pq|v|rs\rangle$ can diverge in plain wave basis.

- MBPT introduces order-by-order specific correlations and we make comparisons with exact calculations like FCI
- At every order, we can calculate all contributions since they are well-known and either tabulated or calculated on the fly.
- MBPT is a non-variational theory and there is no guarantee that higher orders will improve the convergence.
- However, since FCI calculations are limited by the size of the Hamiltonian matrices to diagonalize (today's most efficient codes can attach dimensionalities of ten billion basis states, MBPT can function as an approximative method which gives a straightforward (but tedious) calculation recipe.
- MBPT has been widely used to compute effective interactions for the nuclear shell-model.
- But there are better methods which sum to infinite order important correlations. Coupled cluster theory is one of these methods.

1.15 RPA and TDA

REF: Thesis, https://inis.iaea.org/collection/NCLCollectionStore/_Public/49/023/49023349.pdf?r=1

RPA ground state includes correlations and have more complex structure than HF. But, excited state is described in terms of particle-holes of HF basis. (Note that particle-hole is only well defined for **sub-shell closure**. Sub-shell closure implies that a certain energy shell should be completely filled or empty. In other words, if some shell is partly filled, it is not clear how to define particle and hole states.) In Equation of motion(EOM) method, actual calculation of $|RPA\rangle$ is avoided.

Excitation creation operator(ECO)

$$|\omega\rangle = \hat{Q}^\dagger_\omega |RPA\rangle, \quad \omega = (n, J^\pi, M) \tag{1.167}$$

$$\begin{aligned} \hat{Q}_\omega|\omega\rangle &= |RPA\rangle, \\ \hat{Q}_\omega|RPA\rangle &= 0, \quad \forall\omega. \end{aligned} \tag{1.168}$$

(This imply orthogonality $\langle RPA|\omega\rangle = 0$.) In fact, the detailed form of the ECOs depends on the type of RPA that is used.

$$\begin{aligned} \hat{H}|RPA\rangle &= E_0|RPA\rangle, \\ \hat{H}|\omega\rangle &= E_\omega|\omega\rangle, \quad \forall\omega. \end{aligned} \tag{1.169}$$

From these, we get equation of motion for ECO $\hat{Q}^\dagger_\omega$,

$$[\hat{H}, \hat{Q}^\dagger_\omega]|RPA\rangle = (E_\omega - E_0)\hat{Q}^\dagger_\omega|RPA\rangle = E^{RPA}_\omega \hat{Q}^\dagger_\omega|RPA\rangle. \tag{1.170}$$

Chapter 2

Simple example

2.1 Pairing Model

4 개의 핵자와 4개의 s.p. level 을 생각하자. 각 s.p. level에는 2개의 핵이 있을 수 있다.(spin up and spin down) 항상 paired 된 경우만 생각하면, 2개의 pair가 4개의 paired state에 있는 경우의 수는 ${}_4C_2 = 6$ 가 되어, 4-particle Hamiltonian 은 6×6 matrix 로 나타낼 수 있게 된다. 간단히 energy level이 equally spaced $E_{p\sigma} = \delta(p-1)$ 라고 하고, 하나의 pair가 가지는 interaction을 상수로 두면,

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \hat{V}, \\ \hat{H}_0 &= \delta \sum_{p=1}^{4} \sum_{\sigma=-\frac{1}{2}}^{+\frac{1}{2}} (p-1) a^\dagger_{p\sigma} a_{p\sigma}, \\ \hat{V} &= -\frac{1}{2} g \sum_{p,q=1}^{4} a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+} \end{aligned} \tag{2.1}$$

로 Hamiltonian을 쓸 수 있다. ($\hat{V}$ 는 paired two nucleon state에 대해서만 non-zero matrix element를 준다. 또한, $\hat{V}$는 off-diagonal matrix element를 가져, 하나의 pair를 다른 energy level pair로 바꿀 수 있다. 이 Hamiltonian 하에서는 un-paired states는 존재할 수 없다. One can choose $\delta = 1$.)

- 편의상 pair-creation and pair annihilation operator를 정의하여 사용할 수 있다.

$$\begin{aligned} \hat{P}^+_p &= a^\dagger_{p+} a^\dagger_{p-}, \quad \hat{P}^-_p = a_{p-} a_{p+}, \\ \hat{V} &= -\frac{1}{2} g \sum_{pq} \hat{P}^+_p \hat{P}^-_q \end{aligned} \tag{2.2}$$

  Also sum of operators

$$\begin{aligned} \hat{P}_+ &= \sum_{k>0} \hat{a}^\dagger_k \hat{a}^\dagger_{-k}, \quad \hat{P}_- = (\hat{P}_+)^\dagger, \\ \left[\hat{P}_+, \hat{P}_-\right] &= \sum_{k=1}^{\Omega} (\hat{a}^\dagger_k \hat{a}_k + \hat{a}^\dagger_{-k} \hat{a}_{-k} - 1) = \hat{N} - \Omega \end{aligned} \tag{2.3}$$

  Define

$$\hat{P}_z = \frac{1}{2}(\hat{N} - \Omega), \quad \left[\hat{P}_z, \hat{P}_\pm\right] = \pm \hat{P}_\pm. \tag{2.4}$$

  Even though $\hat{P}_z$ and $\hat{P}_\pm$ is not an angular momentum, they follow the same $SU(2)$ algebra. Also, (여기서, $G = \frac{g}{2}$.)

$$\hat{H} = -G \hat{P}_+ \hat{P}_- = -G \left(\hat{P}^2 - \hat{P}^2_z + \hat{P}_z \right) \tag{2.5}$$

The eigen-value of $\hat{P}^2$ is in form of $p(p+1)$ and $\hat{P}_z$ for given p can be from $-p$ to p integer or half integer. $\hat{P}_z$ 값은 주어진 system의 N과 Ω 로 결정되어 있다. 따라서, 가능한 p값의 범위는 $\frac{1}{2}|N-\Omega| \le p \le \frac{\Omega}{2}$. 일반적으로 $N \le \Omega$ 이므로, $p = \frac{1}{2}(\Omega - v)$ 인 v를 도입하면,pairing Hamiltotnian의 energy는

$$\begin{aligned} E &= -G\left(p(p+1) - (\frac{N-\Omega}{2})^2 + \frac{N-\Omega}{2}\right) \\ &= -\frac{1}{4}G(N-v)(2\Omega+2-N-v) \end{aligned} \tag{2.6}$$

N이 even이면, v도 even, N이 odd이면 v도 odd가 된다. (maximum $v = \Omega - |N-\Omega|$)

This v is called **seniority**.

- spin projection operator와 total spin operator 를 정의하자.

$$\begin{aligned} \hat{S}_z &= \frac{1}{2}\sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma}, \\ \hat{S}^2 &= \hat{S}_z^2 + \frac{1}{2}(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+), \\ \hat{S}_\pm &= \sum_p a^\dagger_{p\pm} a_{p\mp}. \end{aligned} \tag{2.7}$$

이 경우, we can show $[\hat{S}_z, \hat{H}] = 0$ and $[\hat{S}^2, \hat{H}] = 0$. 즉, $\hat{S}^2$ 와 $\hat{S}_z$ 의 eigenvalue는 보존되는 양이다. 따라서, 각 S^2, S_z 값의 state에 대해 Hamiltonian 은 block diagonal이다.

- For example, $N=3$, $\Omega=3$ case: v는 $1,3$이 가능하고, 따라서, $E=-2G, 0$가 가능하다. total number of s.p. states는 $2\Omega = 6$ (1-,1+,2-,2+,3-,3+)이므로, 3-particle state는 ${}_6C_3 = 20$ 가 가능하다. 이중 $S_z = \frac{1}{2}$인 경우는 $|1-,1+,2+\rangle$, $|1-,1+,3+\rangle$, $|1-,2+,3+\rangle$, $|1+,2-,2+\rangle$, $|1+,2-,3+\rangle$, $|1+,2+,3-\rangle$, $|1+,3-,3+\rangle$, $|2-,2+,3+\rangle$, $|2+,3-,3+\rangle$ 의 9 state가 가능하다. 이 state들에 대한 9×9 Hamiltonian matrix($\langle 1-,1+,2+|P_+P_-|1-,1+,2+\rangle = 1$, $\langle 1-,1+,2+|P_+P_-|1-,1+,3+\rangle = 0$, 등)의 eigenvalue를 구해보면, 3개 state는 -2G, 6개 state는 0 값을 가지는 것을 알 수 있다. 즉, diagonalization을 하기 전에 가능한 eigen-value가 얼마인지를 알 수 있다. (사실 가능한 v의 값은 state에서의 broken pair의 수로부터 쉽게 계산이 가능하다. N=3, $S_z = \frac{1}{2}$인 경우는 하나의 pair가 있거나, 하나도 pair가 안되거나 이다.)

- $N=4, \Omega=4$의 $S=0$ 인 경우: Let us index 1,2,3. . . for states $(1+,1-,2+,2-,3-,3+,4-,4+)$. Then, 가능한 4-body state with $M=0$ 는 총 6가지로, $|1234\rangle$, $|1256\rangle$, $1278\rangle$, $|3456\rangle$, $|3478\rangle$, $|5678\rangle$ 이다.

  full Hamiltonian은 다음과 같이 matrix로 표현할 수 있다.

$$H = \begin{pmatrix} 2\delta-g & -g/2 & -g/2 & -g/2 & -g/2 & 0 \\ -g/2 & 4\delta-g & -g/2 & -g/2 & 0 & -g/2 \\ -g/2 & -g/2 & 6\delta-g & 0 & -g/2 & -g/2 \\ -g/2 & -g/2 & 0 & 6\delta-g & -g/2 & -g/2 \\ -g/2 & 0 & -g/2 & -g/2 & 8\delta-g & -g/2 \\ 0 & -g/2 & -g/2 & -g/2 & -g/2 & 10\delta-g \end{pmatrix} \tag{2.8}$$

  여기서 만약 reference space 를 $|1234\rangle$ 로 두면, s.p. states 1,2,3,4 는 hole state, 5,6,7,8은 particle state이다. may-body basis는 첫번째는 $0p0h$, 다른 4개 state는 $2p2h$, 마지막을 $4p4h$ excited 상태로 생각할 수 있다.

- Potential is only non-zero for the types of $\langle ab|v|cd\rangle$, $\langle ij|v|kl\rangle$ and $\langle ab|v|ij\rangle$. (쌍을 이루는 입자는 둘다 hole이거나 particle이어야 한다.) ($\langle ai|v|bj\rangle = 0$.)

- Fock term is (in HF basis) $< p|f|q >=< p|H_0|q > + \sum_{i<=F} < pi|V|qi >$. We only need f_{pp} and f_{hh} type. $< p|H_0|q >$ is diagonal. The second term is non-zero only when p, q are holes and either (12) or (34) pair.
- It was not difficult to construct full Hamiltonian in this example. For more general Hamiltonian, one can compute matrix elements of $\hat{V} = \sum_{p<q,r<s} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_r$. If we list s.p. states $i = 1, \ldots N_{sp}$, then construct possible N-particle states $|\alpha\rangle$. (like $|i_1 < i_2 < \ldots i_N\rangle$) One can make a code to compute $|\alpha'\rangle = a_p^\dagger a_q^\dagger a_s a_r |\alpha\rangle$. Which can be done by brute force or bit-wise operations. For example, $a_2^\dagger a_8^\dagger a_1 a_{12} |1, 3, 9, 12\rangle = -|2, 3, 8, 9\rangle$ (? sign?)
- full configuration interaction(FCI) is to diagonalize the full Hamiltonian.
- (truncated) configuration interaction (CI) is to diagonalize the Hamiltonian in truncated model space. For example, we may use 5×5 matrix excluding $4p4h$ state.

An efficient implementation of these rules requires

- to find the number of single-particle state substitutions between two determinants
- to find which single-particle states are involved in the substitution
- to compute the phase factor if a reordering of the single-particle states has occured
- reference : `https://github.com/scemama/slater_condon`, `https://arxiv.org/abs/0810.2644`

If the eigen state $|\Psi_\lambda\rangle = \sum_p C_{\lambda i} |SD_i\rangle$, in a similar way, we get

$$\langle \Psi_\lambda | O_1 | \Psi_\sigma \rangle = \sum_{pq} \langle p|o_1|q\rangle \sum_{ij} C_{\lambda i}^* C_{\sigma j} \langle SD_i | a_p^\dagger a_q | SD_j \rangle \tag{2.9}$$

We can obtain

$$\langle SD_i^A | a_p^\dagger a_q | SD_j^A \rangle \quad = \quad \sum_l \langle SD_i | a_p^\dagger | SD_l^{(A-1)} \rangle \langle SD_l^{(A-1)} | a_q | SD_j \rangle \tag{2.10}$$

where $\langle SD_l | a_q^\dagger | SD_j^{(A-1)} \rangle$ are spectroscopic factors.

2.2 Bit-wise representation of second quantization

One can express the Slater determinant as a bit-wise integers. For example, if there are 16(starting from zero) possible s.p. states, four particle slater determinant with states $\alpha_3, \alpha_6, \alpha_{10}, \alpha_{13}$ as $\Phi_{3,6,10,13} \to |0001001000010010 0\rangle$. When N particles can be distributed over n single particle states, total number of such N-particle Slater determinant is ${}_nC_N$.

- action of annihilation operator can be done as subtraction of some logical and operation. For example, $a_0 \Phi_{0,1,3,4} = a_0 |11011\rangle = |01011\rangle$ can be done by

$$\begin{aligned} & |\Phi_{0,1,3,4}\rangle - |\Phi_0\rangle \wedge |\Phi_{0,1,3,4}\rangle \\ = \quad & |11011\rangle - |10000\rangle \wedge |11011\rangle = |11011\rangle - |10000\rangle = |01011\rangle \end{aligned} \tag{2.11}$$

- action of creation operator can be done by adding corresponding bit when it is empty. For example $a_2^\dagger |010111\rangle$ can be done by

$$a_2^\dagger |01011\rangle \to |01011\rangle + |00100\rangle = |01111\rangle \tag{2.12}$$

- In addition, one needs to find phase factor $(-1)^l$. This is rather tricky.

Chapter 3

Shell model

3.1 Basics

In shell model approach, we first introduce central spherical potential $\hat{U}$ and then try to solve full hamiltonian for residual interaction $\hat{V} - \hat{U}$

$$\begin{aligned} \hat{H} &= \sum_i^A \left(-\frac{\hbar^2}{2m}\Delta_i \right) + \sum_{i<j}^A W_{i,j} + \sum_{<i<j<k} W_{i,j,k}, \\ &\rightarrow \sum_i^A \left[-\frac{\hbar^2}{2m}\Delta_i + U(i) \right] + \left[\sum_{i<j}^A W_{i,j} - \sum_i^A U(i) \right] = \hat{H}^{(0)} + \hat{V} \end{aligned} \tag{3.1}$$

For a spherical symmetric potential including $\boldsymbol{l} \cdot \boldsymbol{s}$ coupling, the single particle solution of each $\hat{h}(i)$ of $\hat{H}^{(0)} = \sum_i^A \hat{h}(i)$ can be easily obtained and specified by the quantum numbers n, l, s, j.

If the appropriate U is chosen such that residual interaction $\hat{V}$ is weak, we may use perturbative approach from the ground state.

In the independent particle model, ground state is assumed as $a_k|\Phi\rangle = 0$, $k > \epsilon_F$ where a_k is a operator related with single particle state of H_0 and $|\Phi\rangle$ is a A-body slater determinant of lowest lying A-states.

If the residual interaction mixes simple shell model wave functions, we may try to solve the Hamiltonian with linear combination of simple shell model wave functions, $|\Phi_{shell}\rangle = \sum_i c_i |\Phi_{simple,i}\rangle$ where i is an index for many-body states which is a collection of single particle states. This is the shell model with configuration mixing. And it is equivalent to diagonalize the shell model Hamiltonian $H = T + U + (V - U) = H_0 + V'$. In general, the residual interaction will be dependent on the model space and need to be computed as a effective interaction.

single particle state

Spherical Potential(Harmonic oscillator나 Woods Saxon POtential)의 eigen state

$$\phi_{nlj}(\vec{r}) = \frac{R_{nl}(r)}{r} [Y_l(\hat{r}) \otimes \chi_{1/2}]^{(j)}_m \tag{3.2}$$

In a specific example of simple harmonic oscillator,

$$U(r) = \frac{m\omega^2 r^2}{2}, \tag{3.3}$$

the solution is well known and can be specified by the harmonic oscillator length parameter $b = \sqrt{\frac{\hbar}{m\omega}}$ in fm. And Energy level becomes

$$\epsilon_N = \hbar\omega\left(2n + l + \frac{3}{2}\right) = \hbar\omega\left(N + \frac{3}{2}\right). \tag{3.4}$$

The N gives the major shell energy level and LS coupling splits the level further by n, l, j values.

isospin

For the nuclei of (N, Z) nucleons, the possible isospin is

$$T_Z = \frac{1}{2}(N - Z), \quad \frac{1}{2}(N - Z) \leq T \leq \frac{A}{2}. \tag{3.5}$$

The Coulomb interaction

$$\hat{V}_{Coul} = \sum_{i<j}(\frac{1}{2} + t_i^z)(\frac{1}{2} + t_j^z)\frac{e^2}{r_{ij}} \tag{3.6}$$

gives isospin dependence in the energy gives isobaric multiplet mass equation, [1]

$$E(T, T_z) = a(T) + b(T)M_T + c(T)M_T^2 \tag{3.8}$$

3.2 Solution of eigenproblem

When there is no residual interaction, we can easily know the many-body eigen-solution of equation,

$$\hat{H}^{(0)}\Psi_\alpha = E_\alpha^{(0)}\Psi_\alpha. \tag{3.9}$$

In $m-$scheme, Ψ_α is a simply slater determinant of single particle wave function of given $\{\alpha_1 m_1, \alpha_2 m_2, \dots\}$ single particle states, $\alpha_i = (n, l, s, j)_i$ without considering total angular momentum J. So that $E_\alpha^{(0)} = \sum_{i=1}^{A} \epsilon_{\alpha_i}$.

J-scheme에서는 slater determinant가 특정 angular momentum J를 가지고 antisymmetric하도록 만들어야 한다. 예를 들어 두개의 입자가 있는 경우, 적절한 조합을 통해

$$[\phi_\alpha \otimes \phi_\beta]_M^J \tag{3.10}$$

으로 특정 angular momentum을 가지는 상태를 만들수 있으나, 아직 antisymmetric하지는 않다. anti-symmetric하게 만들기 위해서는

$$\Phi_{JMTM_T}^{ab}(1,2) = \left([\phi_a(1) \times \phi_b(2)]_M^{(J)} + (-1)^{j_a+j_b+J+T}\left[\phi_b(1) \times \phi_a(2)\right]_M^{(J)}\right)\frac{\eta_{TM_T}}{\sqrt{2(1+\delta_{ab})}} \tag{3.11}$$

와 같은 과정이 필요하다. (이 때문에 같은 두개의 핵자로 이루어진 상태는 오직 even J 값만 가질 수 있다. isospin을 고려하면, $J + T =$(odd) 인 경우만 가능.)

In J-scheme basis, we construct the many-body basis wave function so that it can have good total angular momentum J (and T). Because it involves a specific combination of single particle wave functions, it can be rather complicate.

[1] This is because the Coulomb interaction is sum of rank-0, rank-1, rank-2 operators in isospin space. This can be proved simply by

$$\langle\sum_i t_i^z\rangle \to M_T, \quad \langle\sum_{i<j} t_i^z t_j^z \to N(N-1-Z) - Z(N-(Z-1)) = (N-Z)^2 - (N-Z). \tag{3.7}$$

In case of many-nucleons, the full wave function will be

$$\Phi^{a^{n_a}b^{n_b}\cdots}_{JMTM_T}(1,2,\ldots,A) \tag{3.12}$$

예를 들어 $(\nu 0f_{7/2})^2$ state는 J-scheme에서,

$$|(\nu 0f_{7/2})^2, J, M, (T=1)\rangle, \quad J=0,2,4,6 \tag{3.13}$$

이고, m-sheme에서는

$$|(\nu 0f_{7/2})^2, m_1, m_2\rangle, \quad m_1 \neq m_2 \tag{3.14}$$

Let us suppose that we have $(N-1)$ identical nucleons in a single j-shell, which forms all possible value of J', with wave function $\Phi^{j^{(N-1)}}_{\chi' J' M'}$. Then to get a wave function of N-nucleons in j-shell with angular momentum J, M, we can write

$$\Phi^{j^{(N)}}_{\chi JM} = \sum_{\chi' J'} \langle j^{N-1}(\chi' J')j|\}j^N \chi J\rangle \Phi^{j^{(N-1)}}_{\chi' J' M'} \phi_{jm} \tag{3.15}$$

The coefficient is called coefficients of fractional parentage.

A many-particle wave functions with nucleons occupying different j-orbitals can be obtained first by creating antisymmetrized wave functions for groups of nucleons in each j-shell and then by coupling and antisymmetrization between different groups.

이러한 normalized, antisymmetrized, Many-body Slater determinant state를 Shell Model basis state 라고 부르고, shell model계산은 이러한 basis를 만드는 것으로부터 시작된다.

Chapter 4

Hartree Fock theory

In Hartree-Fock theory, the ground state of A-body system is assumed to be a slater determinant of single particle states $|\Phi_{HF}\rangle$. However, unlike the shell-model approach, $|\Phi_{HF}\rangle$ is not determined by external single particle potential and rather to be obtained from given Hamiltonian. By minimizing the energy expectation value $\langle\Phi_{HF}|H|\Phi_{HF}\rangle$ by variation of single particle states, one can obtain the HF condition (or equation) for single particle states which would provide best variational ground state.

4.1 Difference between DFT and HF?

The DFT is based on the Hohenberg and Kohn theorem.

For an electronic system, Hamiltonian of N-electrons under external fields(from other ions) is

$$H = \sum_{n=1}^{N} \frac{-\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}\sum_{i\neq j=1}^{N} V(i,j) + \sum_{i=1}^{N} v_{ext}(i). \tag{4.1}$$

The theorem states that the total energy of the system can be written as a functional of the fermion density,

$$E_{v_{ext}}[\rho] = \langle\Psi|\hat{T} + \hat{V} + \hat{v}_{ext}|\Psi\rangle = F[\rho] + \int d^3r v_{ext}(\boldsymbol{r})\rho(\boldsymbol{r}). \tag{4.2}$$

It implies that (1) all system information can be described by density $\rho(\boldsymbol{r})$ instead of wave function Ψ, (2) there exists a universal functional F which does not depends on the external potential. However, the exact form of functional is unknown.

More practical scheme is to use Kohn-Sham scheme, in which it is assumed that the density ρ can be represented in terms of auxiliary single-particle wave functions(orbitals) $\phi_j(\boldsymbol{r})$, and correspondingly the energy can be expressed as

$$\begin{aligned}
\rho(\boldsymbol{r}) &= \sum_j |\phi_j(\boldsymbol{r})|^2, \\
T &= \langle\Psi|\hat{T}|\Psi\rangle = \sum_j \langle j|\frac{-\hbar^2}{2m}\nabla^2|j\rangle, \\
E_{Hartree} &= \frac{e^2}{2}\int d^3r d^3r' \frac{\rho(\boldsymbol{r})\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}, \\
E_{KS} &= T + E_{Hartree} + E_{xc} + \int d^3r v_{ext}(\boldsymbol{r})\rho(\boldsymbol{r})
\end{aligned} \tag{4.3}$$

where the "exchange correlation" E_{xc} is not known yet.

The minimization of functional with respect to density with constraint that the orbitals are orthonormal leads,

$$\begin{aligned} & \frac{\delta}{\delta\rho(\boldsymbol{r})}\left(E_{KS}-\epsilon\int d^3r'\phi_j^*(\boldsymbol{r})\phi_j(\boldsymbol{r}')\right)=0, \\ \rightarrow \quad & \left(-\frac{\hbar^2}{2m}\nabla^2+\frac{e^2}{2}\int d^3r'\frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}+\frac{\delta E_{xc}}{\delta\rho(\boldsymbol{r})}+v_{ext}(\boldsymbol{r})\right)\phi_j(\boldsymbol{r}) \\ = \quad & \left(-\frac{\hbar^2}{2m}\nabla^2+v_{KS}\right)\phi_j(\boldsymbol{r})=\epsilon\phi_j(\boldsymbol{r}) \end{aligned} \tag{4.4}$$

This equation is very similar to HF equation. In other words, one can think HF is a special case of DFT. (In HF nuclear system, there is no external potential. Also, nuclear interaction is short ranged with spin dependent and it can have three-body interactions. Also, usually microscopic nuclear interaction is independent of density. One connection between HF and DFT is the introduction of density dependent interaction in HF theory.)

The actual evaluation of $E_{v_{ext}}$ or E_{KS} is difficult. However, one can do such calculation for uniform matter and can obtain the contribution of E_{xc} for uniform matter. Local Density Approximation(LDA) assumes that in the vicinity of a given point $\boldsymbol{r}$, the exchange correlation energy of any electron system can be approximated with that of the uniform gas with the same density.

$$E_{xc}=\int d^3r e_{xc}^{hom}[\rho(\boldsymbol{r})]\rho(\boldsymbol{r}) \tag{4.5}$$

4.1.1 Thomas-Fermi theory

Wikipedia 참조

Instead of constant density of Fermion gas in whole volume, one may approximate the density varies slowly $\rho(\boldsymbol{r})$ but, in a small volume ΔV still it can be treated as a uniform distribution. This is a Thomas-Fermi theory which relates the local density $\rho(\boldsymbol{r})$ and kinetic energy density $\tau(\boldsymbol{r})$.

$$\tau(\boldsymbol{r})=C_{kin}\rho(\boldsymbol{r})^{5/3}, \quad C_{kin}=\frac{3h^2}{40m}(\frac{3}{\pi})^{\frac{2}{3}} \tag{4.6}$$

자세하게: local $\boldsymbol{r}$ 부근에서 density가 uniform이라고 가정하고, total number of fermion 은 $\Delta N=\rho(\boldsymbol{r})\Delta V$ 라고 쓸 수 있다. 한편, local하게 $p_F(\boldsymbol{r})$ 을 가정하면, phase space volume은 $\frac{4\pi}{3}p_F^3(\boldsymbol{r})\Delta V$ 라고 생각할 수 있다. fermion이 단위 phase space volume $\frac{1}{h^3}$ 당 2개가 있을 수 있다고 하면, phase volume 내에 있는 fermion의 수는 $\Delta N_{ph}=\frac{2}{h^3}\frac{4\pi}{3}p_F^3(\boldsymbol{r})\Delta V$이 된다. 따라서, $\Delta N=\Delta N_{ph}$ 로 두면,

$$\rho(\boldsymbol{r})=\frac{8\pi}{3h^3}p_F^3(\boldsymbol{r}) \tag{4.7}$$

의 관계가 얻어진다. To get the kinetic energy density, using fraction of particles in momentum between p, $p+dp$, $F_r(p)dp=\frac{4\pi p^2dp}{4\pi p_F^3(\boldsymbol{r})/3}$,

$$\tau(\boldsymbol{r})=\int\frac{p^2}{2m}n(\boldsymbol{r})F_r(p)dp=\frac{3h^2}{40m}(\frac{3}{\pi})^{2/3}[n(\boldsymbol{r})]^{5/3} \tag{4.8}$$

4.2 HF energy

Assume HF Hamiltonian and HF statesn such that

$$\begin{aligned} H^{HF} &= \sum_{i=1}^{A} h(i), \\ H^{HF}|\Phi_{HF}(1,\dots A)\rangle &= E|\Phi_{HF}(1,\dots A)\rangle, \\ |\Phi_{HF}(1,\dots A)\rangle &= \frac{1}{\sqrt{A!}}\prod_{i=1}^{A} a_i^\dagger|-\rangle, \\ h(i)\phi_k(i) &= \epsilon_k\phi_k(i), \quad (i)=\{\boldsymbol{r}_i, s_i, t_i\}. \end{aligned} \tag{4.9}$$

s.p. level label convention: (i,j) for hole states(occupied levels in $|HF\rangle$), (m,n) for empty levels(particle states). If we do not distinguish , use (k,l,p,q).

However, note that this H^{HF} is not the same as Hamiltonian of original system H or Hartree-Fock energy,

$$E^{HF} = \langle\Phi_{HF}|H|\Phi_{HF}\rangle \neq \langle\Phi_{HF}|H^{HF}|\Phi_{HF}\rangle = \sum_{i=1}^{A}\epsilon_i \tag{4.10}$$

Single particle wave function can be expressed in terms of s.p. basis functions, χ_l, which corresponds to operators $c_l^\dagger$, c_l.

$$\begin{aligned} \phi_k = \sum_l D_{lk}\chi_l \quad &\leftrightarrow \quad \chi_l = \sum_k D^*_{lk}\phi_k \\ a_k^\dagger = \sum_l c_l^\dagger D_{lk} \quad &\leftrightarrow \quad c_l^\dagger = \sum_k D^*_{lk}a_k^\dagger = \sum_k a_k^\dagger (D^\dagger)_{kl}, \\ a_k = \sum_l D^*_{lk}c_l = \sum_l (D^\dagger)_{kl}c_l \quad &\leftrightarrow \quad c_l = \sum_k D_{lk}a_k = \sum_k a_k (D^*)^\dagger_{kl} \end{aligned} \tag{4.11}$$

Here $c_l^\dagger$ and c_l are defined w.r.t. vacuum, $c_l|-\rangle = 0$. (a_k also gives $a_k|-\rangle = 0$. However, it is because a_k is a linear combinations of c_l.)

For complete and orthogonal sets, D has to be unitary. ($D^\dagger D = DD^\dagger = 1$). Note here the summation runs over all model space. **However, it is not yet specified what is the $h(i)$ and $\phi_k(i)$.** In Shell model, $D_{lk} = 0$ if $l,k > A$ and $D_{lk} = \delta_{lk}$ if $l = k < A$.

For a HF state, $\langle HF|\hat{a}_i^\dagger\hat{a}_j|HF\rangle = \delta_{ij}$ for creation and annihilation operators of HF basis, but $\langle HF|\hat{c}_\alpha^\dagger\hat{c}_\beta|HF\rangle \neq \delta_{\alpha\beta}$ for for creation and annihilation operators of original s.p. basis, rather it becomes a density matrix,

$$\begin{aligned} \rho_{ll'} &= \langle\Phi|c_{l'}^\dagger c_l|\Phi\rangle, \\ &= \sum_{kk'} D_{lk}D^*_{l'k'}\langle\Phi|a_{k'}^\dagger a_k|\Phi\rangle = \sum_{i=1}^{A} D_{li}D^*_{l'i} \end{aligned} \tag{4.12}$$

density matrix satisfies

$$\rho^2 = \rho, \quad \mathrm{Tr}\rho = A \tag{4.13}$$

Then, the HF energy is

$$\begin{aligned}
E^{HF} &= \langle \Phi_{HF}|H|\Phi_{HF}\rangle, \\
H &= \sum_{l_1 l_2} t_{l_1 l_2} c^\dagger_{l_1} c_{l_2} + \frac{1}{4}\sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2, l_3 l_4} c^\dagger_{l_1} c^\dagger_{l_2} c_{l_4} c_{l_3}, \\
\bar{v}_{l_1 l_2, l_3 l_4} &= v_{l_1 l_2, l_3 l_4} - v_{l_1 l_2, l_4 l_3}, \\
E^{HF}[\rho] &= \sum_{l_1 l_2} t_{l_1 l_2} \langle \Phi | c^\dagger_{l_1} c_{l_2} | \Phi \rangle + \frac{1}{4}\sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2, l_3 l_4} \langle \Phi_{HF}| c^\dagger_{l_1} c^\dagger_{l_2} c_{l_4} c_{l_3} |\Phi_{HF}\rangle \\
&= \sum_{l_1 l_2} t_{l_1 l_2} \rho_{l_2 l_1} + \frac{1}{2}\sum_{l_1 l_2 l_3 l_4} \rho_{l_3 l_1} \bar{v}_{l_1 l_2, l_3 l_4} \rho_{l_4 l_2}, \\
&= \mathrm{Tr}[t\rho] + \frac{1}{2}\mathrm{Tr}_1 \mathrm{Tr}_1 (\rho \bar{v} \rho)
\end{aligned} \tag{4.14}$$

In HF basis,

$$E^{HF}[\rho] = \sum_{i=1}^{A} t_{ii} + \frac{1}{2}\sum_{i,j=1}^{A} \bar{v}_{ij,ij} \tag{4.15}$$

(In other words, we want to diagonalize the density matrix which also minimize the HF energy).

4.2.1 Another way to look the problem

Consider a taylor expansion, supposing the variation is allowed only in x, y direction.

$$f(x,y,z) = f(x_0,y_0,z_0) + \frac{\partial f}{\partial x}(x-x_0) + \frac{\partial f}{\partial y}(y-y_0) + \dots \tag{4.16}$$

Then, (x_0, y_0, z_0) to be a minimum is equivalent to the non-existence of first correction terms.

For the Hamiltonian, suppose an expansion around $|\Phi_0\rangle$. By using normal ordering or quasi-particle operator such that $\alpha_k|\Phi_0\rangle = 0$, we may express Hamiltonian as

$$H = \langle \Phi_0|H|\Phi_0\rangle + \sum_{ij} h_{ij}\alpha^\dagger_i \alpha_j + \dots \tag{4.17}$$

If the particle-hole type excitation is allowed for $|\Phi_0\rangle$, $\langle\Phi_0|\alpha^\dagger_p \alpha_h|\delta\Phi\rangle$ can be non-zero and thus the condition of coefficients $h_{ph} = 0$ is equivalent to $|\Phi_0\rangle$ to be a minimum state. [1] Thus, instead of trying variation of expectation value $\langle\Phi_0|H|\Phi_0\rangle$, one can also try to find a quasi-particle expression of Hamiltonian such that the corresponding to lowest order excitation to vanish.

4.3 HF equation

Until now, $h(i)$ and HF basis is not specified.

Consider variation of density. However, the condition that the variation is still a density matrix, one have to keep the properties $\rho^2 = \rho$.

$$(\rho + \delta\rho)^2 = \rho + \delta\rho \quad \Rightarrow \quad \delta\rho \simeq \rho\delta\rho + \delta\rho\rho \tag{4.18}$$

[1] In case of pure shell model, $|\Phi_{shell}\rangle = \prod_{i=1}^{A} c^\dagger_i |-\rangle$, density matrix becomes diagonal $\rho_{ll'} = \delta_{ll'}$ if $l \le \epsilon_F$, or $\rho_{ll'} = 0$ if $i > \epsilon_F$. We can also compute Shell model energy expectation value $\langle\Phi_{shell}|H|\Phi_{shell}\rangle$ which gives similar expression with HF energy. However, the corrections $E = E_{shell} + \dots$ will be non-negligible. On the other hand, HF case $E = E_{HF} + \dots$, at least it has no particle-hole excitation corrections.

In HF basis, ρ is diagonal and $\rho_{ij} = \delta_{ij}$ and $\rho_{mn} = 0$, i.e. particle-particle matrix element or hole-hole matrix element of $\delta\rho$ have to vanish. ($(\delta\rho)_{ij} = (\delta\rho)_{mn} = 0$, or equivalently $\rho\ \delta\rho\ \rho = 0$) . Thus, allowed variations are particle-hole or hole-particle types, $\delta\rho_{im}$ or $\delta\rho_{mi}$.

$$\begin{aligned} \delta E[\rho] &= E[\rho+\delta\rho] - E[\rho] = \sum_{kk'} h_{kk'}\delta\rho_{k'k} = \sum_{mi} h_{mi}\delta\rho_{im} + (c.c.), \\ h_{kk'} &= \frac{\partial E^{HF}[\rho]}{\partial\rho_{k'k}} = t_{kk'} + \Gamma_{kk'}, \quad \Gamma_{kk'} = \sum_{ll'} \bar{v}_{kl'k'l}\rho_{ll'} \end{aligned} \tag{4.19}$$

Because of arbitrary variation $\delta\rho_{im}$, HF condition $\delta E = 0$ means

$$h_{mi} = t_{mi} + \sum_{j=1}^{A} \bar{v}_{mjij} = 0, \quad (\text{for } i \le A, m > A) \tag{4.20}$$

in the basis where ρ is diagonal. (Note that this means that the p-h matrix element should vanish in that basis). Thus,(since there is no mixing between particle and hole),

$$[h, \rho] = [t + \Gamma(\rho), \rho] = 0. \tag{4.21}$$

Thus, h and ρ can be diagonalized at the same time. If we require the h and ρ diagonalized in HF basis,

$$h_{kk'} = t_{kk'} + \sum_{i=1}^{A} \bar{v}_{kik'i} = \epsilon_k \delta_{kk'}. \tag{4.22}$$

This is equivalent in normal basis,

$$\sum_{l'} h_{ll'} D_{l'k} = \sum_{l'} \left(t_{ll'} + \sum_{i=1}^{A} \sum_{pp'} \bar{v}_{lp'l'p} D_{pi} D^*_{p'i} \right) D_{l'k} = \epsilon_k D_{lk} \tag{4.23}$$

This is an non-linear eigen-value problem for D which determines single particle wave function ϕ_k.

Thus, the single particle Hamiltonian h is derived.

$$\begin{aligned} H^{HF} &= \sum_{kk'} h_{kk'} a^\dagger_k a_{k'} = \sum_{kk'} (t+\Gamma)_{kk'} a^\dagger_k a_{k'} \\ &= \sum_{kk'} \left(t_{kk'} + \sum_{j=1}^{A} \bar{v}_{kjk'j} \right) a^\dagger_k a_{k'} = \sum_k \epsilon_k a^\dagger_k a_k \end{aligned} \tag{4.24}$$

However, note that the h contains kinetic energy and self consistent field. (Note that $H^{HF} \neq H$.) Energy expectation value (HF energy)

$$\begin{aligned} E_0^{HF} &= \langle \Phi_{HF} | H | \Phi_{HF} \rangle = \sum_{i=1}^{A} t_{ii} + \frac{1}{2} \sum_{i,j=1}^{A} \bar{v}_{ij,ij} \\ &= \sum_{i=1}^{A} \epsilon_i - \frac{1}{2} \sum_{ij=1}^{A} \bar{v}_{ijij} = \sum_{i=1}^{A} \epsilon_i + \frac{1}{2} \sum_{i=1}^{A} t_i \end{aligned} \tag{4.25}$$

The same equation can be written in Coordinate space,

$$-\frac{\hbar^2}{2m}\Delta\phi_k(\boldsymbol{r}) + \sum_{j=1}^{A} \int d\boldsymbol{r}' v(\boldsymbol{r}, \boldsymbol{r}') \phi^*_j(\boldsymbol{r}') \left(\phi_j(\boldsymbol{r}')\phi_k(\boldsymbol{r}) - \phi_j(\boldsymbol{r})\phi_k(\boldsymbol{r}') \right) = \epsilon_k \phi_k(\boldsymbol{r}) \tag{4.26}$$

Or

$$\left\{-\frac{\hbar^2}{2m}\Delta + \Gamma_H(\boldsymbol{r})\right\}\phi_k(\boldsymbol{r}) + \int d\boldsymbol{r}'\Gamma_{ex}(\boldsymbol{r},\boldsymbol{r}')\phi_k(\boldsymbol{r}') = \epsilon_k\phi_k(\boldsymbol{r}), \tag{4.27}$$

where,

$$\begin{aligned}\Gamma_H(\boldsymbol{r}) &= \int d\boldsymbol{r}' v(\boldsymbol{r},\boldsymbol{r}')\sum_{j=1}^{A}|\phi_j(\boldsymbol{r}')|^2 = \int d\boldsymbol{r}' v(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}'),\\ \Gamma_{ex}(\boldsymbol{r},\boldsymbol{r}') &= -v(\boldsymbol{r},\boldsymbol{r}')\sum_{j=1}^{A}\phi_j^*(\boldsymbol{r}')\phi_j(\boldsymbol{r}) = -v(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r},\boldsymbol{r}')\end{aligned} \tag{4.28}$$

4.4 Symmetry violation

HF solution (and HF potential) may broke some symmetry of the Hamiltonian. Translation invariance, rotational invariance, particle number conservation may be broken. The symmetry is broken because of the simple independent particle picture of HF solution. The symmetry may be restored later.

However, some part of symmetry of Hamiltonian can be conserved. (self-consistent symmetries).

4.5 Numerical Method to solve HF equation

Chapter 5

HF-BCS theory

There exists a paring interaction between nucleons in nuclei. It is originated from nucleon-nucleon interaction. However, usually, the pairing interaction is referred to a specific kind of interaction between nucleons to form a spin 0 states. However, once the pairing interaction is so strong to form a bound state or change the ground state, one can not use perturbation theory and rather have to get a non-perturbative solution with pairing interaction. For a particular kind of paring interaction among the nucleons in the same single particle energy, BCS theory provides such description.

It is observed that the pairing is very important in nuclei with open shells. Thus, one needs a better way to describe pairing interaction. BCS theory represent the wave function for **even-even** nuclei as

$$|BCS\rangle = \prod_{k>0}(u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)|-\rangle \tag{5.1}$$

where conjugate state $\bar{k} < 0$ is to make the whole single particle states are described by $\{k, \bar{k}\}$. 여기서, $k > 0$, $k < 0$ 는 Fermi level에 대한 것이 아니라, s.p. state의 j_z component에 대한 것이다.

(For example, original BCS case, conjugation is for states with opposite momentum and spin. In spherical basis, $|k\rangle = |nljm\rangle$, $\bar{k} = |nlj-m\rangle$ with $m > 0$. Also note that the BCS states only products with $k > 0$. We may use $u_{\bar{k}} = u_k$, $v_{\bar{k}} = -v_k$.) 즉, 다른 말로 BCS ground state는 항상 nucleon pair 를 쌍아 나가는데, 각 pair의 occupation number는 $|v_k|^2$ 라는 것. 다만, Fermi level 밑에서는 $|v_k| = 1$ 이고, Fermi level 위에서는 $|v_k| = 0$ 이고, fractional value를 가지는 것은 Fermi level 부근에서 만이다. [1]

u_k and v_k are not independent,[2]

$$|u_k|^2 + |v_k|^2 = 1. \tag{5.2}$$

In general u_k and v_k are complex. By using overall phase factor, one can fix u_k to be real, but v_k can be complex. But, with some assumption on the interaction, we may use real valued v_k.

BCS state also can be expressed in other ways,

$$|BCS\rangle \propto \exp(A^\dagger)|-\rangle, \quad A^\dagger = \sum_{k>0} \frac{v_k}{u_k} a_k^\dagger a_{\bar{k}}^\dagger. \tag{5.3}$$

[1] In HF case, $|HF\rangle = \sum_{i=1}^{A} a_i^\dagger|-\rangle$ is defined with A- low-lying states. On the other hand, $|BCS\rangle$ has no such constraints. Instead additional constraint is applied with chemical potential. Thus, occupation number distribution changes from sharp function to smooth function in energy with roughly the same volume.

[2] In fact, $|BCS\rangle$ is not properly normalized, $\langle BCS|BCS\rangle = \langle -|\sum_k (|u_k|^2 + |v_k|^2)|-\rangle$.

5.1 BCS equation

Many-body Hamiltonian[3]

$$H = \sum_{k_1 k_2 \gtrless 0} t_{k_1 k_2} a^\dagger_{k_1} a_{k_2} + \frac{1}{4} \sum_{k_1 k_2 k_3 k_4 \gtrless 0} \bar{v}_{k_1 k_2, k_3 k_4} a^\dagger_{k_1} a^\dagger_{k_2} a_{k_4} a_{k_3} \tag{5.4}$$

The expectation values of number operator for BCS states are[4]

$$\langle BCS|\hat{N}|BCS\rangle = \sum_{k>0}(v_k^2 + v_{\bar{k}}^2) = 2\sum_{k>0} v_k^2 = N. \tag{5.5}$$

$$(\Delta N)^2 = \langle BCS|\hat{N}^2|BCS\rangle - N^2 = 4\sum_{k>0} u_k^2 v_k^2. \tag{5.6}$$

To find a minimum of $E_{BCS} = \langle BCS|H|BCS\rangle$ under constraint $\langle BCS|\hat{N}|BCS\rangle = N$ is the same as finding a minimum of expectation value of $H' = H - \lambda N$, $E_{BCS}[\rho, \lambda] = \langle BCS|H'|BCS\rangle$ and chemical potential $\lambda = \frac{dE_{BCS}}{dN}$. Thus, we will deal with Hamiltotnian H', the physical energy is always expectation value H, not H'. (Derivation of following expression will be done later. Be careful for the distinction of $k > 0$ and $\bar{k}$.)

$$\begin{aligned} E_{BCS}[u, v(u)] &= \langle BCS|H'|BCS\rangle \\ &= \sum_{k\gtrless 0}\left[(t_{kk} - \lambda)v_k^2 + \frac{1}{2}\sum_{k'\gtrless 0} \bar{v}_{kk',kk'} v_k^2 v_{k'}^2\right] + \sum_{kk'>0} \bar{v}_{k\bar{k}k'\bar{k}'} u_k v_k u_{k'} v_{k'}. \end{aligned} \tag{5.7}$$

(Actual energy of gound state is $\langle BCS|H|BCS\rangle = \langle BCS|H'|BCS\rangle + \lambda N$.) Variational minimization of energy, $\delta\langle BCS|H'|BCS\rangle = 0$ gives

$$\left(\frac{\partial}{\partial v_k} + \frac{\partial u_k}{\partial v_k}\frac{\partial}{\partial u_k}\right)\langle BCS|H'|BCS\rangle = 0. \tag{5.8}$$

This gives $X = \langle BCS|H'|BCS\rangle$

$$\begin{aligned} \frac{\partial X}{\partial v_l} &= (t_{ll} - \lambda)2v_l + \left(\sum_{k'\gtrless 0}(\bar{v}_{lk',lk'} + \bar{v}_{k'lk'l})v_{k'}^2\right) v_l + \left(\sum_{k'\gtrless 0}(\bar{v}_{l\bar{l},k'\bar{k}'} + \bar{v}_{k'\bar{k}',l\bar{l}})u_{k'}v_{k'}\right) u_l, \\ \frac{\partial X}{\partial u_l} &= \left(\sum_{k'>0}(\bar{v}_{l\bar{l},k'\bar{k}'} + \bar{v}_{k'\bar{k}',l\bar{l}})u_{k'}v_{k'}\right) v_l, \\ \frac{\partial u_l}{\partial v_l} &= -\frac{v_l}{u_l} \end{aligned} \tag{5.9}$$

Thus, above equation becomes, using symmetry of potential,

$$2\tilde{\epsilon}_k u_k v_k + \Delta_k(v_k^2 - u_k^2) = 0, \quad k > 0, \tag{5.10}$$

with [5]

$$\tilde{\epsilon}_k = \frac{1}{2}\left(t_{kk} + t_{\bar{k}\bar{k}} + \sum_{k'\gtrless 0}(\bar{v}_{kk',kk'} + \bar{v}_{\bar{k}k'\bar{k}k'})v_{k'}^2\right) - \lambda \tag{5.11}$$

[3]Note that this Hamiltonian is written in terms of particle operators, $(a^\dagger, a)$, instead of quasi-particle operators, $(c^\dagger, c)$. HF minimization can be separately considered.

[4]These can be shown with explicit calculation of matrix elements.

[5]Error?? $\sum_{k'\gtrless 0} \bar{v}_{k'k,k'k} = \sum_{k'\gtrless 0} \bar{v}_{\bar{k}k'\bar{k}k'}$?

and gap parameter

$$\Delta_k = -\sum_{k'>0} \bar{v}_{k\bar{k},k'\bar{k}'} u_{k'} v_{k'} \tag{5.12}$$

Thus, if we assume $\tilde{\epsilon}_k$ and Δ_k is already known, the solution is

$$v_k^2 = \frac{1}{2}\left(1 - \frac{\tilde{\epsilon}_k}{\sqrt{\tilde{\epsilon}_k^2 + \Delta_k^2}}\right). \tag{5.13}$$

and with particle number condition,

$$2\sum_{k>0} v_k^2 = N. \tag{5.14}$$

Another way to write the BCS equation is the gap equation,

$$\Delta_k = -\frac{1}{2}\sum_{k'>0} \bar{v}_{k\bar{k},k'\bar{k}'} \frac{\Delta_{k'}}{\sqrt{\tilde{\epsilon}_{k'} + \Delta_{k'}^2}}. \tag{5.15}$$

Also, note that when k is far below Fermi level, $v_k \to 1$, $u_k \to 0$, when k is far above Fermi level $v_k \to 0$, $u_k \to 1$, when k is near the Fermi level $v_k \to \frac{1}{\sqrt{2}}$.

So, what is the final energy of the system ? How it is related with the gap energy?

Example of constant paring interaction

We may consider a very simple case of zero-range interaction,

$$-G\sum_{kk'} a_{k+}^\dagger a_{k-}^\dagger a_{k'-} a_{k'+}. \tag{5.16}$$

This gives

$$\langle H' \rangle = 2\sum_k \eta_k |v_k|^2 - G\left(\sum_k (u_k v_k)^* \sum_{k'\neq k} u_{k'} v_{k'} + \sum_k |v_k|^2\right). \tag{5.17}$$

where

$$\eta_k = \epsilon_k - \lambda \tag{5.18}$$

Considering real v_k and ignoring $G\sum_k v_k^2(1-2v_k^2)$,

$$\langle H' \rangle = 2\sum_k \eta_k v_k^2 - G\left(\sum_k v_k\sqrt{1-v_k^2}\right)^2. \tag{5.19}$$

variational minimization of $\langle H' \rangle$ can be obtained when

$$\begin{aligned} u_k &= \sqrt{\frac{1}{2}(1+\eta_k/\Omega_k)}, \quad v_k = \sqrt{\frac{1}{2}(1-\eta_k/\Omega_k)}, \\ \Omega_k &= \sqrt{C^2+\eta_k^2}, \quad C = G\sum_k u_k v_k. \end{aligned} \tag{5.20}$$

Then, from consistency of definitions gives Gap equation and number of particle constraints gives

$$\begin{aligned} \frac{2}{G} &= \sum_k \frac{1}{\Omega_k}, \\ N_0 &= \sum_k (1-\eta_k/\Omega_k) \end{aligned} \tag{5.21}$$

Here C is a constant which corresponds to Δ_k. Note that C and λ determines all η_k and Ω_k for given ϵ_k. Then, this will determine the occupation probability u_k and v_k. Thus, by solving above two equations, one can determine C and λ. This will gives ground state energy,

$$E_0 = \langle H' \rangle + \lambda N_0 = \sum_{ks} \epsilon_k \langle n_{ks} \rangle - \frac{C^2}{G}. \tag{5.22}$$

Note that, if there were no pairing interaction, $\langle n_{ks} \rangle$ will be simply 1 below Fermi level and 0 above Fermi level and energy will be $\sum_{ks} \epsilon_{ks}$. On the other hand, with pairing interaction, the occupation numbers becomes fractional with distribution and there is additional pairing energy contribution.

5.2 Quasi particle

BCS ground state can be written in terms of quasi-particle operators,

$$|BCS\rangle = \prod_{k>0} (u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)|-\rangle \propto \prod_{k>0} \alpha_k \alpha_{\bar{k}} |-\rangle = \prod_{k \gtrless 0} \alpha_k |-\rangle \tag{5.23}$$

where,[6]

$$\begin{aligned} \alpha_k^\dagger &= u_k a_k^\dagger - v_k a_{\bar{p}}, \\ \alpha_{\bar{k}}^\dagger &= u_k a_{\bar{k}}^\dagger + v_k a_k, \end{aligned} \tag{5.26}$$

with

$$\{\alpha_k, \alpha_{k'}\} = 0, \quad \{\alpha_k, \alpha_{k'}^\dagger\} = \delta_{kk'}. \tag{5.27}$$

The last expression implies that $\alpha_k |BCS\rangle = 0$ for any k.

"Bogoliubov" transformation : ground state of pairwise interacting particles $\Rightarrow$ a gas of non-interacting quasi-particles. Also, not only ground state, excited state may be well described by a product of quasi particles.

$$H_{qp} = \langle BCS|H'|BCS\rangle + \sum_{k \gtrless 0} E_k \alpha_k^\dagger \alpha_k \tag{5.28}$$

where

$$\begin{aligned} &\alpha_k |BCS\rangle = 0, \quad \text{for all } k \gtrless 0, \\ &E_k = \langle BCS|\alpha_k H' \alpha_k^\dagger |BCS\rangle - \langle BCS|H'|BCS\rangle = \sqrt{\tilde{\epsilon}_k^2 + \Delta_k^2}. \end{aligned} \tag{5.29}$$

In case of quasi-particle excited state $|k\rangle = \alpha_k^\dagger |BCS\rangle$, gives particle number

$$\langle k|\hat{N}|k\rangle = N + u_k^2 - v_k^2 \tag{5.30}$$

However, Because the energy expectation value $\langle \psi_N|H|\psi_N\rangle$ is strongly depends on particle number simply taking $\langle k|H|k\rangle$ with wrong particle number would results in wrong energy. Thus the energy

[6] Thus, for real values of u, v

$$\begin{aligned} \alpha_k &= u_k a_k - v_k a_{\bar{k}}^\dagger, \\ \alpha_{\bar{k}} &= u_k a_{\bar{k}} + v_k a_k^\dagger. \end{aligned} \tag{5.24}$$

$$\alpha_k \alpha_{\bar{k}} |-\rangle = (u_k a_k - v_k a_{\bar{k}}^\dagger)(u_k a_{\bar{k}} + v_k a_k^\dagger)|-\rangle = (u_k v_k a_k a_k^\dagger - v_k v_k a_{\bar{k}}^\dagger a_k^\dagger)|-\rangle \propto (u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)|-\rangle \tag{5.25}$$

of excited state have to be corrected(or readjust chemical potential for different levels or use $H' = H - \lambda\hat{N}$ for energy expectation value.).

$$\begin{aligned} E^k_{N+1} &= \langle k|H|k\rangle + \frac{dE}{dN}(N+1-\langle k|\hat{N}|k\rangle) \\ &= \langle k|H-\lambda\hat{N}|k\rangle + \lambda(N+1) \\ &= E^{GS}_N + \lambda + E_k \end{aligned} \tag{5.31}$$

On the other hand, the ground state of odd particle system also can be written as

$$\alpha^\dagger_{k_1}|BCS\rangle = a^\dagger_{k_1}\prod_{k\neq k_1>0}(u_k + v_k a^\dagger_k a^\dagger_{\bar{k}})|-\rangle. \tag{5.32}$$

Thus, unpaired particle sitting on k_1 blocks the state. ($v_{k_1} = 1$ and $v_{\bar{k}_1} = 0$ while other u_k, v_k with $k \neq k_1$ are determined by variational principle having smooth variation.) Because of this blocking, the equation of variational method to determine u_k, v_k has difference from even-even ground state $|BCS\rangle$ in the summation should exclude k_1.

$$\Delta = G\sum_{k\neq k_1} u_k v_k \tag{5.33}$$

The level k_1 has to be excluded from the sum because it cannot contribute to the pairing energy. Also chemical potential should be determined from $N = 1 + 2\sum_{k\neq k_1} v_k^2$. These changes in Δ , u and v for odd-nuclei are called **blocking** effect.

The effect of pairing or Δ_k is only important near the Fermi level. In shell model, pairing is only important for partially filled levels.

Chapter 6

Hartree-Fock-Bogoliubov theory

As like BCS theory, paring interaction can have a large effects on the ground state of nuclear system. In Hartree-Fock-Bogoliubov theory, we extends the variational form of ground state to allow the paring between different energy states. But, still it is a variational approach to minimize the energy expectation value.

As an ansatz, the ground state of the system of particles is assumed as a independent quasi-particle states, $|\Phi\rangle$. Then, the energy expectation value of $\langle\Phi|\hat{H}|\Phi\rangle$ becomes a functional of densities, $E[\rho,\tilde{\rho},\tau,J,\tilde{J},\cdots]$ where densities are defined as

$$\begin{aligned}\rho(\boldsymbol{r}\sigma q,\boldsymbol{r}'\sigma' q') &= \langle\Phi|a^\dagger_{\boldsymbol{r}'\sigma' q'}a_{\boldsymbol{r}\sigma q}|\Phi\rangle,\\ \tilde{\rho}(\boldsymbol{r}\sigma q,\boldsymbol{r}'\sigma' q') &= -2\sigma'\langle\Phi|a_{\boldsymbol{r}'-\sigma' q'}a_{\boldsymbol{r}\sigma q}|\Phi\rangle = -2\sigma'\kappa(\boldsymbol{r}\sigma q,\boldsymbol{r}'-\sigma' q').\end{aligned} \tag{6.1}$$

with particle operators $a^\dagger, a$. (Note that if $|\Phi\rangle$ were H.F. states, $\tilde{\rho}$ would be zero.)

In case of time-even quasiparticle states, $\hat{T}|\Phi\rangle = |\Phi\rangle$, from relation,

$$\hat{T}^\dagger a^\dagger_{\boldsymbol{r}\sigma}\hat{T} = 2 - \sigma a^\dagger_{\boldsymbol{r}-\sigma}, \tag{6.2}$$

we get relations between densities, (they are both hermitian and time-even),

$$\begin{aligned}&\rho^*(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') = \rho(\boldsymbol{r}'\sigma',\boldsymbol{r}\sigma), \quad \rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') = 4\sigma\sigma'\rho(\boldsymbol{r}'-\sigma',\boldsymbol{r}-\sigma),\\ &\tilde{\rho}^*(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') = \tilde{\rho}(\boldsymbol{r}'\sigma',\boldsymbol{r},\sigma), \quad \tilde{\rho}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') = 4\sigma\sigma'\tilde{\rho}(\boldsymbol{r}'-\sigma',\boldsymbol{r}-\sigma).\end{aligned} \tag{6.3}$$

Let us define product of densities as

$$(\rho\cdot\tilde{\rho})(\boldsymbol{r}_1\sigma_1,\boldsymbol{r}_2\sigma_2) = \int d\boldsymbol{r}\sum_\sigma \rho(\boldsymbol{r}_1\sigma_1,\boldsymbol{r}\sigma)\tilde{\rho}(\boldsymbol{r}\sigma,\boldsymbol{r}_2\sigma_2). \tag{6.4}$$

For independent quasi-particle states $|\Phi\rangle$, we have (?) commutation ,

$$\rho\cdot\tilde{\rho} - \tilde{\rho}\cdot\rho = 0, \tag{6.5}$$

and relation(?)

$$\rho\cdot\rho + \tilde{\rho}\cdot\tilde{\rho} = \rho. \tag{6.6}$$

In other words, the variation of energy density functional $E[\rho,\tilde{\rho}]$ have constraints on ρ and $\tilde{\rho}$. These relations can be written in a compact way as

$$\mathcal{R}\cdot\mathcal{R} = \mathcal{R}, \quad \mathcal{R} = \begin{pmatrix} \rho & \tilde{\rho} \\ \tilde{\rho} & \delta(\boldsymbol{r}-\boldsymbol{r}')\delta_{\sigma\sigma'} - \rho \end{pmatrix} \tag{6.7}$$

In other words, one have to vary the energy under constraints, $\mathcal{R}\cdot\mathcal{R}=\mathcal{R}$. With another constraint of conservation of particle numbers, with lagrange multiplier λ, the variational equation becomes

$$\delta\left[E'\left[\mathcal{R},\lambda\right]-\mathrm{tr}(\Lambda(\mathcal{R}^2-\mathcal{R}))\right]=0. \tag{6.8}$$

where Λ matrix is a Lagrange multiplier.

According to HFB paper, this variational relation gives, HFB equation as (How? It is not clear how this can be derived from above expression)

$$[\mathcal{W},\mathcal{R}]=0,\quad \mathcal{W}=\begin{pmatrix} h-\lambda & \tilde{h} \\ \tilde{h} & -h+\lambda \end{pmatrix} \tag{6.9}$$

with ($\lambda<0$ will be assumed)

$$h(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma')=\frac{\delta E}{\delta\rho(\boldsymbol{r}'\sigma',\boldsymbol{r}\sigma)},\quad \tilde{h}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma')=\frac{\delta E}{\delta\tilde{\rho}(\boldsymbol{r}'\sigma',\boldsymbol{r}\sigma)} \tag{6.10}$$

In any case, to solve $[\mathcal{W},\mathcal{R}]=0$, one may diagonalize $\mathcal{W}$ and construct R as a projection of set of eigenstates of $\mathcal{W}$, the occupied quasiparticle states.(What does it mean? In other words, eigenstate of $\mathcal{W}$ corresponds to quasi-particle states and by constructing densities in $\mathcal{R}$ with them, one can obtain self-consistent solution of $\mathcal{R}$ and $\mathcal{W}$ which satisfies $[\mathcal{W},\mathcal{R}]=0$.)

The eigen value equation of $\mathcal{W}$ can be written as

$$\int d^3\boldsymbol{r}'\sum_{\sigma'}\begin{pmatrix} h(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') & \tilde{h}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') \\ \tilde{h}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') & -h(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') \end{pmatrix}\begin{pmatrix} \varphi_1(E,\boldsymbol{r}'\sigma') \\ \varphi_2(E,\boldsymbol{r}'\sigma') \end{pmatrix}=\begin{pmatrix} E+\lambda & 0 \\ 0 & E-\lambda \end{pmatrix}\begin{pmatrix} \varphi_1(E,\boldsymbol{r}\sigma) \\ \varphi_2(E,\boldsymbol{r}\sigma) \end{pmatrix} \tag{6.11}$$

Considering asymptotic form of solution, and require at least one solution should be bounded, we should choose $\lambda<0$. (Then , wave functions are such that φ_1 is scattering but φ_2 is bounded for $E>-\lambda$, φ_1 and φ_2 are both bounded for $\lambda<E<-\lambda$, φ_1 is bounded but φ_2 is scattering for $E>-\lambda$.)

The eigenvalues are in pairs of opposite energies and there are doubly degenerate solutions,

$$\varphi_1(-E,\boldsymbol{r}\sigma)=\varphi_2(E,\boldsymbol{r}\sigma),\quad \varphi_2(-E,\boldsymbol{r}\sigma)=-\varphi_1(E,\boldsymbol{r}\sigma) \tag{6.12}$$

$$\varphi_1'(E,\boldsymbol{r}\sigma)=-2\sigma\varphi_1^*(E,\boldsymbol{r}-\sigma),\quad \varphi_2'(E,\boldsymbol{r}\sigma)=-2\sigma\varphi_2^*(E,\boldsymbol{r}-\sigma). \tag{6.13}$$

In other words, if E is an eigenvalue, $-E$ is also an eigenvalue. If φ_1,φ_2 are eigenstate with energy E, φ_1',φ_2' are also eigenstate at the same energy. Also, there will be discrete eigen-values and continuum. ($\lambda<0$ is assumed. $|E|<-\lambda$ are discrete states and $|E|>-\lambda$ are continuous.)

One can construct $\mathcal{R}$ from eigenstates of $\mathcal{W}$,

$$\mathcal{R}=\sum\!\!\!\!\!\!\int dn(E_{occ})\begin{pmatrix} \varphi_1(E,\boldsymbol{r}\sigma) \\ \varphi_2(E,\boldsymbol{r}\sigma) \end{pmatrix}\otimes\left(\varphi_1^*(E,\boldsymbol{r}'\sigma'),\ \varphi_2^*(E,\boldsymbol{r}'\sigma')\right). \tag{6.14}$$

where sum is over the occupied discrete part of the spectrum and integration over the occupied continuous. This implies the relations of φ and densities as

$$\begin{aligned} \rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') &= \sum\!\!\!\!\!\!\int dn(E_{occ})\varphi_1(E,\boldsymbol{r}\sigma)\varphi_1^*(E,\boldsymbol{r}'\sigma'), \\ \tilde{\rho}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') &= \sum\!\!\!\!\!\!\int dn(E_{occ})\varphi_1(E,\boldsymbol{r}\sigma)\varphi_2^*(E,\boldsymbol{r}'\sigma'). \end{aligned} \tag{6.15}$$

and requirements

$$\begin{aligned} &\sum\!\!\!\!\!\!\int dn(E_{occ})\left[\varphi_1(E,\boldsymbol{r}\sigma)\varphi_1(E,\boldsymbol{r}'\sigma')+\varphi_2(E,\boldsymbol{r}\sigma)\varphi_2(E,\boldsymbol{r}'\sigma')\right]=\delta(\boldsymbol{r}-\boldsymbol{r}')\delta_{\sigma\sigma'}, \\ &\sum\!\!\!\!\!\!\int dn(E_{occ})\left[\varphi_1(E,\boldsymbol{r}\sigma)\varphi_2^*(E,\boldsymbol{r}'\sigma')-\varphi_2(E,\boldsymbol{r}\sigma)\varphi_1^*(E,\boldsymbol{r}'\sigma')\right]=0. \end{aligned} \tag{6.16}$$

To satisfy the completeness relation, one must occupy all states with $E<0$ to describe ground state. (Existence of solution does not mean they are occupied. To describe ground state, occupied states should give minumum energy.) Then, for positive quasiparticle energy E states, by using symmetry for $E \to -E$,

$$\begin{aligned}\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') &= \sum\!\!\!\!\!\!\int_0^\infty dn(E_{occ})\varphi_1(E,\boldsymbol{r}\sigma)\varphi_1^*(E,\boldsymbol{r}'\sigma') + \sum\!\!\!\!\!\!\int_{-\infty}^0 dn(E_{occ})\varphi_1(E,\boldsymbol{r}\sigma)\varphi_1^*(E,\boldsymbol{r}'\sigma') \\ &= \sum\!\!\!\!\!\!\int_0^\infty dn(E_{occ})\varphi_2(E,\boldsymbol{r}\sigma)\varphi_2^*(E,\boldsymbol{r}'\sigma')(?) \end{aligned} \tag{6.17}$$

and by discretization of continuum, density can be written as

$$\begin{aligned}\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') &= \sum_{0<E_n<E_{max}} \varphi_2(E_n,\boldsymbol{r}\sigma)\varphi_2^*(E_n,\boldsymbol{r}'\sigma'), \\ \tilde{\rho}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') &= -\sum_{0<E_n<E_{max}} \varphi_2(E_n,\boldsymbol{r}\sigma)\varphi_1^*(E_n,\boldsymbol{r}'\sigma'). \end{aligned} \tag{6.18}$$

In other words, φ_2 is more close to particle states than φ_1.

A canonical basis is defined as a eigenstate of density matrix,

$$\int d^3\boldsymbol{r}\sum_{\sigma'}\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma')\psi_n(\boldsymbol{r}',\sigma') = v_n^2\psi_n(\boldsymbol{r}\sigma). \tag{6.19}$$

This canonical basis ψ_n are physical and entirely localized. (ρ and its $\varphi_2(E,\boldsymbol{r}\sigma)$ for $E<\lambda$ are non-localized.)

In HF-BCS, pairing field is assumed to be local.

$$\tilde{h}_{BCS}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') = -\Delta\delta(\boldsymbol{r}-\boldsymbol{r}')\delta_{\sigma\sigma'} \tag{6.20}$$

In this case, $\varphi_{1,2}$ are proportional to the canonical basis wave function $\psi_n(E>0)$,

$$\varphi_1(E_n,\boldsymbol{r}\sigma) = u_n\psi_n(\boldsymbol{r}\sigma), \quad \varphi_2(E_n,\boldsymbol{r}\sigma) = v_n\psi_n(\boldsymbol{r}\sigma), \tag{6.21}$$

which are eigen functions of the field h,

$$\int d^3\boldsymbol{r}'\sum_{\sigma'}h(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma')\psi_n(\boldsymbol{r}'\sigma') = \epsilon_n\psi_n(\boldsymbol{r}\sigma) \tag{6.22}$$

while E,u_n, v_n are related to ϵ_n, Δ, λ by the BCS formula.

6.1 Quasi Particle

Let us consider quasi-particle operators, which is mixture of particle operators in a model space $1\ldots M$,

$$\beta_k^\dagger = \sum_l U_{lk}c_l^\dagger + V_{lk}c_l, \quad \beta_k = \sum_l U_{lk}^*c_l + V_{lk}^*c_l^\dagger. \tag{6.23}$$

By introducing a vector notation for β and c,

$$\beta_{M\times 1} = \begin{pmatrix}\beta_1\\ \beta_2\\ \vdots\\ \beta_M\end{pmatrix}, \quad \beta_{M\times 1}^\dagger = \begin{pmatrix}\beta_1^\dagger\\ \beta_2^\dagger\\ \vdots\\ \beta_M^\dagger\end{pmatrix} \tag{6.24}$$

we can write in a $2M \times 2M$matrix form,

$$\begin{pmatrix} \beta_{M\times 1} \\ \beta^\dagger_{M\times 1} \end{pmatrix} = \begin{pmatrix} U^\dagger_{M\times M} & V^\dagger_{M\times M} \\ V^T_{M\times M} & U^T_{M\times M} \end{pmatrix} \begin{pmatrix} c_{M\times 1} \\ c^\dagger_{M\times 1} \end{pmatrix} = W^\dagger_{2M\times 2M} \begin{pmatrix} c_{M\times 1} \\ c^\dagger_{M\times 1} \end{pmatrix}. \tag{6.25}$$

We require the matrix W to be unitary,

$$W = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}, \quad W^\dagger W = W W^\dagger = 1 \tag{6.26}$$

Thus, get relations

$$\begin{aligned} U^\dagger U + V^\dagger V = 1, \quad UU^\dagger + V^* V^T = 1, \\ U^T V + V^T U = 0, \quad UV^\dagger + V^* U^T = 0, \end{aligned} \tag{6.27}$$

which allows inverse transform

$$c^\dagger_l = \sum_k U^*_{lk}\beta^\dagger_k + V_{lk}\beta_k, \quad c_l = \sum_k U_{lk}\beta_k + V^*_{lk}\beta^\dagger_k, \tag{6.28}$$

and

$$\begin{pmatrix} c \\ c^\dagger \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = W \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} \tag{6.29}$$

Let us assume that the ground state is defined such as

$$\beta_k |\Phi_{HFB}\rangle = 0 \quad \text{for all } k = 1, \ldots, M. \tag{6.30}$$

Let us define density matrix which is related with HFB wave function $|\Phi_{HFB}\rangle$, normal density matrix and abnormal density matrix

$$\rho_{ll'} \equiv \langle \Phi_{HFB} | c^\dagger_{l'} c_l | \Phi_{HFB}\rangle, \quad \kappa_{ll'} \equiv \langle \Phi_{HFB} | c_{l'} c_l | \Phi_{HFB}\rangle. \tag{6.31}$$

Be careful that the operators are particle operators and order of index.

It can be written, in terms of matrix

$$\begin{aligned} \rho_{ll'} &= \langle \Phi_{HFB}| \left(\sum_k U^*_{l'k}\beta^\dagger_k + V_{l'k}\beta_k \right) \left(\sum_{k'} U_{lk'}\beta_{k'} + V^*_{lk'}\beta^\dagger_{k'} \right) |\Phi_{HFB}\rangle \\ &= \sum_k V_{l'k}V^*_{lk} = (V^* V^T)_{ll'} = \delta_{ll'} - (UU^\dagger)_{ll'}, \\ \kappa_{ll'} &= \langle \Phi_{HFB}| \left(\sum_k U_{l'k}\beta_k + V^*_{l'k}\beta^\dagger_k \right) \left(\sum_{k'} U_{lk'}\beta_{k'} + V^*_{lk'}\beta^\dagger_{k'} \right) |\Phi_{HFB}\rangle \\ &= \sum_k U_{l'k}V^*_{lk} = (V^* U^T)_{ll'} = (-UV^\dagger)_{ll'} \end{aligned} \tag{6.32}$$

Note here that ρ is Hermitian but κ is skew Hermitian.

Another derivation of HFB equation(Need verification and clarify.):

In fact, we can introduce generalized density matrix such as

$$\mathcal{R} = \begin{pmatrix} \langle \Phi_{HFB}|c^\dagger_{l'}c_l|\Phi_{HFB}\rangle & \langle \Phi_{HFB}|c_{l'}c_l|\Phi_{HFB}\rangle \\ \langle \Phi_{HFB}|c^\dagger_{l'}c^\dagger_l|\Phi_{HFB}\rangle(?) & \langle \Phi_{HFB}|c_{l'}c^\dagger_l|\Phi_{HFB}\rangle(?) \end{pmatrix} = \begin{pmatrix} \rho_{ll'} & \kappa_{ll'} \\ \kappa^\dagger(?) & (1-\rho)_{ll'}(?) \end{pmatrix} \tag{6.33}$$

The minimization of energy $E'[\mathcal{R},\lambda] = \langle\Phi_{HFB}|H-\lambda N|\Phi_{HFB}\rangle$ under requirement of the ground state is the quasi-particle vacuum gives,

$$\mathcal{R}\cdot\mathcal{R} = \mathcal{R} \tag{6.34}$$

leads to HFB equation,

$$\delta\left[E'\left[\mathcal{R},\lambda\right] - \mathrm{tr}(\Lambda(\mathcal{R}^2-\mathcal{R}))\right] = 0 \tag{6.35}$$

where Λ matrix is a Lagrange multiplier.

6.1.1 Bloch-Messiah theorem and cannonical basis

Unitary matrix W can always be decomposed into three matrices,

$$\begin{aligned}
\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} &= \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix}\begin{pmatrix} c \\ c^\dagger \end{pmatrix} = W^\dagger \begin{pmatrix} c \\ c^\dagger \end{pmatrix}, \\
W &= \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix}\begin{pmatrix} \bar{U} & \bar{V} \\ \bar{V} & \bar{U} \end{pmatrix}\begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix}
\end{aligned} \tag{6.36}$$

such as $\bar{U}^\dagger = \bar{U}$, $\bar{V}^\dagger = -\bar{V}$, or

$$U = D\bar{U}C, \quad V = D^*\bar{V}C. \tag{6.37}$$

In other words, the transformation can be done in three-steps

$$\begin{aligned}
\begin{pmatrix} a \\ a^\dagger \end{pmatrix} &= \begin{pmatrix} D^\dagger & 0 \\ 0 & D^T \end{pmatrix}\begin{pmatrix} c \\ c^\dagger \end{pmatrix}, \\
\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} &= \begin{pmatrix} \bar{U}^\dagger & \bar{V}^\dagger \\ \bar{V}^\dagger & \bar{U}^\dagger \end{pmatrix}\begin{pmatrix} a \\ a^\dagger \end{pmatrix}, \\
\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} &= \begin{pmatrix} C^\dagger & 0 \\ 0 & C^T \end{pmatrix}\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix},
\end{aligned} \tag{6.38}$$

The D-transformation $a^\dagger$ is called connonical basis, corresponding to HF states. In this basis, the density matrix is diagonal.

A special Bogoliubov transformation $\bar{U}$ and $\bar{V}$ involves paired levels $(p,\bar{p})$ and "blocked" levels (i,m)(Each is a $M\times M$ matrix is block diagonal. Some levels are occupied, some are empty, and some levels are paired.). This corresponds to BCS pairing.

$$\begin{aligned}
\alpha_p^\dagger &= u_p a_p^\dagger - v_p a_{\bar{p}}, \\
\alpha_{\bar{p}}^\dagger &= u_p a_{\bar{p}}^\dagger + v_p a_p,
\end{aligned} \tag{6.39}$$

$$\begin{aligned}
&\alpha_i^\dagger = a_i, \quad \alpha_m^\dagger = a_m^\dagger, \quad \text{occupied } v_i = 1, u_i = 0, \\
&\alpha_i = a_i^\dagger, \quad \alpha_m = a_m, \quad \text{empty } v_m = 0, u_m = 1,
\end{aligned} \tag{6.40}$$

The C-transformation mix quasi-particle themselves.

6.2 Hamiltonian for quasi-particle excitation

From the Hamiltonian given for particles, we may obtain the Hamiltonian in quasi-particle form using the inverse transformation.

6.2.1 One-body Operator

$$\hat{F} = \sum_{ll'} f_{ll'} c_l^\dagger c_{l'} + \frac{1}{2}(g_{ll'} c_l^\dagger c_{l'}^\dagger + h.c.) \tag{6.41}$$

from inverse transformation, the first term (be careful for the order ll' is different from density matrix definition)

$$\begin{aligned}
\sum_{ll'} f_{ll'} c_l^\dagger c_{l'} &= \sum_{ll'} f_{ll'} \left(\sum_k U_{lk}^* \beta_k^\dagger + V_{lk} \beta_k \right) \left(\sum_{k'} U_{l'k'} \beta_{k'} + V_{l'k'}^* \beta_{k'}^\dagger \right) \\
&= \sum_{ll'} \sum_{kk'} f_{ll'} U_{lk}^* U_{l'k'} \beta_k^\dagger \beta_{k'} + f_{ll'} U_{lk}^* V_{l'k'}^* \beta_k^\dagger \beta_{k'}^\dagger + f_{ll'} V_{lk} U_{l'k'} \beta_k \beta_{k'} + f_{ll'} V_{lk} V_{l'k'}^* \beta_k \beta_{k'}^\dagger \\
&= \sum_{ll'} \sum_{kk'} f_{ll'} V_{lk} V_{l'k'}^* \delta_{kk'} + f_{ll'} U_{lk}^* U_{l'k'} \beta_k^\dagger \beta_{k'} - f_{ll'} V_{lk} V_{l'k'}^* \beta_{k'}^\dagger \beta_k \\
&\quad + f_{ll'} U_{lk}^* V_{l'k'}^* \beta_k^\dagger \beta_{k'}^\dagger + f_{ll'} V_{lk} U_{l'k'} \beta_k \beta_{k'} \\
&= \sum_{kk'} (V^T f V^*)_{kk'} \delta_{kk'} + (U^\dagger f U)_{kk'} \beta_k^\dagger \beta_{k'} - (V^\dagger f^T V)_{kk'} \beta_k^\dagger \beta_{k'} \\
&\quad + (U^\dagger f V^*)_{kk'} \beta_k^\dagger \beta_{k'}^\dagger + (V^T f U)_{kk'} \beta_k \beta_{k'}
\end{aligned} \tag{6.42}$$

where the relation $\beta_k \beta_{k'}^\dagger = -\beta_{k'}^\dagger \beta_k + \delta_{kk'}$ is used and rename parameters. We may write the last line in a symmetric form by using

$$\begin{aligned}
\sum_{kk'} (U^\dagger f V^*)_{kk'} \beta_k^\dagger \beta_{k'}^\dagger &= -\sum_{kk'} (U^\dagger f V^*)_{kk'} \beta_{k'}^\dagger \beta_k^\dagger = -\sum_{kk'} (V^\dagger f^T U^*)_{kk'} \beta_k^\dagger \beta_{k'}^\dagger \\
&= \frac{1}{2} \sum_{kk'} (U^\dagger f V^* - V^\dagger f^T U^*)_{kk'} \beta_k^\dagger \beta_{k'}^\dagger
\end{aligned} \tag{6.43}$$

similarly for the $\beta_k \beta_{k'}$.

Then the other terms becomes [1]

$$\begin{aligned}
\sum_{ll'}\frac{1}{2}(g_{ll'}c_l^\dagger c_{l'}^\dagger + h.c.) &= \sum_{ll'}\frac{1}{2}g_{ll'}\left(\sum_k U_{lk}^*\beta_k^\dagger + V_{lk}\beta_k\right)\left(\sum_{k'} U_{l'k'}^*\beta_{k'}^\dagger + V_{l'k'}\beta_{k'}\right) + (h.c.) \\
&= \frac{1}{2}\sum_{ll'}\sum_{kk'} g_{ll'}U_{lk}^*V_{l'k'}\beta_k^\dagger\beta_{k'} + g_{ll'}V_{lk}U_{l'k'}^*\beta_k\beta_{k'}^\dagger + g_{ll'}U_{lk}^*U_{l'k'}^*\beta_k^\dagger\beta_{k'}^\dagger + g_{ll'}V_{lk}V_{l'k'}\beta_k\beta_{k'} + (h.c.) \\
&= \frac{1}{2}\sum_{kk'}(U^\dagger gV)_{kk'}\beta_k^\dagger\beta_{k'} + (V^T gU^*)_{kk'}\beta_k\beta_{k'}^\dagger + (U^\dagger gU^*)_{kk'}\beta_k^\dagger\beta_{k'}^\dagger + (V^T gV)_{kk'}\beta_k\beta_{k'} \\
&\quad +(V^\dagger g^\dagger U)_{kk'}\beta_k^\dagger\beta_{k'} + (U^T g^\dagger V^*)_{kk'}\beta_k\beta_{k'}^\dagger + (U^T g^\dagger U)_{kk'}\beta_k\beta_{k'} + (V^\dagger g^\dagger V^*)_{kk'}\beta_k^\dagger\beta_{k'}^\dagger \\
&= \frac{1}{2}\sum_{kk'}(U^\dagger gV + V^\dagger g^\dagger U - V^T gU^* - U^T g^\dagger V^*)_{kk'}\beta_k^\dagger\beta_{k'} + (V^T gU^* + U^T g^\dagger V^*)_{kk'}\delta_{kk'} \\
&\quad +(U^\dagger gU^* + V^\dagger g^\dagger V^*)_{kk'}\beta_k^\dagger\beta_{k'}^\dagger + (V^T gV + U^T g^\dagger U)_{kk'}\beta_k\beta_{k'} \qquad (6.47)
\end{aligned}$$

Thus, we can rewrite

$$\hat{F} = F_0 + \sum_{kk'}F_{kk'}^{11}\beta_k^\dagger\beta_{k'} + \frac{1}{2}\sum_{kk'}(F_{kk'}^{20}\beta_k^\dagger\beta_{k'}^\dagger + h.c.), \qquad (6.48)$$

where, [2]

$$\begin{aligned}
F_0 &= \sum_{kk'}\left(V^T fV^* + \frac{1}{2}(V^T gU^* - U^T g^* V^*)\right)_{kk'} \\
&= \mathrm{Tr}(f\rho) - \frac{1}{2}\mathrm{Tr}(g\kappa^* + g^*\kappa), \\
F_{kk'}^{11} &= \left(U^\dagger fU - V^\dagger f^T V + U^\dagger gV - V^\dagger g^* U\right)_{kk'}, \\
F_{kk'}^{20} &= \left(U^\dagger fV^* - V^\dagger f^T U^* + U^\dagger gU^* - V^\dagger g^* V^*\right)_{kk'} \qquad (6.49)
\end{aligned}$$

6.2.2 Two-body Operator

Two-body operator case,

$$\frac{1}{4}\sum_{l_1l_2l_3l_4}\bar{v}_{l_1l_2l_3l_4}c_{l_1}^\dagger c_{l_2}^\dagger c_{l_4}c_{l_3} \qquad (6.50)$$

proof to be added later

---

[1] For convenience,

$$c_l^\dagger = (U^*\beta^\dagger + V\beta)_l, \quad c_l = (U\beta + V^*\beta^\dagger)_l \qquad (6.44)$$

Noet here that congugation changes $\beta \leftrightarrow \beta^\dagger$ and $(U, V) \leftrightarrow (U^*, V^*)$ but does not change order.

On the other hand ,

$$\left(\sum_{ll'}f_{ll'}c_l^\dagger c_{l'}\right)^\dagger = \sum_{ll'}f_{ll'}^* c_{l'}^\dagger c_l = \sum_{ll'}f_{ll'}^\dagger c_l^\dagger c_{l'}, \qquad (6.45)$$

where hermitian conjugation change order of c operators. Thus, (g must be such as $g^\dagger = -g^*$)

$$\left(\sum_{ll'}g_{ll'}c_l^\dagger c_{l'}^\dagger\right)^\dagger = \sum_{ll'}g_{ll'}^* c_{l'}c_l = \sum_{ll'}g_{ll'}^\dagger c_l c_{l'} = -\sum_{ll'}g_{ll'}^* c_l c_{l'} \qquad (6.46)$$

[2] Use $g^\dagger = -g^*$ and Note $U^\dagger gV + V^\dagger g^\dagger U$ is hermitian and thus gives factor2.

6.2.3 Hamiltonian

$$\begin{aligned}
\hat{H} &= \sum_{l_1 l_2} \epsilon_{l_1 l_2} c^\dagger_{l_1} c_{l_2} + \frac{1}{4} \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} c^\dagger_{l_1} c^\dagger_{l_2} c_{l_4} c_{l_3} \\
&= H^0 + \sum_{kk'} H^{11}_{kk'} \beta^\dagger_k \beta_{k'} \\
&\quad + \frac{1}{2} \sum_{kk'} (H^{20}_{kk'} \beta^\dagger_k \beta^\dagger_{k'} + h.c.) \\
&\quad + \sum_{k_1 k_2 k_3 k_4} (H^{40}_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4} + h.c.) \\
&\quad + \sum_{k_1 k_2 k_3 k_4} (H^{31}_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta_{k_4} + h.c.) \\
&\quad + \frac{1}{4} \sum_{k_1 k_2 k_3 k_4} H^{22}_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta_{k_4} \beta_{k_3}. \qquad (6.51)
\end{aligned}$$

With definitions

$$\begin{aligned}
h &= \epsilon + \Gamma, \\
\Gamma_{lm} &= \sum_{pq} \bar{v}_{lqmp} \rho_{pq} := \mathrm{Tr}_1(\bar{v}\rho)_{lm}, \\
\Delta_{lm} &= \frac{1}{2} \sum_{pq} \bar{v}_{lmpq} \kappa_{pq} := -\frac{1}{2} \mathrm{Tr}_2(\bar{v}\kappa)_{lm} \qquad (6.52)
\end{aligned}$$

Matrix elements are

$$\begin{aligned}
H^0 &= \mathrm{Tr}(\epsilon\rho + \frac{1}{2}\Gamma\rho - \frac{1}{2}\Delta\kappa^*) \\
&= \mathrm{Tr}(\epsilon\rho) + \frac{1}{2}\mathrm{Tr}_1\mathrm{Tr}_1(\rho\bar{v}\rho) + \frac{1}{4}\mathrm{Tr}_2\mathrm{Tr}_2(\kappa^*\bar{v}\kappa), \\
H^{11} &= U^\dagger h U - V^\dagger h^T V + U^\dagger \Delta V - V^\dagger \Delta^* U, \\
H^{20} &= U^\dagger h V^* - V^\dagger h^T U^* + U^\dagger \Delta U^* - V^\dagger \Delta^* V^*, \qquad (6.53)
\end{aligned}$$

$$\begin{aligned}
H^{40}_{k_1 k_2 k_3 k_4} &= \frac{1}{4} \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} U^*_{l_1 k_1} U^*_{l_2 k_2} V^*_{l_4 k_3} V^*_{l_3 k_4}, \\
H^{31}_{k_1 k_2 k_3 k_4} &= \frac{1}{2} \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} \left(U^*_{l_1 k_1} V^*_{l_4 k_2} V^*_{l_3 k_3} V_{l_2 k_4} + V^*_{l_3 k_1} U^*_{l_2 k_2} U^*_{l_1 k_3} U_{l_4 k_4} \right), \\
H^{22}_{k_1 k_2 k_3 k_4} &= \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} \big((U^*_{l_1 k_1} V^*_{l_4 k_2} V_{l_2 k_3} U_{l_3 k_4} - (k_1 \leftrightarrow k_2)) - (k_3 \leftrightarrow k_4) \\
&\quad + U^*_{l_1 k_1} U^*_{l_2 k_2} U_{l_3 k_3} U_{l_4 k_4} + V^*_{l_3 k_1} V^*_{l_4 k_2} V_{l_1 k_3} V_{l_2 k_4} \big) \qquad (6.54)
\end{aligned}$$

The HF-BCS corresponds to set U and V to be diagonal, $U_{l_1 l_2} = U_{l_1}\delta_{l_1 l_2}$, $V_{l_1 l_2} = V_{l_1}\delta_{l_1 l_2}$ and ignoring H^{40}, H^{31}, H^{22}.

The HF corresponds to U_k or V_k is zero depending on k is above or below fermi level and take H^0 term for ground state energy.

The RPA considers excitation from ground state $|\Phi_{HFB}\rangle$ too, but usually only consider some set of excitations.

6.3 HFB equation

Since the HFB ground state is $\beta|\Phi_{HFB}\rangle = 0$, the energy expectation value of HFB state is

$$\langle\Phi_{HFB}|H|\Phi_{HFB}\rangle = E^{HFB}[\rho,\kappa] = H^0 = \mathrm{Tr}(\epsilon\rho + \frac{1}{2}\Gamma\rho - \frac{1}{2}\Delta\kappa^*) \tag{6.55}$$

However, we need to first determine what is the $U_{M\times M}$ and $V_{M\times M}$. In HFB theory, we obtain the variational solution which minimize the HFB energy. Thus, as like HF, it is a variational approximation to the tru ground state. But as like BCS, HFB state does not conserve particle number N, one minimizes expectation value of $\langle\Phi_{HFB}|H' = H - \lambda N|\Phi_{HFB}\rangle$ with lagrange multiplier λ, instead of $\langle\Phi_{HFB}|H|\Phi_{HFB}\rangle$.

There are may ways to derive HFB theory from variational equation,

$$\delta\frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle} \tag{6.56}$$

with small variation $|\delta\Phi\rangle$.

6.3.1 Thouless theorem

According to Touless theorem, variation of HFB state $|\Phi'\rangle = |\Phi\rangle + |\delta\Phi\rangle$ can be expressed

$$|\Phi'\rangle = \exp\left(\sum_{k<k'} Z_{kk'}\beta^\dagger_k\beta^\dagger_{k'}\right)|\Phi\rangle \tag{6.57}$$

The, from Hamiltonian in quasi-particle operator form,

$$H = H^0 + \sum_{k_1k_2} H^{11}_{k_1k_2}\beta^\dagger_{k_1}\beta_{k_2} + \sum_{k_1<k_2}(H^{20}_{k_1k_2}\beta^\dagger_{k_1}\beta^\dagger_{k_2} + h.c.) + H_{int} \tag{6.58}$$

we get

$$\frac{\langle\Phi'|H|\Phi'\rangle}{\langle\Phi'|\Phi'\rangle} = H^0 + \begin{pmatrix} H^{20*} & H^{20}\end{pmatrix}\begin{pmatrix} Z \\ Z^*\end{pmatrix} + \frac{1}{2}\begin{pmatrix} Z^* & Z\end{pmatrix}\begin{pmatrix} A & B \\ B^* & A^*\end{pmatrix}\begin{pmatrix} Z \\ Z^*\end{pmatrix}, \tag{6.59}$$

where index runs over all pairs $k < k'$, and

$$\begin{aligned} H^0 &= \langle\Phi|H|\Phi\rangle, & A_{kk'll'} &= \langle\Phi|[\beta_{k'}\beta_k,[H,\beta^\dagger_l\beta^\dagger_{l'}]]|\Phi\rangle, \\ H^{20}_{kk'} &= \langle\Phi|[\beta_{k'}\beta_k,H]|\Phi\rangle, & B_{kk'll'} &= -\langle\Phi|[\beta_{k'}\beta_k,[H,\beta_{l'}\beta_l]]|\Phi\rangle. \end{aligned} \tag{6.60}$$

then

$$\frac{\partial}{\partial Z^*_{kk'}}\frac{\langle\Phi'|H|\Phi'\rangle}{\langle\Phi'|\Phi'\rangle}\Big|_{Z=0} = H^{20}_{kk'} = 0, \tag{6.61}$$

By the Bogoliubov transformation, one can make $H^{20} = 0$ and diagnonalize H^{11} at the same time. This corresponds to diagonalization of supermatrix,

$$\begin{pmatrix} H^{11} & H^{20} \\ -H^{20*} & -H^{11*}\end{pmatrix} = \begin{pmatrix} \langle\Phi|\{[\beta_k,H],\beta^\dagger_{k'}\}|\Phi\rangle & \langle\Phi|\{[\beta_k,H],\beta_{k'}\}|\Phi\rangle \\ \langle\Phi|\{[\beta^\dagger_k,H],\beta^\dagger_{k'}\}|\Phi\rangle & \langle\Phi|\{[\beta^\dagger_k,H],\beta_{k'}\}|\Phi\rangle\end{pmatrix} \tag{6.62}$$

In the space of the basis operators $c_l, c^\dagger_l$, this matrx has the form

$$\mathcal{K} = W\begin{pmatrix} H^{11} & H^{20} \\ -H^{20*} & -H^{11*}\end{pmatrix}W^\dagger = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^*\end{pmatrix} \tag{6.63}$$

with

$$\begin{aligned} h_{ll'} &= \langle\Phi|\{[c_l.H], c^\dagger_{l'}\}|\Phi\rangle = (\epsilon+\Gamma-\lambda)_{ll'}, \\ \Gamma_{ll'} &= \sum_{qq'} \bar{v}_{lq'l'q}\rho_{qq'}, \\ \Delta_{ll'} &= \langle\Phi|\{[c_l.H], c_{l'}\}|\Phi\rangle = \frac{1}{2}\sum_{qq'} \bar{v}_{ll'qq'}\kappa_{qq'}. \end{aligned} \tag{6.64}$$

Thus, the problem is a diagonalization of $\mathcal{K}$,

$$\begin{pmatrix} \epsilon+\Gamma-\lambda & \Delta \\ -\Delta^* & -\epsilon-\Gamma^*+\lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} E_k \tag{6.65}$$

where the columns U_k, V_k of the matrices U and V determine the quasi-particle operators β_k

6.3.2 Another deriation

Using the theorem of Wick, we expand the Hamiltonian in normal order with respect to the ground state $|\Phi\rangle$.(Normal ordering is defined as $:O:=O-\langle\Phi|O|\Phi\rangle$ so that $\langle\Phi|:O:|\Phi\rangle=0$.)

Let us consider normal ordering,[3]

$$:c^\dagger_l c_{l'}: \;=\; -:c_{l'}c^\dagger_l:=c^\dagger_l c_{l'}-\langle\Phi|c^\dagger_l c_{l'}|\Phi\rangle, \tag{6.66}$$

Thus, we can express in terms of normal ordering,

$$\begin{aligned} c^\dagger_l c_{l'} &= :c^\dagger_l c_{l'}: +\langle\Phi|c^\dagger_l c_{l'}|\Phi\rangle = \rho_{l'l}+:c^\dagger_l c_{l'}:, \\ c_{l'}c^\dagger_l &= :c_{l'}c^\dagger_l: +\langle\Phi|c_{l'}c^\dagger_l|\Phi\rangle = -:c^\dagger_l c_{l'}: -\langle\Phi|c^\dagger_l c_{l'}|\Phi\rangle+\delta_{ll'}, \\ c^\dagger_l c^\dagger_{l'} &= :c^\dagger_l c^\dagger_{l'}: +\langle\Phi|c^\dagger_l c^\dagger_{l'}|\Phi\rangle, \\ c_l c_{l'} &= :c_l c_{l'}: +\langle\Phi|c_l c_{l'}|\Phi\rangle. \end{aligned} \tag{6.67}$$

Note that for any operator,

$$A:B:=:AB: \tag{6.68}$$

For two-body operators,

$$\begin{aligned} c^\dagger_{l_1}c^\dagger_{l_2}c_{l_4}c_{l_3} &= \rho_{l_3l_1}\rho_{l_4l_2}-\rho_{l_3l_2}\rho_{l_4l_1}+\kappa^*_{l_1l_2}\kappa_{l_3l_4} \\ &\quad +\rho_{l_3l_1}:c^\dagger_{l_2}c_{l_4}:+\rho_{l_4l_2}:c^\dagger_{l_1}c_{l_3}:-\rho_{l_4l_1}:c^\dagger_{l_2}c_{l_3}:-\rho_{l_3l_2}:c^\dagger_{l_1}c_{l_4}: \\ &\quad +\kappa^*_{l_1l_2}:c_{l_4}c_{l_3}:+\kappa_{l_3l_4}:c^\dagger_{l_1}c^\dagger_{l_2}: \\ &\quad +:c^\dagger_{l_1}c^\dagger_{l_2}c_{l_4}c_{l_3}: \end{aligned} \tag{6.69}$$

Then, with the definition,

$$\Gamma_{ll'}\equiv\sum_{qq'}\bar{v}_{lq'l'q}\rho_{qq'}, \quad \Delta_{ll'}\equiv\frac{1}{2}\sum_{qq'}\bar{v}_{ll'qq'}\kappa_{qq'} \tag{6.70}$$

[3]Thus,

$$\langle c_{l'}c^\dagger_l\rangle=-\langle c^\dagger_l c_{l'}\rangle+\delta_{ll'}$$

. If $\langle c^\dagger_l c_{l'}\rangle=\delta_{ll'}\theta(F-l)$, $\langle c_{l'}c^\dagger_l\rangle=\delta_{ll'}(1-\theta(F-l))$.

we can re-write the Hamiltonian as

$$\begin{aligned}
H &= \sum_{n_1 n_2} e_{n_1 n_2}(\rho_{n_2 n_1} + : c^\dagger_{n_1} c_{n_2} :) + \frac{1}{4}\sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4}\left(\rho_{n_3 n_1}\rho_{n_4 n_2} - \rho_{n_3 n_2}\rho_{n_4 n_1} + \kappa_{n_1 n_2}\kappa_{n_3 n_4}\right) \\
&+\frac{1}{4}\sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4}\Big(\rho_{n_3 n_1} : c^\dagger_{n_2} c_{n_4} : + \rho_{n_4 n_2} : c^\dagger_{n_1} c_{n_3} : - \rho_{n_4 n_1} : c^\dagger_{n_2} c_{n_3} : - \rho_{n_3 n_2} : c^\dagger_{n_1} c_{n_4} : \\
&\quad + \kappa^*_{n_1 n_2} : c_{n_4} c_{n_3} : + \kappa_{n_3 n_4} : c^\dagger_{n_1} c^\dagger_{n_2} : \Big) \\
&+\frac{1}{4}\sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} : c^\dagger_{n_1} c^\dagger_{n_2} c_{n_4} c_{n_3} :
\end{aligned} \tag{6.71}$$

(Note that in the normal ordering, $: c_{n_2} c^\dagger_{n_1} := - : c^\dagger_{n_1} c_{n_2} :$ regardless whether n_1 and n_2 are the same or not.) We may use symmetry of the $\rho, \kappa, \Gamma, \Delta$,

$$\begin{aligned}
\kappa^T &= -\kappa, \quad \rho^\dagger = \rho, \\
(\Gamma^*)_{ll'} &= \sum_{qq'} \bar{v}^*_{lq'l'q}\rho^*_{qq'} = \sum_{qq'} \bar{v}_{l'qlq'}\rho^\dagger_{q'q} = \Gamma_{l'l} \\
(\Delta^*)_{ll'} &= \frac{1}{2}\sum_{qq'} \bar{v}^*_{ll'qq'}\kappa^*_{qq'} = \frac{1}{2}\sum_{qq'} \bar{v}_{qq'll'}\kappa^*_{qq'}
\end{aligned} \tag{6.72}$$

then the part with normal ordered operators,

$$\begin{aligned}
&\sum_{n_1 n_2} e_{n_1 n_2} : c^\dagger_{n_1} c_{n_2} := \frac{1}{2}\sum_{n_1 n_2} e_{n_1 n_2} : c^\dagger_{n_1} c_{n_2} : - \frac{1}{2}\sum_{n_1 n_2} e_{n_1 n_2} : c_{n_2} c^\dagger_{n_1} : \\
&\frac{1}{4}\sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4}\Big(\rho_{n_3 n_1} : c^\dagger_{n_2} c_{n_4} : - \rho_{n_4 n_1} : c^\dagger_{n_2} c_{n_3} :\Big) = \frac{1}{2}\sum_{n_2 n_4} \Gamma_{n_2 n_4} : c^\dagger_{n_2} c_{n_4} : \\
&\frac{1}{4}\sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4}\Big(\rho_{n_4 n_2} : c^\dagger_{n_1} c_{n_3} : - \rho_{n_3 n_2} : c^\dagger_{n_1} c_{n_4} :\Big) = \frac{1}{2}\sum_{n_1 n_3} \Gamma_{n_1 n_3} : c^\dagger_{n_1} c_{n_3} : \\
&\quad = -\frac{1}{2}\sum_{n_1 n_3} \Gamma^*_{n_3 n_1} : c_{n_3} c^\dagger_{n_1} : \\
&\frac{1}{4}\sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4}\Big(\kappa^*_{n_1 n_2} : c_{n_4} c_{n_3} : + \kappa_{n_3 n_4} : c^\dagger_{n_1} c^\dagger_{n_2} :\Big) = \frac{1}{2}\Delta^*_{n_3 n_4} : c_{n_4} c_{n_3} : + \frac{1}{2}\Delta_{n_1 n_2} : c^\dagger_{n_1} c^\dagger_{n_2} : \\
&\quad = -\frac{1}{2}\Delta^*_{n_3 n_4} : c_{n_3} c_{n_4} : + \frac{1}{2}\Delta_{n_1 n_2} : c^\dagger_{n_1} c^\dagger_{n_2} :
\end{aligned} \tag{6.73}$$

Thus, by reform the Hamiltonian as a super-matrix form,

$$\begin{aligned}
H &= H^0 + : \frac{1}{2}\begin{pmatrix} c^\dagger & c \end{pmatrix}\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}\begin{pmatrix} c \\ c^\dagger \end{pmatrix} : + \frac{1}{4}\sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} : c^\dagger_{l_1} c^\dagger_{l_2} c_{l_4} c_{l_3} :, \\
H^0 &= \langle\Phi|H|\Phi\rangle = \mathrm{Tr}[(e + \frac{1}{2}\Gamma)\rho] - \frac{1}{2}\mathrm{Tr}[\Delta\kappa^*], \\
h &= e + \Gamma,
\end{aligned} \tag{6.74}$$

The last term corresponds to four quasi-particles, H^{40}, H^{31}, H^{22} and can be ignored in HFB. The rest can be diagonalized as previuos derivation. And thus, we get the same HFB equation.

6.3.3 Yet another derivation

Another possible way is to minimize $\langle\Phi_{HFB}|H|\Phi_{HFB}\rangle = E[\rho, \kappa]$ by varying ρ and κ as like HF. case.

6.4 HFB equations

There seems to be various representation of HFB equations.

$$\begin{pmatrix} \epsilon+\Gamma-\lambda & \Delta \\ -\Delta^* & -\epsilon-\Gamma^*+\lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} E_k, \tag{6.75}$$

where

$$\begin{aligned} h_{ll'} &= \langle\Phi|\{[c_l.H], c^\dagger_{l'}\}|\Phi\rangle = (\epsilon+\Gamma-\lambda)_{ll'}, \\ \Gamma_{ll'} &= \sum_{qq'} \bar{v}_{lq'l'q}\rho_{qq'}, \\ \Delta_{ll'} &= \langle\Phi|\{[c_l.H], c_{l'}\}|\Phi\rangle = \frac{1}{2}\sum_{qq'} \bar{v}_{ll'qq'}\kappa_{qq'}. \end{aligned} \tag{6.76}$$

where index l, l' are particle state index. U_k is a column vector such that $(U_k)_l = U_{lk}$ and k is a quasi-particle index. This equation can be solved by

- Define particle model space $l = 1 \ldots M$.
- construct matrix elements $h_{ll'}$,$\Gamma_{ll'}$,'$\Delta_{ll'}$ with assumptions on U,V and λ.
- solve $2M \times 2M$ matrix eigen-value equation for a particular k. get U_k,V_k and E_k
- compute ρ, κ and thus reconstruct matrix.
- iterate until convergence achieved.

Another form of HFB equation is to write them in position space. Since l index corresponds to basis wave function $\phi_l(\boldsymbol{r}, s)$, in position space (**why sign difference and factor in spin?** This equation comes from the HFBRAD manual.)

$$\begin{aligned} \rho(\boldsymbol{r},\sigma,q,\boldsymbol{r}',\sigma',q') &= \sum_{ll'} \rho_{ll'}\phi(\boldsymbol{r},\sigma,q)\phi^*_{l'}(\boldsymbol{r}',\sigma',q') = \langle\Phi|a^\dagger(\boldsymbol{r}'\sigma'q')a(\boldsymbol{r},\sigma,q)|\Phi\rangle \\ \tilde{\rho}(\boldsymbol{r},\sigma,q,\boldsymbol{r}',\sigma',q') &= \langle\Phi|a(\boldsymbol{r}',-\sigma',q')a(\boldsymbol{r},\sigma,q)|\Phi\rangle(-2\sigma) \end{aligned} \tag{6.77}$$

where σ is spin, q is an isospin index. Then,

$$\int d^3\boldsymbol{r}' \sum_{\sigma'} \begin{pmatrix} h(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') & \tilde{h}(\boldsymbol{r}\sigma\boldsymbol{r}'\sigma') \\ \tilde{h}(\boldsymbol{r}\sigma\boldsymbol{r}'\sigma') & -h(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') \end{pmatrix} \begin{pmatrix} U(E,\boldsymbol{r}',\sigma') \\ V(E,\boldsymbol{r}',\sigma') \end{pmatrix} = \begin{pmatrix} E+\lambda & 0 \\ 0 & E-\lambda \end{pmatrix} \begin{pmatrix} U(E,\boldsymbol{r},\sigma) \\ V(E,\boldsymbol{r},\sigma) \end{pmatrix} \tag{6.78}$$

where

$$h(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') = \frac{\delta E[\rho,\tilde{\rho}]}{\delta\rho(\boldsymbol{r}\sigma\boldsymbol{r}'\sigma')}, \quad \tilde{h}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') = \frac{\delta E[\rho,\tilde{\rho}]}{\delta\tilde{\rho}(\boldsymbol{r}\sigma\boldsymbol{r}'\sigma')} \tag{6.79}$$

Or in RHB (Relativistic Hartree Bogoliubov) equation(from Lulu Li et.al., arxiv:1202.0070)

$$\sum_{s'p'} \int d^3\boldsymbol{r}' \begin{pmatrix} h_D(\boldsymbol{r}sp,\boldsymbol{r}'s'p') - \lambda & \Delta(\boldsymbol{r}sp,\boldsymbol{r}'s'p') \\ -\Delta^*(\boldsymbol{r}sp,\boldsymbol{r}'s'p') & -h_D(\boldsymbol{r}sp,\boldsymbol{r}'s'p') + \lambda \end{pmatrix} \begin{pmatrix} U_k(\boldsymbol{r}'s'p') \\ V_k(\boldsymbol{r}'s'p') \end{pmatrix} = E_k \begin{pmatrix} U_k(\boldsymbol{r}sp) \\ V_k(\boldsymbol{r}sp) \end{pmatrix} \tag{6.80}$$

where E_k is a quasiparticle energy, λ is a chemical potential, p is a index for upper component and lower component.

To solve the HFB equation what we needs are

(1) How to obtain the matrix elements in h_D and Δ from U and V.

(2) How to obtain E_k and U_k, V_k by solving the equation.

(3) How to compute the ground state energy.

Chapter 7

Skyrme Hartree-Fock functional

7.1 Skyrme Hartree-Fock-Bogoliubov functional

The Skyrme interaction is a zero-range, density-dependent, non-local interaction.

$$\begin{aligned} V_{12}(\boldsymbol{r}_1,\boldsymbol{r}_2) &= t_0(1+x_0P_\sigma)\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)+\frac{1}{2}t_1(1+x_1P_\sigma)(\boldsymbol{k}'^2\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)+\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\boldsymbol{k}^2) \\ &\quad +t_2(1+x_2P_\sigma)\boldsymbol{k}'\cdot\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\boldsymbol{k}+\frac{1}{6}t_3(1+x_3P_\sigma)\rho^\gamma\delta(\boldsymbol{r}_1-\boldsymbol{r}_2) \\ &\quad +iW_0(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot(\boldsymbol{k}'\times\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\boldsymbol{k}) \end{aligned} \tag{7.1}$$

where $\boldsymbol{k}=\boldsymbol{k}_1-\boldsymbol{k}_2$, $\boldsymbol{k}'=\boldsymbol{k}'_1-\boldsymbol{k}'_2$. The functional of Skyrme interaction can be expressed (but with some simplifications like omitting J^2 terms) in terms of densities. (HF functional corresponds to ignore all pairing densities.)

Energy Functional is a functional of local densities, particle and pairing densities,

$$\rho(\boldsymbol{r})=\sum_i\varphi_2(E_i,\boldsymbol{r})^2,\quad \tilde{\rho}(\boldsymbol{r})=-\sum_i\varphi_1(E_i,\boldsymbol{r})\varphi_2(E_i,\boldsymbol{r}) \tag{7.2}$$

and its derivatives. (only real valued solution?)

non-local term introduce the kinetic density dependence,

$$\tau(\boldsymbol{r})=\sum_i|\nabla\varphi_2(E_i,\boldsymbol{r})|^2,\quad \tilde{\tau}(\boldsymbol{r})=-\sum_i\nabla\varphi_1(E_i,\boldsymbol{r})\cdot\nabla\varphi_2(E_i,\boldsymbol{r}) \tag{7.3}$$

spin-orbit term introduce spin current dependence,

$$\boldsymbol{J}(\boldsymbol{r})=i\sum_i\varphi_2(E_i,\boldsymbol{r})\nabla\varphi_2(E_i,\boldsymbol{r})\langle\sigma'|\hat{\boldsymbol{\sigma}}|\sigma\rangle,\quad \tilde{\boldsymbol{J}}(\boldsymbol{r})=-i\sum_i\varphi_1(E_i,\boldsymbol{r})\nabla\varphi_2(E_i,\boldsymbol{r})\langle\sigma'|\hat{\boldsymbol{\sigma}}|\sigma\rangle. \tag{7.4}$$

For spherical symmetric solution, with quantum number $(nljmq)$,

$$\varphi_i(E,\boldsymbol{r}\sigma)=\frac{u_i(nlj,r)}{r}Y^{(l)}_{m_l}(\hat{r})\langle lm_l\frac{1}{2}\sigma|jm\rangle. \tag{7.5}$$

Then, in terms of radial wave function, each densities can be written as radial functions

$$\rho(r)=\frac{1}{4\pi r^2}\sum_{nlj}(2j+1)u_2^2(nlj,r),\quad \tilde{\rho}(r)=-\frac{1}{4\pi r^2}\sum_{nlj}(2j+1)u_1(nlj,r)u_2(nlj,r). \tag{7.6}$$

$$\begin{aligned} \tau(r) &= \sum_{nlj}\frac{(2j+1)}{4\pi r^2}\left[\left(u_2'(nlj,r)-\frac{u_2(nlj,r)}{r}\right)^2+\frac{l(l+1)}{r^2}u_2^2(nlj,r)\right], \\ \tilde{\tau}(r) &= -\sum_{nlj}\frac{(2j+1)}{4\pi r^2}\left[\left(u_1'(nlj,r)-\frac{u_1(nlj,r)}{r}\right)\left(u_2'(nlj,r)-\frac{u_2(nlj,r)}{r}\right)+\frac{l(l+1)}{r^2}u_1(nlj,r)u_2(nlj,r)\right] \end{aligned} \tag{7.7}$$

Spin current vector densities have only one non-vanishing component,

$$J(r) = \frac{1}{4\pi r^3}\sum_{nlj}(2j+1)\left[j(j+1)-l(l+1)-\frac{3}{4}\right]u_2^2(nlj,r),$$
$$\tilde{J}(r) = -\frac{1}{4\pi r^3}\sum_{nlj}(2j+1)\left[j(j+1)-l(l+1)-\frac{3}{4}\right]u_1(nlj,r)u_2(nlj,r). \tag{7.8}$$

The energy density functional can be obtained by $\langle\Phi|H|\Phi\rangle$ directly. (Derivation required).

$$\begin{aligned} E &= K + E_{Skyrme} + E_{pair} + E_{Coul} \\ &= \int d^3\boldsymbol{r}\left[\mathcal{K}(r) + \mathcal{E}_{Skyrme}(r) + \mathcal{E}_{pair}(\boldsymbol{r}) + \mathcal{E}_{Coul}(r)\right] \end{aligned} \tag{7.9}$$

Kinetic energy with c.m. correction,

$$\mathcal{K}(r) = \frac{\hbar^2}{2m}\tau(r)(1-\frac{1}{A}) \tag{7.10}$$

Skyrme energy density

$$\begin{aligned} \mathcal{E}_{Skyrme}(r) &= \frac{1}{2}t_0\left[(1+\frac{x_0}{2})\rho^2 - (x_0+\frac{1}{2})\sum_q\rho_q^2\right] \\ &+\frac{t_1}{4}\left\{\left(1+\frac{x_1}{2}\right)\left[\rho\tau+\frac{3}{4}(\nabla\rho)^2\right] - (x_1+\frac{1}{2})\sum_q\left[\rho_q\tau_q+\frac{3}{4}(\nabla\rho_q)^2\right]\right\} \\ &+\frac{t_2}{4}\left\{\left(1+\frac{x_2}{2}\right)\left[\rho\tau-\frac{1}{4}(\nabla\rho)^2\right] + (x_2+\frac{1}{2})\sum_q\left[\rho_q\tau_q-\frac{1}{4}(\nabla\rho_q)^2\right]\right\} \\ &+\frac{1}{12}t_3\rho^\gamma\left[\left(1+\frac{x_3}{2}\right)\rho^2 - \left(x_3+\frac{1}{2}\right)\sum_q\rho_q^2\right] \\ &-\frac{1}{16}(t_1x_1+t_2x_2)J^2 + \frac{1}{16}(t_1-t_2)\sum_q J_q^2 \\ &+\frac{1}{2}W_0\left(J\nabla\rho + \sum_q J_q\nabla\rho_q\right). \end{aligned} \tag{7.11}$$

last two lines are often ignored.

Pairing energy density

$$\begin{aligned} \mathcal{E}_{pair} &= \sum_q\left\{\frac{t_0'}{4}(1-x_0')\tilde{\rho}_q^2 + \frac{t_1'}{4}(1-x_1')\left[\tilde{\rho}_q\tilde{\tau}_q+\frac{1}{4}(\nabla\tilde{\rho}_q)^2\right]\right. \\ &\left.+\left[\frac{t_2'}{8}(1+x_2')+\frac{1}{4}W_0'\right]\tilde{J}_q^2 + \frac{t_3'}{24}(1-x_3')\rho^{\gamma'}\tilde{\rho}_q^2\right\}. \end{aligned} \tag{7.12}$$

(In HFBRAD, only t_0' and t_3' term are used.)

Coulomb energy density is approximated as

$$\begin{aligned} \mathcal{E}_{coul} &= \mathcal{E}_{coul}^{dir} + \mathcal{E}_{coul}^{ex}, \\ \mathcal{E}_{coul}^{dir} &= \frac{e^2}{2}\int\int d^3\boldsymbol{r}d^3\boldsymbol{r}'\frac{\rho_{ch}(\boldsymbol{r})\rho_{ch}(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}, \\ \mathcal{E}_{coul}^{ex} &= -\frac{3}{4}e^2\left(\frac{3}{\pi}\right)^{1/3}\int d^3\boldsymbol{r}\rho_p^{4/3}(\boldsymbol{r}) \end{aligned} \tag{7.13}$$

(It seems that the equation is for energy E not energy density.)

Now from the energy density functional, one can obtain the HFB equation.(Note that ρ and $\tilde{\rho}$ are independent variables. Thus, do not consider derivative of abnoarmal density over normal density.)

$$h(r) = \frac{\delta E}{\delta \rho(r)} = \left(\frac{\partial}{\partial \rho} + \frac{\partial \tau}{\partial \rho}\frac{\partial}{\partial \tau} + \frac{\partial J}{\partial \rho}\frac{\partial}{\partial J} + \cdots \right) E[\rho, \tilde{\rho}] \tag{7.14}$$

For the derivative of kinetic density, $\frac{\partial \tau}{\partial \rho} = -\nabla^2$, one gets effective mass term,

$$\begin{aligned} M_q &= \frac{\partial}{\partial \tau_q} E[\rho, \tilde{\rho}] = \frac{\hbar^2}{2m^*} \\ &= \frac{\hbar^2}{2m} + \frac{t_1}{4}\left\{ \left(1 + \frac{x_1}{2}\right)\rho - (x_1 + \frac{1}{2})\rho_q \right\} + \frac{t_2}{4}\left\{ \left(1 + \frac{x_2}{2}\right)\rho + (x_2 + \frac{1}{2})\rho_q \right\} \end{aligned} \tag{7.15}$$

For the derivative of abnormal kinetic density, $\frac{\partial \tilde{\tau_q}}{\partial \tilde{\rho}_q} = -\nabla^2$, abnormal effective mass

$$\tilde{M}_q = \frac{\partial}{\partial \tilde{\tau}_q} E[\rho, \tilde{\rho}] = \frac{t_1'}{4}(1 - x_1')\tilde{\rho}_q. \tag{7.16}$$

For derivative of normal density, effective potential as

$$\begin{aligned} U_q &= \frac{\partial}{\partial \rho_q} E[\rho, \tilde{\rho}] \\ &= t_0\left[(1 + \frac{x_0}{2})\rho - (x_0 + \frac{1}{2})\rho_q \right] \\ &\quad + \frac{t_1}{4}\left\{ \left(1 + \frac{x_1}{2}\right)\left[\tau - \frac{3}{2}\nabla^2\rho \right] - (x_1 + \frac{1}{2})\left[\tau_q - \frac{3}{2}\nabla^2\rho_q \right] \right\} \\ &\quad + \frac{t_2}{4}\left\{ \left(1 + \frac{x_2}{2}\right)\left[\tau + \frac{1}{2}\nabla^2\rho \right] + (x_2 + \frac{1}{2})\left[\tau_q + \frac{1}{2}\nabla^2\rho_q \right] \right\} \\ &\quad + \frac{1}{12}t_3\left[\left(1 + \frac{x_3}{2}\right)(\gamma + 2)\rho^{\gamma+1} - \left(x_3 + \frac{1}{2}\right)\left(\gamma\rho^{\gamma-1}\sum_{q'}\rho_{q'}^2 + 2\rho^{\gamma}\rho_q \right) \right] \\ &\quad - \frac{1}{2}W_0\left(\nabla J + \nabla J_q\right) \\ &\quad + \frac{t_3'}{24}(1 - x_3')\gamma'\rho^{\gamma'-1}\sum_{q'}\tilde{\rho}_{q'}^2. \end{aligned} \tag{7.17}$$

which have additional Coulomb potential for proton case,

$$V_c(\boldsymbol{r}) = \frac{e^2}{2}\int d^3\boldsymbol{r}' \frac{\rho_p(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} - e^2(\frac{3}{\pi})^{1/3}\rho_p^{1/3}(\boldsymbol{r}) \tag{7.18}$$

for derivative of abnormal density $\tilde{\rho}_q$,

$$\tilde{U}_q = \frac{\partial}{\partial \tilde{\rho}_q} E[\rho, \tilde{\rho}] = \frac{t_0'}{2}(1 - x_0')\tilde{\rho}_q + \frac{t_1'}{4}(1 - x_1')\left[\tilde{\tau}_q - \frac{1}{2}(\nabla^2\tilde{\rho}_q) \right] + \frac{t_3'}{12}(1 - x_3')\rho^{\gamma'}\tilde{\rho}_q \tag{7.19}$$

for derivative of J_q,

$$B_q = \frac{\partial}{\partial J_q} E[\rho, \tilde{\rho}] = -\frac{1}{8}(t_1x_1 + t_2x_2)J + \frac{1}{8}(t_1 - t_2)J_q + W_0\nabla(\rho + \rho_q). \tag{7.20}$$

for derivative of $\tilde{J}_q$,

$$\tilde{B}_q = \frac{\partial}{\partial \tilde{J}_q} E[\rho, \tilde{\rho}] = \left[\frac{t_2'}{2}(1 + x_2') + W_0' \right]\tilde{J}_q. \tag{7.21}$$

In summary,

$$h = -M_q\nabla^2 + U_q + B_q, \quad \tilde{h} = -\tilde{M}_q\nabla^2 + \tilde{U}_q + \tilde{B}_q \tag{7.22}$$

Inserting this into the HFB equation and expands for $nljq$, we gets the differential equations for $u_1(nlj;r)$ and $u_2(nlj;r)$ as

$$\mathcal{M} = \begin{pmatrix} M & \tilde{M} \\ \tilde{M} & -M \end{pmatrix}, \quad \mathcal{U} = \begin{pmatrix} U-\lambda & \tilde{U} \\ \tilde{U} & -U+\lambda \end{pmatrix}, \tag{7.23}$$

$$\mathcal{U}_{so} = \begin{pmatrix} B & \tilde{B} \\ \tilde{B} & -B \end{pmatrix} \frac{j(1j+1) - l(l+1) - \frac{3}{4}}{2r}, \tag{7.24}$$

$$\left[-\frac{d}{dr}\mathcal{M}\frac{d}{dr} + \mathcal{U} + \mathcal{M}\frac{l(l+1)}{r^2} + \frac{\mathcal{M}'}{r} + \mathcal{U}_{so}\right]\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = E\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}. \tag{7.25}$$

This equation can be re-arranged so that there's no derivative on the coupling.

$$\begin{aligned} -M^*\frac{d}{dr^2}f_1 + Vf_1 + Wf_2 &= Ef_1, \\ M^*\frac{d}{dr^2}f_2 - Vf_2 + Wf_1 &= Ef_2. \end{aligned} \tag{7.26}$$

(How one determine λ_q? As a last occupied level energy?) Exact definition of $f_{1,2}$ M^*, V, W are given in NPA422(1984)103. In any way, important point is that the above expression can be solved by using Numerov method for each s.p. states $(nljq)$ with box boundary conditions $f_i(r = R_{box}) = 0$.

Once $u_{1,2}$ and E_i is obtained, one can extract corresponding physical quantities.

- Occupation number $n_i = \int dr u_2^2(nlj;r)$ for state E_i.
- H-F equivalent energy $\bar{\epsilon}_i = \lambda + E_i(2n_i - 1)$.
- equivalent gap $\Delta_i = 2E_i\sqrt{n_i(1-n_i)}$.
- rms raidus is from $\int_0^{R_{box}} d^3\boldsymbol{r}\boldsymbol{r}^2\varphi_{2,i}^2(\boldsymbol{r})$
- number of nodes are counted for component of greatest amplitude.

7.2 Nuclear Matter case

- 중성자별이라고 중성자만 있는 것은 아니다. chemical and charge equilibrium을 생각해야한다. (beta-equilibrium) $b_1 \to b_2 + l + \bar{\nu}_l$ and $b_2 + l \to b_1 + \nu_l$의 평형상태. (b_1의 beta decay를 생각하기 때문.)
- symmetric nuclear matter saturation density and energy per baryon,

$$\begin{aligned} \rho_0 &\simeq 0.16 \pm 0.02 \text{ fm}^{-3}, \\ \mathcal{E}_0 &= \frac{B}{A} = -15.6 \pm 0.2 \text{ MeV} \end{aligned} \tag{7.27}$$

Energy density $\epsilon = E/V$,

$$\mathcal{E} = \frac{E}{A} = \frac{E}{V}\frac{V}{A} = \frac{\epsilon}{\rho} \tag{7.28}$$

- Pressure and chemical potential: for fixed $A = \rho V$, from $dE = -PdV$, [1]

$$\begin{aligned} P &= -\frac{dE}{dV} = -A\frac{d}{dV}(\mathcal{E}) = -\rho V\frac{d\mathcal{E}}{dV} \\ &= \rho^2\frac{\partial}{\partial\rho}\mathcal{E} = \rho\frac{\partial\epsilon}{\partial\rho} - \epsilon \end{aligned} \tag{7.29}$$

for fixed volume V, chemical potential $dE = \mu_i dA_i$,

$$\begin{aligned} \mu_i &= \left(\frac{\partial E}{\partial A_i}\right)_V = \left(\frac{\partial}{\partial\rho_i}\frac{E}{V}\right)_V \\ &= \left(\frac{\partial\epsilon}{\partial\rho_i}\right) \end{aligned} \tag{7.30}$$

Baryon density $\rho = \sum_i \rho_i$. For proton and neutron, define proton fraction,

$$x_p = \frac{\rho_p}{\rho} \tag{7.31}$$

- Fermi momentum is defined as

$$\rho = \frac{g(=4)}{6\pi^2}k_F^3 = x_p\rho + (1-x_p)\rho = \frac{g(=2)}{6\pi^2}k_{Fp}^3 + \frac{g(=2)}{6\pi^2}k_{Fn}^3 \tag{7.32}$$

this comes from, number density of Fermi gas

$$\rho_i = g\int_0^{k_{Fi}}\frac{dpp^2(4\pi)}{(2\pi)^3} = \frac{g}{6\pi^2}k_{Fi}^3 \tag{7.33}$$

which is related with kinetic energy density of Fermi gas (non-relativistic)

$$\mathcal{K} = g\int^{k_F}\frac{dpp^2(4\pi)}{(2\pi)^3}E_p\left(=\frac{p^2}{2m}\right) = \frac{3}{5}\frac{k_F^2}{2m}\rho \tag{7.34}$$

In other words, In the limit of nuclear matter, a constant $\rho(r)$, the kinetic energy term for a Fermi gas become (No C.M. energy correction, Same Nucleon mass)

$$\mathcal{K}_{NM} = \frac{3}{5}\frac{\hbar^2}{2m}k_{p,F}^2\rho_p + \frac{3}{5}\frac{\hbar^2}{2m}k_{n,F}^2\rho_n \tag{7.35}$$

- Energy per Baryon $\mathcal{E}(\rho, x_p)$: for symmetric nuclear matter $\mathcal{E}(\rho, \frac{1}{2})$. for pure neutron matter, $\mathcal{E}(\rho, 0)$. Symmetry energy is defined as

$$\mathcal{S}(\rho) = \mathcal{E}(\rho, x_p = 0) - \mathcal{E}(\rho, x_p = 1/2) \tag{7.36}$$

Expansion around $x_p = \frac{1}{2}$,

$$\mathcal{E}(\rho, x_p) = \mathcal{E}(\rho, x_p = \frac{1}{2}) + \frac{1}{2}\frac{d^2\mathcal{E}}{dx_p^2}(x_p - \frac{1}{2})^2 + \cdots \tag{7.37}$$

neglecting higher order terms, empirically we may associate symmetry energy ,

$$\frac{1}{8}\frac{d^2\mathcal{E}(\rho, x_p = \frac{1}{2})}{dx_p^2} \simeq \mathcal{S}(\rho)?$$

However, it is an approximation.

[1] $\rho dV + V d\rho = 0$, and $\rho\frac{\partial}{\partial\rho} = -V\frac{\partial}{\partial V}$.

- In neutron star, the proton fraction is important. (not pure neutron matter). proton fraction can be determined from beta-equilibrium conditions, (Need derivation!)

$$\hbar c(3\pi^2\rho x_p)^{1/3} = 4\mathcal{S}(\rho)(1-2x_p) \tag{7.38}$$

  In other words, if we know $\mathcal{S}(\rho)$, we can determine the proton fraction. (electron chemical potential $\mu_e = \hbar c k_F$ determines density ρ)

- One may try to obtain $\mathcal{S}(\rho)$ from finite nuclei $\mathcal{E}(\rho, x_p)$, it is limited to ρ_0 and $x_p \simeq \frac{1}{2}$

- 실제 Nuclear Matter 계산의 경우, plane wave의 periodic boundary condition을 생각한다. 먼저 particle number A 를 정하고, density ρ 또는 k_F 를 정한다. 그러면,

$$\rho = \frac{A}{L^3} = g\frac{k_F^3}{6\pi^2} \tag{7.39}$$

  으로 L이 정해지고, momentum 값은

$$\Delta k = \frac{2\pi}{L} \tag{7.40}$$

  로 정해지게 된다. 이 때, particle number 는 closed shell의 형태가 되도록 plane wave magic number[2] 2,14,38,54,66,114 등으로 정한다(하나의 nucleon 에 대해서).

The Skyrme energy density of nuclear matter is easy to get by taking constant $\rho(r)$ limit. (What about spin density J?) It is not clear whether there is a pairing energy density for nuclear matter. The Coulomb energy density are ignored in nuclear matter EOS.

The energy density for Symmetric Nuclear Matter(SNM) and Pure Neutron Matter(PNM) can be expressed in terms of $\rho = \rho_n + \rho_p$ and $\delta = \frac{\rho_n - \rho_p}{\rho}$.[3] Then,

$$\begin{aligned}
\mathcal{K}_{NM}(\rho,\delta) &= C_{kin}\left(\rho_p^{5/3} + \rho_n^{5/3}\right), \quad C_{kin} = \frac{\hbar^2}{2m}\frac{3}{5}(3\pi^2)^{2/3}, \\
&= C_{kin}\rho^{5/3}\left((\frac{1+\delta}{2})^{5/3} + (\frac{1-\delta}{2})^{5/3})\right), \\
\mathcal{E}_{Skyrme}(\rho,\delta) &= \ldots.
\end{aligned} \tag{7.41}$$

For Symmetric Nuclear Matter, saturation properties at normal nuclear matter density gives

$$\begin{aligned}
\mathcal{E}(\rho_0, 0) &= -16\text{MeV}, \\
L &= \frac{d\mathcal{E}(\rho,0)}{d\rho}|_{\rho_0} = 0. \\
K &= 9\rho^2\frac{d^2}{d\rho^2}(\frac{\mathcal{E}(\rho,0)}{\rho})|_{\rho_0}, \\
Q &= 27\rho^3\frac{d^3\mathcal{E}(\rho,0)}{d\rho^3}|_{\rho_0}, \\
R &= 81\rho^4\frac{d^4\mathcal{E}(\rho,0)}{d\rho^4}|_{\rho_0},
\end{aligned} \tag{7.42}$$

Symmetry energy ,which is the difference of SNM and PNM, is

$$S(\rho) = \mathcal{E}(\rho,1) - \mathcal{E}(\rho,0) \tag{7.43}$$

[2] $n_x^2 + n + y^2 + n_z^2 \le N$ 조건과 spin degeneracy

[3] Thus, $\rho_p = \frac{1}{2}\rho(1-\delta)$ and $\rho_n = \frac{1}{2}\rho(1+\delta)$

One can define similar quantities at saturation density

$$\begin{aligned} J_{sym} &= S(\rho_0), \\ L_{sym} &= \rho \frac{dS(\rho)}{d\rho}|_{\rho_0}, \\ K_{sym} &= , \\ Q_{sym} &= , \\ R_{sym} &= \end{aligned} \tag{7.44}$$

Chapter 8

Brueckner Hartree-Fock theory

T-matrix equation (from P.Ring's book)

$$T^E_{\boldsymbol{k}_1\boldsymbol{k}_2,\boldsymbol{k}'_1\boldsymbol{k}'_2} = \bar{v}_{\boldsymbol{k}_1\boldsymbol{k}_2,\boldsymbol{k}'_1\boldsymbol{k}'_2} + \frac{1}{2}\sum_{\boldsymbol{p}_1\boldsymbol{p}_2} \bar{v}_{\boldsymbol{k}_1\boldsymbol{k}_2,\boldsymbol{p}_1\boldsymbol{p}_2} \frac{1}{E - (\boldsymbol{p}_1^2/2m) - (\boldsymbol{p}_2^2/2m) + i\eta} T^E_{\boldsymbol{p}_1\boldsymbol{p}_2,\boldsymbol{k}'_1\boldsymbol{k}'_2} \tag{8.1}$$

In nuclear medium, modifications (1) change plane wave to shell model basis (2) energy in denominator to shell model energy (3) sum over intermediate states with Pauli operator

$$G^E_{ab,cd} = \bar{v}_{ab,cd} + \frac{1}{2}\sum_{mn>\epsilon_F} \bar{v}_{ab,mn} \frac{1}{E - \epsilon_m - \epsilon_n + i\eta} G^E_{mn,cd} \tag{8.2}$$

or with

$$\begin{aligned} Q_F &= \sum_{m<n,m,n>\epsilon_F} |mn\rangle\langle mn|, \\ G &= \bar{v} + \bar{v}\frac{Q_F}{E - H_0} G. \end{aligned} \tag{8.3}$$

[1]

The scattered wave function,

$$|\psi_{ab}\rangle = \bar{v}^{-1} G|ab\rangle = \left(1 + \frac{G_F}{E - H_0}\right)|ab\rangle = |ab\rangle + \frac{Q_F}{E - H_0}\bar{v}|\psi_{ab}\rangle \tag{8.4}$$

note that $|ab\rangle$ is a normalized anti-symmetric wave function.

BHF equation,

$$\begin{aligned} &\sum_{l'}\left(t_{ll'} + \sum_{pp'}\sum_{i=1}^{A} G^{\epsilon_k+\epsilon_i}_{lp',l'p} D_{pi} D^*_{p'i}\right) D_{l'k} = \epsilon_k D_{lk}, \\ &E_0^{BHF} = \sum_{i=1}^{A} t_{ii} + \frac{1}{2}\sum_{ij=1}^{A} G^{\epsilon_i+\epsilon_j}_{ij,ij} \\ &\quad = \sum_{i=1}^{A}\epsilon_i - \frac{1}{2}\sum_{ij=1}^{A} G^{\epsilon_i+\epsilon_j}_{ij,ij}. \end{aligned} \tag{8.5}$$

[1] I am not sure the equation of T-matrix and G-matrix: (1) $\bar{v}$ represent anti-symmetric matrix elements ? (2) factor 1/2?

There is an ambiguity. In standard convention,

$$\begin{aligned}\Gamma^{BHF}_{kk'} &= \frac{1}{2}\sum_{i=1}^{A}(G^{\epsilon_k+\epsilon_i}_{ki,k'i}+G^{\epsilon_{k'}+\epsilon_i}_{ki,k'i}) \quad \text{for } k,k'\le\epsilon_F,\\ &= \sum_{i=1}^{A}G^{\epsilon_k+\epsilon_i}_{ki,k'i} \quad \text{for } k\le\epsilon_F, k'>\epsilon_F,\\ &= \sum_{i=1}^{A}G^{\epsilon_{k'}+\epsilon_i}_{ki,k'i} \quad \text{for } k'\le\epsilon_F, k>\epsilon_F,\end{aligned} \tag{8.6}$$

and

$$\Gamma^{BHF}_{kk'}=0, \quad \text{for } k,k'>\epsilon_F. \tag{8.7}$$

But, original BHF gives unsatisfactory results, while density dependent effective interaction or Skyrme force gives better results.

8.1 BHF(Bruckner Hartree-Fock) calculation for nuclear matter

This section is based on the Haftel and Tabakin, NPA158(1970)1-42.

In nuclear matter, we can approximate single particle wave functions to be plane waves,

$$\phi_\mu(\boldsymbol{r}_i)=\langle \boldsymbol{r}_i|\mu\rangle=\frac{e^{i\boldsymbol{k}_\mu\cdot\boldsymbol{r}_i}}{\Omega^{\frac{1}{2}}}|s_\mu t_\mu\rangle \tag{8.8}$$

Note that this corresponds to the normalization convention,

$$\langle \boldsymbol{k}|\boldsymbol{k}'\rangle=\frac{(2\pi)^3}{\Omega}\delta^{(3)}(\boldsymbol{k}-\boldsymbol{k}'), \quad \sum_\mu \to \frac{\Omega}{(2\pi)^3}\sum_{s_\mu}\sum_{t_\mu}\int d^3k_\mu \tag{8.9}$$

[2] [3] However, because of the effects of interaction, s.p. energy would be modified, $e(k)\neq\frac{k^2}{2m_N}$. We may consider the average effects of other particles can appear as (1) s.p. mean field potential and (2) Pauli-exclusion in scattering of two particles.

[2] In other words,

$$\begin{aligned}&\langle \boldsymbol{x}|\boldsymbol{x}'\rangle=\delta^{(3)}(\boldsymbol{x}-\boldsymbol{x}'), \quad \int_{L^3}d^3x|\boldsymbol{x}\rangle\langle\boldsymbol{x}|=1,\\ &\langle \boldsymbol{k}|\boldsymbol{k}'\rangle=\frac{(2\pi)^3}{\Omega}\delta^{(3)}(\boldsymbol{k}-\boldsymbol{k}'), \quad \frac{\Omega}{(2\pi)^3}\int d^3k|\boldsymbol{k}\rangle\langle\boldsymbol{k}|=1.\end{aligned} \tag{8.10}$$

[3] The two particle state

$$\begin{aligned}|m_1m_2\rangle &= |\boldsymbol{k}_1s_1t_1\rangle\otimes|\boldsymbol{k}_2s_2t_2\rangle\\ &= \sum_{SM_S,TT_z}|\boldsymbol{k}\boldsymbol{K}SM_STT_z\rangle C^{SM_S}_{s_1s_2}C^{TT_z}_{t_1t_2},\\ |\boldsymbol{k}\boldsymbol{K}\rangle &= \frac{1}{\sqrt{\Omega}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\frac{1}{\sqrt{\Omega}}e^{i\boldsymbol{K}\cdot\boldsymbol{R}}, \quad \boldsymbol{k}=\frac{(\boldsymbol{k}_1-\boldsymbol{k}_2)}{2},\boldsymbol{K}=\boldsymbol{k}_1+\boldsymbol{k}_2.\end{aligned} \tag{8.11}$$

Further partial wave expansion,

$$\begin{aligned}|m_1m_2\rangle &= \sum_{SM_S,TT_z}|\boldsymbol{K}\rangle\otimes(4\pi)\sum_{lm}i^l|\frac{1}{\sqrt{\Omega}}j_l(kr)\rangle Y^*_{lm}(\hat{k})Y_{lm}(\hat{r})|SM_STT_z\rangle C^{SM_S}_{s_1s_2}C^{TT_z}_{t_1t_2}\\ &= |\boldsymbol{K}\rangle\otimes\sum_{SM_S,TT_z}\sum_{lm}\sum_{JM}i^lY^*_{lm}(\hat{k})C^{SM_S}_{s_1s_2}C^{TT_z}_{t_1t_2}C^{JM}_{lmSM_S}|\frac{1}{\sqrt{\Omega}}j_l(kr)|\mathcal{Y}^M_{lSJ}(\hat{r})\rangle,\end{aligned} \tag{8.12}$$

However, because of the hard-core or short range repulsion of NN interaction, naive perturbative calculation based on the expansion of V would be not correct. (If we start from the free-particles or some single-particle basis and compute perturbation, we need matrix element $\langle\phi_i\phi_j|V|\phi_i\phi_j\rangle$ which integral becomes very large. Because uncorrelated two single particle wave functions $\phi(r)$ will be non-zero at short distance, the integral will be very large. This is as if a situation $f(x) = x/(1+x)$ cannot be well approximated by perturbative series $x + \ldots$. However, even though individual V is large, the infinite sum $f(x)$ can be well defined. Thus, if we can compute non-perturvative sum of diagrams directly, they can be well-behaved. This is a G-matrix. In a sense, it is introducing a correlated two-particle wave functions ψ, such that it vanishes at short distance but restores/heals at large distance. (So that the matrix elements $\langle\phi|V|\psi\rangle = \langle\phi|G|\phi\rangle$ is well defined where $|\psi\rangle$ contains infinite sum of $\langle\phi|V|\phi\rangle$.)

)

For infinite symmetric nuclear matter, $\Omega \to \infty$ and $A \to \infty$, but particle number density $\rho = A/\Omega$ is finite. This corresponds to a fixed Fermi momentum by,

$$\begin{aligned}\rho &= \frac{A}{\Omega} = \frac{1}{\Omega}\frac{\Omega}{(2\pi)^3} g\int_F d^3k = \frac{2k_F^3}{3\pi^2}, \quad g=4, \\ \langle T\rangle &= \frac{\Omega}{(2\pi)^3} g\int_F d^3k \frac{\hbar^2k^2}{2M_N} = \frac{3}{5}\epsilon_F A, \quad \epsilon_F = \frac{\hbar^2k_F^2}{2m_N}, g=4 \end{aligned} \tag{8.14}$$

where ϵ_F is a kinetic energy of highest level state. Note that this is not the single particle energy ϵ_α of highest level state. (We would expect nuclear matter saturation , $E/A = -15.8$ MeV/A at $k_F = 1.36$ fm^{-1})

The base of BHF is to consider each particles are in the single particle potential which is a mean field generated from other particles, but instead of bare potential like HF, from G-matrix as an effective interaction. Also, the independent pair approximation assumes that the correction from one interaction only affects to the wave function of the pair,

$$\mathcal{A}|\phi_1\phi_2\phi_3\cdots\rangle \to \mathcal{A}|\psi_{12}\phi_3\cdots\rangle. \tag{8.15}$$

Though it will be necessary to go beyond the independent pair approximation, let us follow the standard procedure of BHF theory.

In case of infinite Nuclear Matter, single particle wave function ϕ_k is known, one only have to obtain self consistent single particle energies ϵ_k. Procedure are

- (1) Initial Guess of ϵ_k. This defines Q(Pauli operator).
- (2) compute G-matrix from Brueckner equation.
- (3) compute single particle potential $U(k) = \langle k|U|k\rangle$ from G-matrix.
- (4) obtain new ϵ_k from $U(k)$.

For anti-symmetric state

$$\begin{aligned}|m_1m_2\rangle - |m_2m_1\rangle &= |\boldsymbol{K}\rangle \otimes \sum_{SM_S,TT_z}\sum_{lm}\sum_{JM} i^l \left(Y^*_{lm}(\hat{k})C^{SM_S}_{s_1s_2}C^{TT_z}_{t_1t_2} - Y^*_{lm}(-\hat{k})C^{SM_S}_{s_2s_1}C^{TT_z}_{t_2t_1}\right) \\ &\quad \times C^{JM}_{lmSM_S}|\frac{1}{\sqrt{\Omega}}j_l(kr)\rangle|\mathcal{Y}^M_{lSJ}(\hat{r})\rangle \\ &= |\boldsymbol{K}\rangle \otimes \sum_{SM_S,TT_z}\sum_{lm}\sum_{JM} i^l Y^*_{lm}(\hat{k})C^{SM_S}_{s_1s_2}C^{TT_z}_{t_1t_2}\left(1-(-1)^l(-1)^{1+S}(-1)^{1+T}\right) \\ &\quad \times C^{JM}_{lmSM_S}|\frac{1}{\sqrt{\Omega}}j_l(kr)\rangle|\mathcal{Y}^M_{lSJ}(\hat{r})\rangle \end{aligned} \tag{8.13}$$

- (5) repeat [2-4] until convergence in ϵ_k
- (6) compute nuclear matter properties using G-matrix and U.

In case of finite nuclei, the single particle wave function is not known, one have to obtain self-consistent ϕ_α by Hartree-Fock problem. Thus, we require self-consistencies in both ϕ_α and ϵ_α. Procedure are

- (1) Initial guess on U_α.
- (2) Given U_α gives ϕ_α,ϵ_α and thus Q for given nuclei.
- (3) Obtain self consistent ϵ_k from the above Bruecker procedure.
- (4) Compute $\langle k|H_0|a\rangle$ and by solving H-F problem, obtain new ϕ_α and ϵ_α.
- (5) repeat [2-4] until convergence in ϕ_α and ϵ_α.
- (6) compute nuclear properties from ϕ_α and ϵ_α.

Here, let us focus on the infinite matter case.

In BHF, G-matrix which satisfies following equation acts as a effective interaction between particles in medium,

$$G(\omega) = V + V\frac{Q}{\omega - h_0}G(\omega) \tag{8.16}$$

, where ω is two-particle starting energy(just a parameter) Q is a Pauli projection operator for the outside of Fermi level. The h_0 includes both kinetic energy and potential.

$$Q|\alpha\beta\rangle = \begin{cases} 1 & \text{for } \alpha \text{ and } \beta \text{ above } \epsilon_F, \\ 0 & \text{for } \alpha \text{ and } \beta \text{ at or below } \epsilon_F \end{cases}, \tag{8.17}$$

$$\begin{aligned} h_0|\alpha\beta\rangle &= (\epsilon_\alpha + \epsilon_\beta)|\alpha\beta\rangle, \\ \epsilon_\alpha &= \langle\alpha|\frac{p^2}{2m_N} + U|\alpha\rangle. \end{aligned} \tag{8.18}$$

Then, the single particle energy is determined from the G-matrix which depends on the single particle energy.(Actually, this choice is similar as HF choice but it comes from the BBP theorem.) [4]

$$\langle\mu|U|\mu\rangle = U(k_\mu) = \sum_{\nu<F}\langle\mu\nu|G(\epsilon_\mu + \epsilon_\nu)|\mu\nu - \nu\mu\rangle, \text{ for } \mu \le F, \tag{8.20}$$

Since G-matrix itself depends on single particle energy, the G-matrix have to satisfy self-consistent relations and require iteration to solve. Once G-matrix is determined, it can be used to obtain the total energy of the system.

$$E = \sum_{\mu<F}\langle\mu|\frac{p^2}{2M}|\mu\rangle + \frac{1}{2}\sum_{\mu\nu<F}\langle\mu\nu|G(\epsilon_\mu + \epsilon_\nu)|\mu\nu - \nu\mu\rangle \tag{8.21}$$

However, exactly solving these equation is complicate and following approximations are introduced usually,

[4] It is un-clear. In some paper, the relation was given as

$$\langle\mu|U|\mu\rangle = U(k_\mu) = \sum_{\nu<F}\langle\mu\nu|\frac{1}{2}[G(\epsilon_\mu + \epsilon_\nu) + G(\epsilon_{\mu'} + \epsilon_{\nu'})]|\mu\nu - \nu\mu\rangle, \text{ for } \mu \le F, \tag{8.19}$$

- Effective Mass approximation: approximate $U(k)$ up to second power of k. Then, single particle energy can be simply represented by effective mass M^*. Near k_0, we expand

$$U(k) \simeq U(k_0^2) + \frac{\hbar^2}{2M_N}(k^2 - k_0^2)U_1 \tag{8.22}$$

$$\begin{aligned} \epsilon_k &= \langle k|\frac{p^2}{2M_N} + U|k\rangle \simeq \frac{\hbar^2 k^2}{2M_N} + U(k_0^2) + \frac{\hbar^2}{2M_N}(k^2 - k_0^2)U_1 \\ &\simeq \frac{\hbar^2 k^2}{2M_N^*} - U_0, \quad \text{for } k \le k_F \end{aligned} \tag{8.23}$$

  for occupied states $k \le k_F$.

  Of course, this simple form would not be correct for all momenta. Since we want to match Fermi energy, with $k_0 \simeq k_F$ choice

$$\frac{M^*}{M} = \frac{1}{1+U_1}, \quad U_1 = \frac{M}{\hbar^2 k_F}\frac{dU}{dk}|_{k=k_F} \tag{8.24}$$

  In this case U_0 becomes

$$-U_0 = U(k_F^2) - \frac{\hbar^2 k_F^2}{2M_N}U_1, \quad U(k_F^2) = \frac{\hbar^2 k_F^2}{2M_N}U_1 - U_0 \tag{8.25}$$

- Zero s.p. potential approximation for unoccupied states: there is no clear way to defined s.p. potential above Fermi sea. (Though BBP theorem provides some recommendation.) Zero s.p. potential approximation is

$$\epsilon_k = \frac{\hbar^2 k^2}{2M}, \quad k > k_F \tag{8.26}$$

- In terms of self energy, the above relation can be written as

$$\begin{aligned} \epsilon &= \frac{\hbar^2 k^2}{2m} + \Sigma(k,\epsilon) = \frac{\hbar^2 k^2}{2m^*}, \\ \frac{m^*}{m} &= \left(1 + \frac{m}{\hbar^2 k}\frac{\partial \Sigma}{\partial k}\right)\left(1 - \frac{\partial \Sigma}{\partial \epsilon}\right)^{-1}, \\ \Sigma_{\sigma\tau}(k,\epsilon) &= \sum_{\sigma'\tau'}\frac{\Omega}{(2\pi)^3}\int d^3k' \langle \boldsymbol{k},\sigma,\tau;\boldsymbol{k}',\sigma',\tau'|V(1-P_{12})|\boldsymbol{k},\sigma,\tau;\boldsymbol{k}',\sigma',\tau'\rangle \end{aligned} \tag{8.27}$$

Further simplification is needed to solve Brueckner equation.

- Solve G-matrix equation.

$$\langle \mu'\nu'|G(\omega)|\mu\nu\rangle = \langle \mu'\nu'|V|\mu\nu\rangle + \langle \mu'\nu'|V\frac{Q}{\omega - h_0}G(\omega)|\mu\nu\rangle, \tag{8.28}$$

  with $\omega = \epsilon_\mu + \epsilon_\nu$ (? or $\omega = \epsilon_{\mu'} + \epsilon_{\nu'}$?).

  Inserting complete set of states, we gets equivalent equation

$$G(\boldsymbol{K}|\boldsymbol{k},\boldsymbol{k}_0) = V(\boldsymbol{k},\boldsymbol{k}_0) - \int d\boldsymbol{k}'\frac{V(\boldsymbol{k},\boldsymbol{k}')Q(\boldsymbol{k}',\boldsymbol{K})G(\boldsymbol{K}|\boldsymbol{k}',\boldsymbol{k}_0)}{E(\boldsymbol{k}',\boldsymbol{K}) - E(\boldsymbol{k}_0,\boldsymbol{K})}. \tag{8.29}$$

  This equation will be simplified further.

- Angle Average approximation on Q : The original Q-operator and energy denominator in G-matrix equation depends on the angles between $\boldsymbol{K}$, $\boldsymbol{k}'$, $\boldsymbol{k}_0$. This makes the Q can couple different relative angular momentum J states. To simplify the problem, one introduces angle average approximation, which makes $Q(\boldsymbol{k}', \boldsymbol{K}) \to \bar{Q}(k', K)$ depends only on the magnitudes,

$$\begin{aligned} \bar{Q}(k', K) = & \quad 0, & \text{for } k' \le \sqrt{k_F^2 - K^2}, \\ = & \quad 1, & \text{for } k' \ge k_F + K, \\ = & \quad \tfrac{K^2 + k'^2 - k_F^2}{2Kk'}, & \text{for } \sqrt{k_F^2 - K^2} < k' \le k_F + K \end{aligned} \tag{8.30}$$

  where $\bar{Q}(k', K)$ has discontinuous derivatives at $k' = \sqrt{k_F^2 - K^2}$ and $k' = k_F + K$. [5]

- Effective mass approximation simplifies the denominator: Original denominator depends on angles

$$E(\boldsymbol{k}', \boldsymbol{K}) \quad = \quad \frac{\hbar^2 K^2}{M_N} + \frac{\hbar^2 k'^2}{M_N} + U(|\boldsymbol{K} + \boldsymbol{k}'|) + U(|\boldsymbol{K} - \boldsymbol{k}'|). \tag{8.32}$$

  However, in effective mass approximation they becomes,

$$\begin{aligned} E(k', K) &\simeq \frac{\hbar^2}{M_N}(K^2 + k'^2) = E_>(k', K), \quad k', K \text{ pair are above } k_F \ , \\ E(k_0, K) &\simeq \frac{\hbar^2(K^2 + k_0^2)}{M_N^*} - 2U_0 = E_<(k_0, K), \quad k_0, K \text{ pair are below } k_F \end{aligned} \tag{8.33}$$

  These approximation partly removes angle dependence from the equation.

- partial wave component :

  Let us assume that the potential only changes orbital angular momentum and does not depend on the spin(let us treat isospin separately). Then, one may define partial wave component of G or V as

$$V_{LL'}^{SJ}(k, k') \equiv \left(\frac{\pi}{2}\frac{M}{\hbar^2}\right) \int d\Omega_k \int d\Omega_{k'} \left(i^L \mathcal{Y}_{LS}^{JM}(\hat{k})\right)^\dagger V(\boldsymbol{k}, \boldsymbol{k}') \left(i^{L'} \mathcal{Y}_{L'S}^{JM}(\hat{k}')\right), \tag{8.34}$$

  where overall factor is just a normalization convention for $V_{LL'}^{SJ}(k, k')$ and one may write,

$$V(\boldsymbol{k}, \boldsymbol{k}') = \frac{2}{\pi}\frac{\hbar^2}{M} \sum_{LL'SJM} \left(i^L \mathcal{Y}_{LS}^{JM}(\hat{k})\right) V_{LL'}^{SJ}(k, k') \left(i^{L'} \mathcal{Y}_{L'S}^{JM}(\hat{k}')\right)^\dagger \tag{8.35}$$

  Thus, above Bethe-Goldstone equation becomes after partial wave expansion (by multiplying tensor spherical harmonics and doing angle integration)

$$G_{LL'}^{\alpha}(K|k, k_0) = V_{LL'}^{\alpha}(k, k_0) - \frac{2}{\pi} \sum_l \int_0^\infty dk' \frac{k'^2 V_{Ll}^{\alpha}(k, k') \bar{Q}(k', K) G_{lL'}^{\alpha}(K|k', k_0)}{E_>(k', K) - E_<(k_0, K)} \tag{8.36}$$

[5] The form can be derived by averaging over all angles for fixed k' and K. Since initial states were within Fermi sea, $K \le k_F$. Letting z as a $\cos\theta$ of $\boldsymbol{k}'$ and $\boldsymbol{K}$,

$$\bar{Q}(k', K) = \frac{1}{2}\int_{-1}^{1} dz Q(k', K, z) \tag{8.31}$$

$Q(k', K, z) = 1$ if $-\frac{k'^2 + K^2 - k_F^2}{2k'K} \le z \le \frac{k'^2 + K^2 - k_F^2}{2k'K}$. This condition is always satisfied if $\frac{k'^2 + K^2 - k_F^2}{2k'K} > 1$, i.e. $k' \ge k_F + K$, but both fails if $k'^2 + K^2 - k_F^2 < 0$, i.e. $k' \le \sqrt{k_F^2 - K^2}$. In between, range of z is determined by above condition.

Note that there is no singularity in the integral because denominator never become zero.

Also, Note in this particular convention, dimensions are

$$\begin{aligned} [V(\boldsymbol{r},\boldsymbol{r}')] &= MeV^4, \quad \left[V(\boldsymbol{k},\boldsymbol{k}')\right] = MeV^{-2}, \\ [V^\alpha_{LL'}(k,k')] &= MeV^{-1}, \quad [G^\alpha_{LL'}(k,k')] = MeV^{-1} \end{aligned} \tag{8.37}$$

- The G-matrix can be solved by using the Matrix-inversion method. Letting,

$$\int_0^\infty dk f(k) \to \sum_{j=1}^N w_j f(k_j), \quad k_0 \to k_{N+1} \tag{8.38}$$

The partial wave expansion form becomes (in case of coupled channels, index k_j actually implies (L,j) pairs.)

$$\begin{aligned} G^\alpha_{LL'}(K|k_i,k_{N+1}) &= V^\alpha_{LL'}(k_i,k_{N+1}) \\ &\quad -\sum_l \sum_{j=1}^N V^\alpha_{Ll}(k_i,k_j) \left(\frac{2}{\pi} \frac{w_j k_j^{'2} \bar{Q}(k_j,K)}{E_>(k_j,K) - E_<(k_{N+1},K)} \right) G^\alpha_{lL'}(K|k_j,k_{N+1}), \\ &= V^\alpha_{LL'}(k_i,k_{N+1}) - \sum_l \sum_{j=1}^{N+1} V^\alpha_{Ll}(k_i,k_j) u_j G^\alpha_{lL'}(K|k_j,k_{N+1}) \end{aligned} \tag{8.39}$$

with

$$\begin{aligned} u_{j\le N} &= \frac{2}{\pi} \frac{w_j k_j^{'2} \bar{Q}(k_j,K)}{E_>(k_j,K) - E_<(k_{N+1},K)}, \\ u_{j=N+1} &= 0 \end{aligned} \tag{8.40}$$

This equation can be solved by $(N+1)\times(N+1)$ matrix inversion.

- It seems that $N \times N$ matrix may be enough? Unlike the T-matrix, the equation of G-matrix do not have singularity when k_0 is the same as the grid point k_i. Thus, one can simply solve the equation for $G(K|k_i,k_j)$. In that case, we may simply use $k_{i=1,\dots N}$, with

$$\begin{aligned} G^\alpha_{LL'}(K|k_i,k_j) &= V^\alpha_{LL'}(k_i,k_j) \\ &\quad -\sum_l \sum_{n=1}^N V^\alpha_{Ll}(k_i,k_n) \left(\frac{2}{\pi} \frac{w_n k_n^{'2} \bar{Q}(k_n,K)}{E_>(k_n,K) - E_<(k_j,K)} \right) G^\alpha_{lL'}(K|k_n,k_j), \\ &= V^\alpha_{LL'}(k_i,k_j) - \sum_l \sum_{n=1}^N F(k_i,k_n) G^\alpha_{lL'}(K|k_n,k_j) \end{aligned} \tag{8.41}$$

with

$$F(k_i,k_n) = \frac{2}{\pi} \frac{w_n k_n^{'2} \bar{Q}(k_n,K)}{E_>(k_n,K) - E_<(k_i,K)} ??? \tag{8.42}$$

In other words, actually choosing

$$G(K|k_i,k_j,\omega), \quad \text{with } \omega = E(k_i,K)?E(k_j,K)? \tag{8.43}$$

So that

$$G = V - FG \quad \to \quad G = (1+F)^{-1} V. \tag{8.44}$$

Calculation of single particle spectrum

Once G-matrix is obtained, using the G-matrix, one can calculate single particle energy, $U(k_\mu)$ for $|\boldsymbol{k}_\mu| \le k_F$.

$$\langle \mu|U|\mu\rangle = U(k_\mu) = \sum_{\nu<F} \langle \mu\nu|G(\epsilon_\mu+\epsilon_\nu)|\mu\nu-\nu\mu\rangle, \text{ for } \mu \le F, \tag{8.45}$$

If there is no spin dependence in the potential, we may average over spin projection over m_μ. Also, the anti-symmetrization in the right hand part will give $1-(-1)^{L+S+T}$ factors when partial wave decomposed. Thus, as long as we only consider partial waves such that $L+S+T=$ odd, it gives factor 2.(**Is this correct**?) Thus,

$$\begin{aligned}
U(k_\mu) &= \frac{1}{2}\sum_{m_\mu}\langle m_\mu|U(\boldsymbol{k}_\mu)|m_\mu\rangle \\
&= \frac{1}{2}\sum_{m_\mu}\int_F d^3k_\nu \sum_{m_\nu}\left(\langle \boldsymbol{k}_\mu\boldsymbol{k}_\nu, m_\mu m_\nu|G(\omega)|\boldsymbol{k}_\mu\boldsymbol{k}_\nu, m_\mu m_\nu\rangle - \langle \boldsymbol{k}_\mu\boldsymbol{k}_\nu, m_\mu m_\nu|G(\omega)|\boldsymbol{k}_\nu\boldsymbol{k}_\mu, m_\nu m_\mu\rangle\right) \\
&\to \sum_{m_\mu}\sum_{m_\nu}\int_F d^3k_\nu \langle \boldsymbol{k}_\mu\boldsymbol{k}_\nu, m_\mu m_\nu|G(\omega)|\boldsymbol{k}_\mu\boldsymbol{k}_\nu, m_\mu m_\nu\rangle, \quad \text{only L+S+T=odd waves} \\
&= \sum_{m_\mu}\sum_{m_\nu}\int_F d^3k_\nu \langle m_\mu m_\nu|G(\boldsymbol{K}|\boldsymbol{k},\boldsymbol{k})|m_\mu m_\nu\rangle
\end{aligned} \tag{8.46}$$

Since the $\boldsymbol{k}_\mu$ is fixed , we have to find range of $\boldsymbol{k}, \boldsymbol{K}$ satisfying both $k_\mu \le k_F$ and $k_\nu \le k_F$. Change of variable $\boldsymbol{k}_\nu$ as

$$\boldsymbol{k}_\nu = \boldsymbol{k}_\mu - 2\,\boldsymbol{k}, \quad d^3k_\nu \to (-2)^3 d^3k \tag{8.47}$$

For given $\boldsymbol{k}_\mu$, the angle between $\boldsymbol{k}$ and $\boldsymbol{k}_\mu$ can be rewritten in terms of K(for given k),

$$\boldsymbol{k}_\mu - \boldsymbol{k} = \boldsymbol{K} \;\to\; \cos\theta = \frac{K^2-k^2-k_\mu^2}{-2kk_\mu} \tag{8.48}$$

$$\begin{aligned}
\sum_{\nu<F} &\to \frac{\Omega}{(2\pi)^3}\int_F d^3k_\nu \to \int_F (-2)^3 d^3k \to \int_F (-2)^3 dk k^2 d\cos\theta(2\pi) \\
&\to \int_F (-2)^3 dk k^2 dK \frac{2K}{-2kk_\mu}(2\pi) \to \frac{16\pi}{k_\mu}\int dkk \int dKK
\end{aligned} \tag{8.49}$$

where,$\frac{\Omega}{(2\pi)^3}$ cancels with the normalization of wave function.

Now, if we introduce partial wave expansion of G-matrix

$$\begin{aligned}
U(k_\mu) &\to \sum_{m_\mu m_\nu}\frac{16\pi}{k_\mu}\int dkk\int dKK\langle m_\mu m_\nu|G(\boldsymbol{K}|\boldsymbol{k},\boldsymbol{k})|m_\mu m_\nu\rangle \\
&= \frac{16\pi}{k_\mu}\int dkk\int dKK\frac{2}{\pi}\frac{\hbar^2}{M}\sum_{LL'SJM}\langle m_\mu m_\nu|\left(i^L\mathcal{Y}_{LS}^{JM}(\hat{k})\right)G_{LL'}^{SJ}(\boldsymbol{K},k,k)\left(i^{L'}\mathcal{Y}_{L'S}^{JM}(\hat{k})\right)^\dagger|m_\mu m_\nu\rangle \\
&= \frac{16\pi}{k_\mu}\frac{2}{\pi}\frac{\hbar^2}{M}\int dkk\int dKK\sum_{LL'SJM}\sum_{m_\mu m_\nu}G_{LL'}^{SJ}(\boldsymbol{K},k,k) \\
&\quad \times i^{L-L'}\left(\langle m_\mu m_\nu|\mathcal{Y}_{LS}^{JM}(\hat{k})\rangle\right)\left(\langle m_\mu m_\nu|\mathcal{Y}_{L'S}^{JM}(\hat{k})\rangle\right)^\dagger
\end{aligned} \tag{8.50}$$

here, $\hat{k}$ is actually a function of k and K. By decomposing tensor spherical harmonics,

$$\langle m_\mu m_\nu|\mathcal{Y}_{LS}^{JM}(\hat{k})\rangle = \sum_{M_L M_S} Y_{LM_L}(\hat{k})\langle\frac{1}{2}m_\mu\frac{1}{2}m_\nu|SM_S\rangle\langle LM_L SM_S|(LS)JM\rangle \tag{8.51}$$

Then,

$$U(k_\mu) = \frac{16\pi}{k_\mu}\frac{2}{\pi}\frac{\hbar^2}{M}\int dkk\int dKK\sum_{LL'SJM}\sum_{m_\mu m_\nu}\sum_{M_L M_S}\sum_{M'_L M'_S} G^{SJ}_{LL'}(\boldsymbol{K},k,k)i^{L-L'}Y_{LM_L}(\hat{k})Y^*_{L'M'_L}(\hat{k})$$
$$\times\langle\frac{1}{2}m_\mu\frac{1}{2}m_\nu|SM_S\rangle\langle LM_L SM_S|(LS)JM\rangle\langle\frac{1}{2}m_\mu\frac{1}{2}m_\nu|SM'_S\rangle\langle L'M'_L SM'_S|(LS)JM\rangle$$

then, sum over m_μ, m_ν gives $\delta_{M_S M'_S}$ and sum over M, M_S gives $\delta_{LL'}\delta_{M'_L M_L}$,

$$\sum_{m_1 m_2}\langle JM|j_1 m_1 j_2 m_2\rangle\langle j_1 m_1 j_2 m_2|J'M'\rangle = \delta_{JJ'}\delta_{MM'}$$
$$\sum_{Mm_1}\langle JM|j_1 m_1 j_2 m_2\rangle\langle j_1 m_1 j'_2 m'_2|JM\rangle = \frac{(2J+1)}{(2j_2+1)}\delta_{j_2 j'_2}\delta_{m_2 m'_2} \tag{8.52}$$

Thus,

$$U(k_\mu) = \frac{16\pi}{k_\mu}\frac{2}{\pi}\frac{\hbar^2}{M}\int dkk\int dKK\sum_{LL'SJM}\sum_{M_L M_S}\sum_{M'_L} G^{SJ}_{LL'}(\boldsymbol{K},k,k)i^{L-L'}Y_{LM_L}(\hat{k})Y^*_{L'M'_L}(\hat{k})$$
$$\times\langle LM_L SM_S|(LS)JM\rangle\langle L'M'_L SM_S|(LS)JM\rangle$$
$$= \frac{16\pi}{k_\mu}\frac{2}{\pi}\frac{\hbar^2}{M}\int dkk\int dKK\sum_{LSJ}\sum_{M_L} G^{SJ}_{LL}(\boldsymbol{K},k,k)\frac{(2J+1)}{(2L+1)}|Y_{LM_L}(\hat{k})|^2 \tag{8.53}$$

From the relation

$$\sum_M\frac{1}{2L+1}|Y_{LM}|^2 = \frac{1}{4\pi} \tag{8.54}$$

We get

$$U(k_\mu) = \frac{8}{\pi}\frac{\hbar^2}{M}\frac{1}{k_\mu}\sum_{LSJT}(2J+1)(2T+1)\int dkk\int dKK G^{SJT}_{LL}(\boldsymbol{K},k,k). \tag{8.55}$$

where I included isospin by assuming potential does not depend on the isospin projection. Also note that the sum should be done only for $L+S+T$ =odd cases.

Now let us consider the range of integration. From the constraint, $k_\mu \le k_F$ and $k_\nu \le k_F$,

$$0 \le (k_\nu^2 = k_\mu^2 + 4k^2 - 4kk_\mu\cos\theta) \le k_F^2,$$
$$-1 \le (\cos\theta = \frac{K^2 - k^2 - k_\mu^2}{-2kk_\mu}) \le 1. \tag{8.56}$$

The these relation gives $k \le \frac{1}{2}(k_F + k_\mu)$, $|k - k_\mu| < K < k + k_\mu$ for given k. Also, replacing $\cos\theta$ in the first relation,

$$0 \le 2k^2 - k_\mu^2 + 2K^2 \le k_F^2,$$
$$\rightarrow \quad \sqrt{\frac{k_\mu^2 - 2k^2}{2}} \le K \le \sqrt{\frac{k_F^2 + k_\mu^2 - 2k^2}{2}} \tag{8.57}$$

Thus,

$$\text{if } 0 \le k \le \frac{1}{2}(k_F - k_\mu),\ k_\mu - k \le K \le k_\mu + k,$$
$$\text{if } \frac{1}{2}(k_F - k_\mu) \le k \le \frac{1}{2}(k_F + k_\mu),\ |k_\mu - k| \le K \le \sqrt{\frac{k_F^2 + k_\mu^2 - 2k^2}{2}}. \tag{8.58}$$

Thus we get the equation in (3.17) of the Haftel and Tabakin. (**up to factor 2**?)

$$U(k_\mu) = \frac{\mathbf{8}}{\pi}\frac{\hbar^2}{M_N}\frac{1}{k_\mu}\sum_{JSTL}(2J+1)(2T+1)\left\{\left[\int_0^{\frac{1}{2}(k_F-k_\mu)} dk_0 k_0 \int_{k_\mu-k_0}^{k_\mu+k_0} dKK + \int_{\frac{1}{2}(k_F-k_\mu)}^{\frac{1}{2}(k_F+k_\mu)} dk_0 k_0 \int_{|k_\mu-k_0|}^{\sqrt{\frac{k_F^2+k_\mu^2-2k_0^2}{2}}} dKK\right]\right\} G^\alpha_{LL}(K|k_0,k_0). \tag{8.59}$$

To reduce the integral, one can introduce another approximation.

- Average c.m. momentum approximation: If we approximate,

$$G^\alpha_{LL}(K|k_0,k_0) \simeq G^\alpha_{LL}(K_{av}|k_0,k_0) \tag{8.60}$$

we may simplify the integral over K. Then, in two cases of k_0, average c.m. momentum becomes[6]

$$\begin{aligned} K^2_{av} &= k_\mu^2 + k_0^2, \quad \text{for } 2k_0 \le k_F - k_\mu, \\ &= k_\mu^2 + k_0^2 - \frac{1}{4}(2k_0+k_\mu-k_F)(2k_0+k_\mu+k_F), \quad \text{for } k_F-k_\mu \le 2k_0 \le k_F+k_\mu \end{aligned}$$

With this approximation, integral over K can be done simply, and we get eq.(3.20) of Haftel and Tabakin up to some typo. (factor 2?)

$$\begin{aligned} U(k_\mu) &= \frac{\mathbf{8}}{\pi}\frac{\hbar^2}{M_N}\frac{1}{k_\mu}\sum_{JSTL}(2J+1)(2T+1)\left\{\int_0^{\frac{1}{2}(k_F-k_\mu)} dk_0 k_0 \times 2k_\mu k_0 G^\alpha_{LL}(K_{av,1}|k_0,k_0) \right. \\ &\quad \left. + \int_{\frac{1}{2}(k_F-k_\mu)}^{\frac{1}{2}(k_F+k_\mu)} dk_0 k_0 \times \frac{1}{4}(k_F^2-k_\mu^2-4k_0^2+4k_\mu k_0) G^\alpha_{LL}(K_{av,2}|k_0,k_0)\right\} \\ &= \frac{\mathbf{16}}{\pi}\frac{\hbar^2}{M_N}\sum_{JSTL}(2J+1)(2T+1)\left\{\int_0^{\frac{1}{2}(k_F-k_\mu)} dk_0 k_0^2 G^\alpha_{LL}(K_{av,1}|k_0,k_0) \right. \\ &\quad \left. + \frac{1}{2k_\mu}\int_{\frac{1}{2}(k_F-k_\mu)}^{\frac{1}{2}(k_F+k_\mu)} dk_0 k_0 \frac{1}{4}(k_F^2-k_\mu^2-4k_0^2+4k_\mu k_0) G^\alpha_{LL}(K_{av,2}|k_0,k_0)\right\} \end{aligned} \tag{8.61}$$

One have to determine U_0 and M^* of effective mass approximation from $U(k_\mu)$. It is not clearly written in the reference, how one determine new M^* and U_0 from $U(k_\mu)$ for next iteration. However, I think these values should be fixed around $k_\mu = k_F$ instead of $k_\mu = 0$.

Calculation of the binding energy of nuclear matter

Once the G-matrix and single particle energy is obtained, one can compute energy density of nuclear matter, E/A

$$E = \sum_{\mu<F}\langle\mu|\frac{p^2}{2M}|\mu\rangle + \frac{1}{2}\sum_{\mu\nu<F}\langle\mu\nu|G(\epsilon_\mu+\epsilon_\nu)|\mu\nu-\nu\mu\rangle. \tag{8.62}$$

The first term is simply[7],

$$\sum_{\mu<F}\langle\mu|\frac{p^2}{2M}|\mu\rangle = \frac{\Omega}{(2\pi)^3}\int_F d^3k\frac{\hbar^2k^2}{2M_N} = \Omega\epsilon_F = \frac{3}{5}\epsilon_F A \tag{8.63}$$

[6]It is simply average of K^2 values in range, $K \in [a,b]$, $K^2_{av} = \frac{1}{2}(a^2+b^2)$.

[7]sum over μ implies also the spin and isospin of a nucleon

Note that this expression is rather different from $U(k_\mu)$ because now k_μ is not fixed. Thus,

$$\sum_{\mu\nu<F} \to \frac{\Omega^2}{(2\pi)^6}\int d^3k \int d^3K \sum_{S,T} \tag{8.64}$$

$$\begin{aligned}\int_F d^3k_1 \int_F d^3k_2(..) &= \int d^3k d^3K \Theta(k_F - |\boldsymbol{K}+\boldsymbol{k}|)\Theta(k_F - |\boldsymbol{K}-\boldsymbol{k}|)(..) \\ &= \int dk k^2 d\cos\theta (2\pi) dK K^2 (4\pi)\Theta(k_F - |\boldsymbol{K}+\boldsymbol{k}|)\Theta(k_F - |\boldsymbol{K}-\boldsymbol{k}|)(..),\end{aligned}$$

In case of partial wave expansion, there will be spherical harmonics of $Y_L(\theta)Y^*_{L'}(\theta)$. Thus, the angle integration over θ will be changed into $\delta_{LL'}$. (No restriction on angle??) and the range of integration is determined by the condition, $|\boldsymbol{k}_0 \pm \boldsymbol{K}| \le k_F$. C.M. part of wave function removes the K integral. On the other hand, the condition gives constraint on

$$-\frac{k_F^2 - K^2 - k_0^2}{2k_0K} \le \cos\theta \le \frac{k_F^2 - K^2 - k_0^2}{2k_0K}, \tag{8.65}$$

and thus angle integration of k can be replaced by integration over K for given k. (More discussion on the range of integration required)

For the second term, the similar procedure as the calculation of $U(k_\mu)$ gives (**Needs confirmation**)

$$\begin{aligned}\frac{E}{A} &= \frac{3}{5}\epsilon_F + \frac{3}{\pi^2}\frac{\hbar^2}{M_N}\frac{1}{k_F^3}\sum_{LSJT}(2J+1)(2T+1)\left\{4\pi\int_0^{k_F} dk_0 k_0^2 \left[\int_0^{k_F-k_0} dK K^2 \right.\right. \\ &\left.\left. + \frac{1}{2}\int_{k_F-k_0}^{\sqrt{k_F^2-k_0^2}} dK K^2 \frac{k_F^2 - K^2 - k_0^2}{k_0 K}\right] G^\alpha_{LL}(K|k_0,k_0)\right\}.\end{aligned} \tag{8.66}$$

We may simplify the integration over K by approximation.

- average value of K approximation in energy:

$$G^\alpha_{LL}(K|k_0,k_0) \simeq G^\alpha_{LL}(\tilde{K}_{av}|k_0,k_0) \tag{8.67}$$

with the average value of K,

$$\tilde{K}^2_{av} = \frac{3}{5}k_F^2(1-\frac{k_0}{k_F})[1+\frac{k_0^2/k_F^2}{3(2+k_0/k_F)}] \tag{8.68}$$

This average is obtained from average of K -value with fixed k in the region where each particle are in the Fermi sea. (Need confirmation)

Then, in this approximation, we get (Need confirmation)

$$\frac{E}{A} = \frac{3}{5}\epsilon_F + \frac{4}{\pi}\frac{\hbar^2}{M_N}\sum_{LSJT}(2J+1)(2T+1)\int_0^{k_F} dk_0 k_0^2 \left(1 - \frac{3}{2}\frac{k_0}{k_F} + \frac{1}{2}\frac{k_0^3}{k_F^3}\right) G^\alpha_{LL}(\tilde{K}_{av};k_0,k_0) \tag{8.69}$$

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[8]From

$$\int_0^{k_F-k_0} dK K^2 + \frac{1}{2}\int_{k_F-k_0}^{\sqrt{k_F^2-k_0^2}} dK K^2 \frac{k_F^2 - K^2 - k_0^2}{k_0 K} = \frac{k_F^3}{3}\left(1 - \frac{3}{2}\frac{k_0}{k_F} + \frac{1}{2}\frac{k_0^3}{k_F^3}\right) \tag{8.70}$$

8.2 Another derivation

This time let us try to do the same derivation in different convention. Basically, I am trying to use the same convention as "Nuclear structure from Nuclei to Neutron stars" lecture given by M. Hjorth-Jensen.

First convention

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \langle \boldsymbol{r}|\boldsymbol{k}\rangle = 4\pi \sum_{lm} i^l j_l(kr) Y^*_{lm}(\hat{k}) Y_{lm}(\hat{r}) \tag{8.71}$$

$$\langle \boldsymbol{k}'\boldsymbol{K}'|V|\boldsymbol{k}\boldsymbol{K}\rangle = \int d\boldsymbol{r} d\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} V(\boldsymbol{r}',\boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \delta(\boldsymbol{K}',\boldsymbol{K}) \tag{8.72}$$

where it is not clear for the definition(or normalization) of $\langle \boldsymbol{K}'|\boldsymbol{K}\rangle = \delta(\boldsymbol{K}',\boldsymbol{K})$, but we can rewrite relative momentum dependence part, Assuming potential is not spin-dependent,(because of conservation of spin, the z-component of orbital angular momentum also should conserve. Thus no summation over m')

$$\begin{aligned}
\langle \boldsymbol{k}', S'M'_S|V|\boldsymbol{k}, SM_S\rangle &= \delta_{SS'}\delta_{M_S M'_S}(4\pi)^2 \sum_{ll'}\sum_{m} i^{-l'+l} Y_{l'm}(\hat{k}') Y^*_{lm}(\hat{k}) \\
&\quad \times \int dr' r'^2 dr r^2 j_{l'}(k'r') \Big[\int d\Omega_r d\Omega_{r'} Y^*_{l'm}(\hat{r}') \langle SM_S|V(\boldsymbol{r}',\boldsymbol{r})|SM_S\rangle Y_{lm}(\hat{r}) \Big] j_l(kr) \\
&= \delta_{SS'}\delta_{M_S M'_S}(4\pi)^2 \sum_{ll'}\sum_{m}\sum_{J} i^{-l'+l} Y_{l'm}(\hat{k}') Y^*_{lm}(\hat{k}) C^{JM}_{l'mSM_S} C^{JM}_{lmSM_S} \\
&\quad \times \langle k'l'STJM|V|klSTJM\rangle
\end{aligned} \tag{8.73}$$

where,

$$\begin{aligned}
\langle k'l'STJM|V|klSTJM\rangle &\equiv \int dr' r'^2 dr r^2 j_{l'}(k'r') \langle l'STJM|V(r',r)|lSTJM\rangle j_l(kr), \\
\langle l'STJM|V(r',r)|lSTJM\rangle &\equiv \int d\Omega_r d\Omega_{r'} \mathcal{Y}^M_{l'SJ}(\hat{r}')^\dagger V(\boldsymbol{r}',\boldsymbol{r}) \mathcal{Y}^M_{lSJ}(\hat{r})
\end{aligned} \tag{8.74}$$

This partial wave expansion have difference from previous one, in the normalization and i factors.

For the G-matrix equation,

$$G(\omega) = V + V\frac{Q}{\omega - H_0} G \tag{8.75}$$

where ω is a starting energy of two particle and H_0 is s.p. energies of two particles.

Chapter 9

Relativistic mean-field : QHD theory

Chapter 10

Relativistic Hartree-Bogoliubov theory

RHB (Relativistic Hartree Bogoliubov) equation(from Lulu Li et.al., arxiv:1202.0070) is

$$\sum_{s'p'}\int d^3\boldsymbol{r}' \begin{pmatrix} h_D(\boldsymbol{r}sp,\boldsymbol{r}'s'p')-\lambda & \Delta(\boldsymbol{r}sp,\boldsymbol{r}'s'p') \\ -\Delta^*(\boldsymbol{r}sp,\boldsymbol{r}'s'p') & -h_D(\boldsymbol{r}sp,\boldsymbol{r}'s'p')+\lambda \end{pmatrix} \begin{pmatrix} U_k(\boldsymbol{r}'s'p') \\ V_k(\boldsymbol{r}'s'p') \end{pmatrix} = E_k \begin{pmatrix} U_k(\boldsymbol{r}sp) \\ V_k(\boldsymbol{r}sp) \end{pmatrix} \quad (10.1)$$

where E_k is a quasiparticle energy, λ is a chemical potential, p is a index for upper and lower component. The potential depends on the densities,

$$\begin{aligned} \rho_s(\boldsymbol{r}) &= \sum_{k>0} V_k^\dagger(\boldsymbol{r})\gamma_0 V_k(\boldsymbol{r}), \\ \rho_v(\boldsymbol{r}) &= \sum_{k>0} V_k^\dagger(\boldsymbol{r}) V_k(\boldsymbol{r}), \\ \rho_3(\boldsymbol{r}) &= \sum_{k>0} V_k^\dagger(\boldsymbol{r})\tau_3 V_k(\boldsymbol{r}), \\ \rho_c(\boldsymbol{r}) &= \sum_{k>0} V_k^\dagger(\boldsymbol{r})\frac{1-\tau_3}{2} V_k(\boldsymbol{r}), \\ \kappa(\boldsymbol{r}) &= \sum_{k} V_k^\dagger(\boldsymbol{r}) U_k(\boldsymbol{r}). \end{aligned} \quad (10.2)$$

I am going to follow Lulu Li et.al., arxiv:1202.0070 for details of how to solve this equation. For the derivation of RHB equation and meanings will be added later.

10.1 Central field Dirac equation

Let us assume fermion under central potential. Dirac equation becomes

$$\begin{aligned} h_D\phi_k &= \epsilon_k\phi_k, \\ h_D &= c\boldsymbol{\alpha}\cdot\boldsymbol{p} + c^2\beta[M+S(r)] + V(r), \quad V(r) = V_c(r) + V_{nuc}(r) \end{aligned} \quad (10.3)$$

where k is an eigen-state index, ϵ_k can be $-mc^2 < \epsilon_k < mc^2$ for bound state, $\epsilon_k > mc^2$ for positive continuum state, $\epsilon_k < -mc^2$ for negative continuum state. If one use solutions as a complete basis, one have to include both positive and negative solutions regardless one use "no-sea" approximation or not.

Because of rotational symmetry, total angular momentum $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$ is conserved. In other words, jm is a conserved quantity. For given jlm, spinor spherical harmonics is defined as

$$\Omega_{jlm}(\theta,\phi) = \sum_\mu C(lm-\mu,\frac{1}{2}\mu;jm) Y_{l,-m-\mu}(\theta,\phi)\chi_\mu \quad (10.4)$$

In explicit form,

$$\begin{aligned}\Omega_{j=l+\frac{1}{2},lm} &= \begin{pmatrix} \sqrt{\frac{l+m+1/2}{2l+1}}Y_{lm-\frac{1}{2}}(\theta,\phi) \\ \sqrt{\frac{l-m+1/2}{2l+1}}Y_{lm+\frac{1}{2}}(\theta,\phi) \end{pmatrix} \\ \Omega_{j=l-\frac{1}{2},lm} &= \begin{pmatrix} -\sqrt{\frac{l-m+1/2}{2l+1}}Y_{lm-\frac{1}{2}}(\theta,\phi) \\ \sqrt{\frac{l+m+1/2}{2l+1}}Y_{lm+\frac{1}{2}}(\theta,\phi) \end{pmatrix} \end{aligned} \tag{10.5}$$

where it is written in column in χ_+ and χ_- basis. This spinor spherical harmonic is an eigen function of $\boldsymbol{\sigma}\cdot\boldsymbol{L}$ or $\hat{K}=-1-\boldsymbol{\sigma}\cdot\boldsymbol{L}$ operator.

$$\hat{K}\Omega_{jlm}(\theta,\phi)=\kappa\Omega_{jlm}(\theta,\phi), \quad \left\{ \begin{array}{cc} \kappa=-l-1 & \text{for } j=l+\frac{1}{2} \\ \kappa=l & \text{for } j=l-\frac{1}{2} \end{array} \right\} \tag{10.6}$$

Thus, one can use κm instead of jm.

$$\int d\Omega_r \Omega^\dagger_{\kappa' m'}(\hat{r})\Omega_{\kappa m}(\hat{r})=\delta_{\kappa\kappa' mm'} \tag{10.7}$$

($\kappa>0$ means $j=l+\frac{1}{2}$, $l=-\kappa-1$ and $\kappa<0$ means $j=l-\frac{1}{2}$,$l=|\kappa|$)
Then,

$$\begin{aligned} &\boldsymbol{\sigma}\cdot\hat{r}\Omega_{\kappa m}(\theta,\phi)=-\Omega_{-\kappa m}(\theta,\phi), \\ &\boldsymbol{\sigma}\cdot\boldsymbol{p}f(r)\Omega_{\kappa m}(\theta,\phi)=i\left(\frac{df}{dr}+\frac{\kappa+1}{r}f(r)\right)\Omega_{-\kappa m}(\theta,\phi) \end{aligned} \tag{10.8}$$

and solution of Dirac equation can be written as

$$\phi_{\kappa m}(r)=\frac{1}{r}\begin{pmatrix} iP_\kappa(r)\Omega_{\kappa m}(\hat{r}) \\ Q_\kappa(r)\Omega_{-\kappa m}(\hat{r}) \end{pmatrix}. \tag{10.9}$$

(Note this is a 4-component.) and $P_\kappa(r)$ and Q_κ satisfies (need verification..)

$$\begin{aligned} &(V(r)+m+S(r))P_\kappa(r)+c\left(\frac{d}{dr}-\frac{\kappa}{r}\right)Q_\kappa(r)=\epsilon_\kappa P_\kappa, \\ &-c\left(\frac{d}{dr}+\frac{\kappa}{r}\right)P_\kappa(r)+(V(r)-m-S(r))Q_\kappa(r)=\epsilon_\kappa Q_\kappa. \end{aligned} \tag{10.10}$$

with normalization

$$\int_0^\infty dr[P^2_\kappa(r)+Q^2_\kappa(r)]=1. \tag{10.11}$$

10.2 WS basis ?

We may use coordinate space representation $x=(\boldsymbol{r}sp)$, where s is the spin coordinate and p describes large(or upper) ($p=1$ or $p=+$) and small (or lower) ($p=2$ or $p=-$) components. Also, we may define W-S shape basis, $|n\kappa m\rangle$ such that

$$\langle \boldsymbol{r}sp|n\kappa m\rangle=\phi_{n\kappa m}(\boldsymbol{r}sp)=i^p\frac{R_{n\kappa}(r,p)}{r}Y^{l(p)}_{\kappa m}(\Omega,s) \tag{10.12}$$

In other words,

$$\phi_{n\kappa m}(\boldsymbol{r}s)=\frac{1}{r}\begin{pmatrix} iG_{n\kappa}(r)Y^{l(p=1)}_{jm}(\Omega s) \\ -F_{n\kappa}(r)Y^{l(p=2)}_{jm}(\Omega s) \end{pmatrix}=\begin{pmatrix} \phi_{n\kappa m}(\boldsymbol{r}s1) \\ \phi_{n\kappa m}(\boldsymbol{r}s2) \end{pmatrix} \tag{10.13}$$

where orbital angular momentum $l(p=1) = j + \frac{1}{2}\text{sign}(\kappa)$ and $l(p=2) = j - \frac{1}{2}\text{sign}(\kappa)$, $R_{n\kappa}(r,1) = G_{n\kappa}(r)$, $R_{n\kappa}(r,2) = F_{n\kappa}(r)$ and $Y^l_{\kappa m}$ is

$$Y^l_{\kappa m}(\Omega, s) = \sum_{m_l, m_s} C(\frac{1}{2} m_s l m_l | jm) Y_{lm_l}(\Omega) \chi_{\frac{1}{2}, m_s} \tag{10.14}$$

Time-reversal state

$$\bar{\phi}_{n\kappa m}(\boldsymbol{r} sp) = (-1)^{p+l(p)+j-m} \phi_{n\kappa -m}(\boldsymbol{r} sp). \tag{10.15}$$

For given $(n\kappa)$ value, there are two solutions with $\epsilon_{n\kappa} > 0$ and $\epsilon_{n\kappa} < 0$. Thus, complete basis should include both solutions(?).

We can define WS basis with WS potentials $S^{(0)}(r)$ and $V^{(0)}(r)$, which are not mean fields,

$$h_D^{(0)} = \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta[M + S^{(0)}(r)] + V^{(0)}(r). \tag{10.16}$$

Then, original Hamiltonian can be written by expanding in Legendre polynomials

$$\begin{aligned} h_D &= \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta[M + S(\boldsymbol{r})] + V(\boldsymbol{r}) \\ &= h_D^{(0)} + \sum_\lambda [\beta S'_\lambda(r) + V'_\lambda(r)] P_\lambda(\hat{r}). \end{aligned} \tag{10.17}$$

with $S'_0(r) = S_0(r) - S^{(0)}(r)$ and $S'_\lambda(r) = S_\lambda(r)$ for $\lambda \neq 0$, $V'_0(r) = V_0(r) - V^{(0)}(r)$ and $V'_\lambda(r) = V_\lambda(r)$ for $\lambda \neq 0$.

coupled equation for basis function?

The quasiparticle wave functions U_k and V_k are represented as

$$\begin{aligned} U_k(\boldsymbol{r} sp) &= \sum_{n\kappa} u^{(m)}_{k,(n\kappa)} \phi_{n\kappa m}(\boldsymbol{r} sp), \\ V_k(\boldsymbol{r} sp) &= \sum_{n\kappa} v^{(m)}_{k,(n\kappa)} \bar{\phi}_{n\kappa m}(\boldsymbol{r} sp) \end{aligned} \tag{10.18}$$

where the sum $\sum_{k>0}$ needs cutoffs. Smooth cutoff is introduced with two parameters, $E^{q.p}_{cut}$ and $\Gamma^{q.p}_{cut}$ such as $\sqrt{s(E_k)}$ factors is multiplied to V_k of $v^2 < 1/2$.

$$s(E_k) = \frac{1}{2}\left(1 - \frac{E_k - E^{q.p}_{cut}}{\sqrt{(E_k - E^{q.p}_{cut})^2 + (\Gamma^{q.p}_{cut})^2}}\right) \tag{10.19}$$

To include continuum, one may introduce large spherical box for discretized states.

RHB equation in WS basis is

$$\begin{pmatrix} \mathcal{A} - \lambda & \mathcal{B} \\ \mathcal{B}^\dagger & -\mathcal{A}^* + \lambda \end{pmatrix} \begin{pmatrix} \mathcal{U}_k \\ \mathcal{V}_k \end{pmatrix} = E_k \begin{pmatrix} \mathcal{U}_k \\ \mathcal{V}_k \end{pmatrix} \tag{10.20}$$

where

$$\mathcal{U}_k = \left(u^{(m)}_{k,(n\kappa)}\right), \ \mathcal{V}_k = \left(v^{(m)}_{k,(n\kappa)}\right), \tag{10.21}$$

and

$$\begin{aligned} \mathcal{A} &= \left(h^{(m)}_{D(n\kappa)(n'\kappa')}\right) = \left(\langle n\kappa m | h_D | n'\kappa' m \rangle\right), \\ \mathcal{B} &= \left(\Delta^{(m)}_{(n\kappa)(n'\kappa')}\right) = \left(\langle n\kappa m | \Delta | \overline{n'\kappa' m} \rangle\right) \end{aligned} \tag{10.22}$$

Matrix elements in WS basis,

$$\langle n\kappa m | h_D | n'\kappa' m' \rangle, \quad \langle n\kappa m | \Delta | n'\kappa' m' \rangle \tag{10.23}$$

should be obtained. If h_D or Δ are axial symmetric, one can expand potentials, densities with Legendre Polynomials,

$$\begin{aligned} f(\boldsymbol{r}) &= \sum_\lambda f_\lambda(r) P_\lambda(\cos\theta), \quad \lambda = 0, 2, 4 \ldots, \\ f_\lambda(r) &= \frac{2\lambda+1}{4\pi} \int d\Omega f(\boldsymbol{r}) P_\lambda(\Omega) \end{aligned} \tag{10.24}$$

For local potentials, we need basis function product,

$$\sum_s \phi_{n\kappa m}(\boldsymbol{r}sp)\phi^*_{n'\kappa' m}(\boldsymbol{r}sp) \tag{10.25}$$

$$\left[\sum_s \phi_{n\kappa m}(\boldsymbol{r}sp)\phi^*_{n'\kappa' m}(\boldsymbol{r}sp)\right]_\lambda = \frac{R_{n\kappa}(r,p)}{r}\frac{R_{n'\kappa'}(r,p)}{r}\langle \kappa m|P_\lambda|\kappa' m\rangle \tag{10.26}$$

For even values of $l+\lambda+l'$,

$$\langle \kappa m|P_\lambda|\kappa' m\rangle = (-1)^{m-\frac{1}{2}}\hat{j}\hat{j}' \begin{pmatrix} j & \lambda & j' \\ -m & 0 & m \end{pmatrix} \begin{pmatrix} j & \lambda & j' \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \tag{10.27}$$

where $\hat{j} = \sqrt{2j+1}$ and odd values of $l+\lambda+l'$, the matrix element vanishes.

10.3 Matrix elements of DRHB Hamiltonian

For DRHB, we may write

$$\begin{aligned} U_k(\boldsymbol{r}, s, t) &= \begin{pmatrix} i\frac{G_U^{\alpha lj}(r)}{r} \\ \frac{F_U^{\alpha lj}(r)}{r}\boldsymbol{\sigma}\cdot\hat{r} \end{pmatrix} Y^l_{jm}(\theta,\phi)\chi_t \\ V_k(\boldsymbol{r}, s, t) &= \begin{pmatrix} i\frac{G_V^{\alpha lj}(r)}{r} \\ \frac{F_V^{\alpha lj}(r)}{r}\boldsymbol{\sigma}\cdot\hat{r} \end{pmatrix} Y^l_{jm}(\theta,\phi)\chi_t \end{aligned} \tag{10.28}$$

For given spherical $S(r)$ and $V(r)$, one can numerically obtain basis wave functions. For each κ, there is a positive and negative eigenvalues $\epsilon_{n\kappa}$.

One can rewrite the DRHB equations into coupled equations for F and G:...

For Hartree approximation and local paring interaction, we can let

$$\begin{aligned} &h_D(\boldsymbol{r}sp, \boldsymbol{r}'s'p') = h_D(\boldsymbol{r}, sp, s'p')\delta(\boldsymbol{r}-\boldsymbol{r}'), \\ &\Delta(\boldsymbol{r}p, \boldsymbol{r}'p') = \delta_{pp'}\Delta(\boldsymbol{r}p)\delta(\boldsymbol{r}-\boldsymbol{r}') \end{aligned} \tag{10.29}$$

where pairing is assumed only in spin $S=0$ (thus no spin index s dependence) and diagonal in p. Then, expansion is Legendre Polynomial,

$$h_D = h_D^{(0)} + \sum_\lambda [\beta S'_\lambda(r) + V'_\lambda(r)]P_\lambda(\Omega) \tag{10.30}$$

where $S'_0 = S_0 - S^{(0)}$, $V'_0 = V_0 - V^{(0)}$, and $S'_\lambda = S_\lambda$ and $V'_\lambda = V_\lambda$ for $\lambda > 0$.

$$\begin{aligned} \langle n\kappa|h_D|n'\kappa'\rangle &= \epsilon_{n\kappa}\delta_{nn'}\delta_{\kappa\kappa'} + \sum_\lambda \langle \kappa m|P_\lambda|\kappa' m\rangle \int dr[G_{n\kappa}(r)(V'_\lambda(r)+S'_\lambda(r))G_{n'\kappa'}(r) \\ &\quad + F_{n\kappa}(r)(V'_\lambda(r)-S'_\lambda(r))F_{n'\kappa'}(r)], \end{aligned} \tag{10.31}$$

Projection onto spin $S = 0$,

$$\phi_{n\kappa m}(\boldsymbol{r}s)\bar{\phi}_{n'\kappa' m}(\boldsymbol{r}s) \rightarrow \sum_s (-1)^{\frac{1}{2}-s}\phi_{n\kappa m}(s)\bar{\phi}_{n'\kappa' m}(-s) = \sum_s \phi_{n\kappa m}(s)\phi^*_{n\kappa' m}(s) \tag{10.32}$$

$$\begin{aligned}
\langle n\kappa|\Delta^{++}|n'\kappa'\rangle &= \sum_\lambda \langle \kappa m|P_\lambda|\kappa' m\rangle \int dr G_{n\kappa}(r)\Delta_\lambda(r)G_{n'\kappa'}(r), \\
\langle n\kappa|\Delta^{--}|n'\kappa'\rangle &= \sum_\lambda \langle \kappa m|P_\lambda|\kappa' m\rangle \int dr F_{n\kappa}(r)\Delta_\lambda(r)F_{n'\kappa'}(r),
\end{aligned} \tag{10.33}$$

10.3.1 Calculation of the densities

Chapter 11

Neutron Star application

REF : 'Nuclear structure from Nuclei to Neutron stars', M. Hjorth-Jensen., 'Neutron stars for Undergraduates' , R.R. Silbar and S. Reddy, `https://arxiv.org/abs/nucl-th/0309041v2`.

11.1 TOV equation

One of the application of nuclear matter study os to compute the neutron star mass and radius by using the equation of states from nuclear matter study. The TOV equation basically gives the relation for balance between gravitational pressure and pressure from matter interaction or Pauli exclusion. Let us denote the mass density at neutron star radius r as $\rho(r)$ and corresponding energy density as $\epsilon(r)$ and total accumulated mass up to r as $m(r)$. Then, mass relation is

$$\begin{aligned} m(r) &= 4\pi\int_0^r dr' r'^2\rho(r') = 4\pi\int_0^r dr' r'^2\epsilon(r')/c^2, \\ \frac{dm(r)}{dr} &= 4\pi r^2\rho(r) = \frac{4\pi r^2\epsilon(r)}{c^2} \end{aligned} \tag{11.1}$$

The balance of pressure and gravity is in non-relativistic case,

$$\frac{dp(r)}{dr} = -\frac{G\rho(r)m(r)}{r^2} = -\frac{G\epsilon(r)m(r)}{r^2c^2} \tag{11.2}$$

in (general) relativistic case,

$$\frac{dp(r)}{dr} = -\frac{G\epsilon(r)m(r)}{c^2r^2}\left[1+\frac{p(r)}{\epsilon(r)}\right]\left[1+\frac{4\pi r^3p(r)}{m(r)c^2}\right]\left[1-\frac{2Gm(r)}{c^2r}\right]^{-1} \tag{11.3}$$

Or

$$\begin{aligned} \frac{dP(r)}{dr} &= -\frac{1}{r^2}(\rho(r)+P(r))(M(r)+4\pi r^3P(r))e^{2\Lambda(r)}, \\ e^{2\Lambda(r)} &= e^{-2\phi(r)} = (1-\gamma(r))^{-1}, \end{aligned} \tag{11.4}$$

with [1]

$$\begin{aligned}\gamma(r) &= 2M(r)/r, \quad r \le R_s \\ & \quad 2M_s/r, \quad r \ge R_s \end{aligned} \tag{11.7}$$

Note that the pressure at point r is determined by EOS as a function of local number density.

The neutron star mass and radius is determined by the condition $p(r = R_s) = 0$. The initial condition $m(r = 0) = 0$ but $\rho(r = 0) = \rho_c$ is treated as an input parameter. [2] [3]

In other words, by using coupled equations,

$$\frac{dm(r)}{dr} \propto r^2\epsilon(r), \quad \frac{dP(r)}{dr} \propto \epsilon(r)m(r)/r^2 \tag{11.9}$$

we want to obtain accumulated mass $m(r)$ and pressures $P(r)$ as a function of r which requires energy density $\epsilon(r)$. We may relate pressure and energy density with

$$P(n) = -\frac{\partial E}{\partial V} = n\frac{\partial \rho(n)}{\partial n} - \rho(n). \tag{11.10}$$

where $n(r)$ is a number density of nucleons.

In other words, start integration of $m(r)$ and $P(r)$ from initial values $m(r_0)$, $P(r_0)$, $\epsilon(r_0)$, using differential equation to get $m(r_0 + \delta r)$, $P(r_0 + \delta_r)$. Then,one gets new number density from $P(n) = -\frac{\partial E}{\partial V} = n\frac{\partial \rho(n)}{\partial n} - \rho(n)$. And one gets new $\epsilon(r + \delta r)$ by using the new number density. And the cycle repeats.

In other words, we need EOS in form of $\epsilon(r) = \epsilon(n(r))$ or $\epsilon(r) = \epsilon(P(r))$.)

A typical poly-trope form is $\epsilon(r) = Kp^{1/\gamma}(r)$.

Since energy density is given usually as $\epsilon(k_F)$, and $p(k_F)$, one can obtain a relation $\epsilon(p)$.

Because the equation involves very large and small numbers at the same time, it is better to reform the equation for dimensionless variables.

11.1.1 EOS: simple Bethe-Johnson form

$$\rho(n) = 236n^{2.54} + nm_nc^2. \tag{11.11}$$

This leads to relation

$$P(n) = 363.44n^{2.54} \tag{11.12}$$

Thus, once $P(r+\delta r)$ is obtained, one get obtain new energy density $\rho(r+\delta r) = \rho(n = (\frac{P(r+\delta r)}{363.44})^{\frac{1}{2.54}})$

[1] This relativistic form, the metric function follows

$$\frac{d\phi(r)}{dr} = -\frac{1}{\rho(r) + P(r)}\frac{dP}{dr}, \tag{11.5}$$

with boundary condition,

$$\phi(r = R_s) = \frac{1}{2}\ln(1 - \gamma(R_s)). \tag{11.6}$$

and $P(R_s) = 0$.

[2] If non-zero cosmological constant is assumed,

$$\left[1 + \frac{4\pi r^3 p(r)}{m(r)c^2}\right] \to \left[1 + \frac{4\pi r^3 p(r)}{m(r)c^2} - \frac{\Lambda r^3}{2Gm(r)}\right] \tag{11.8}$$

[3] How to know starting radius and starting density? Because neutron star have differnt layers, each layer should have different equation of states...

11.1.2 EOS: Fermi gas model for electron in white dwarf

The white dwarf is made of atoms and sustained by the pressure coming from the degenerate atomic electrons. In Fermi gas of electrons, number density of electron is $n_e = \frac{k_F^3}{3\pi^2\hbar^3}$. Then, the number density of nucleons in the atom is $\frac{A}{Z}n_e$. (Assume there are only one kind of atoms in the white dwarf.) Then, energy density of electrons is

$$\epsilon_e(k_F) = \frac{8\pi}{(2\pi\hbar)^3}\int_0^{k_F}(k^2c^2 + m_e^2c^4)^{1/2}k^2dk \tag{11.13}$$

Neglecting nuclear interaction, the energy density of atom is

$$\epsilon = \frac{A}{Z}n_e m_N c^2 + \epsilon_e(k_F) \tag{11.14}$$

The pressure is (note the density depends on volume $n_e = N_e/V$),

$$p = -\frac{\partial U}{\partial V}|_{T=0} = n^2\frac{d(\epsilon/n)}{dn} = n\frac{d\epsilon}{dn} - \epsilon \tag{11.15}$$

We may approximate the integration in electron energy density as

$$\begin{aligned} p(k_F) &\simeq K_{rel}\epsilon^{4/3}, \quad K_{rel} = \frac{\hbar c}{12\pi^2}\left(\frac{3\pi^2 Z}{Am_N c^2}\right)^{4/3}, \quad \text{if } k_F \gg m_e \\ &\simeq K_{nonrel}\epsilon^{5/3}, \quad K_{nonrel} = \frac{\hbar^2}{15\pi^2 m_e}\left(\frac{3\pi^2 Z}{Am_N c^2}\right)^{5/3}, \quad \text{if } k_F \ll m_e. \end{aligned} \tag{11.16}$$

11.1.3 EOS: Fermi gas model for neutron star

Ignoring small fraction of electrons in the neutron star and nuclear interaction, the model is similar to the white dwarf. However, now the energy density is simply

$$\epsilon = \epsilon_n(k_F) = \frac{8\pi}{(2\pi\hbar)^3}\int_0^{k_F}(k^2c^2 + m_n^2c^4)^{1/2}k^2dk \tag{11.17}$$

Thus,

$$\begin{aligned} p(k_F) &\simeq K^{(n)}_{nonrel}\epsilon^{5/3} \quad \text{if } k_F \ll m_N, \\ &\simeq K^{(n)}_{rel}\epsilon \quad \text{if } k_F \gg m_N. \end{aligned} \tag{11.18}$$

Or instead of trying to find $\epsilon(p)$, one can first obtain new $p(r)$ and compute n or k_F from $p(n)$ relation and get energy from $\epsilon(n)$.

If we include electrons, but still using Fermi gas model ignoring nuclear interaction, we will need to consider the balance of chemical potentials of electron, protons and neutrons. The electron is necessary to prevent the weak decay of neutrons($n \to p + e^- + \bar{\nu}_e$) . Then, we need charge neutrality $k_F^{(p)} = k_F^{(e)}$ and chemical potential $\mu_n = \mu_p + \mu_e$. For Fermi gas, chemical potential is

$$\mu_i(k_F^{(i)}) = \frac{d\epsilon_i}{dn_i} = (k_F^{(i)2} + m_i^2)^{1/2}, \quad i = n, p, e. \tag{11.19}$$

This gives $k_F^{(p)}$ as a function of $k_F^{(n)}$. Then, total energy density and pressure can be obtained from,

$$\begin{aligned} \epsilon_i(k_F^{(i)}) &= \int_0^{k_F^{(i)}}(k^2 + m_i^2)^{1/2}k^2dk, \\ p_i(k_F^{(i)}) &= \int_0^{k_F^{(i)}}(k^2 + m_i^2)^{-1/2}k^4dk. \end{aligned} \tag{11.20}$$

11.1.4 EOS: Mass formula for nuclear matter

One easy way to include the effects of nuclear interaction is to use mass formula. For symmetric nuclear matter, $N = Z$ and thus $n_p = n_n$ and total nucleon density is $n = n_p + n_n$.

Let us consider symmetric nuclear matter. We may put constraints for $E/A = \epsilon(n)/n$, from the information at normal nuclear density,

$$\begin{aligned}
&\frac{\epsilon(n)}{n} - m_N = BE \text{ at } n = n_0, \\
&\frac{d}{dn}(\frac{E}{A}) = \frac{d}{dn}(\frac{\epsilon(n)}{n}) = 0 \text{ at } n = n_0, \\
&K(n = n_0) = K_0, \text{ with } K(n) = 9\frac{dp(n)}{dn} = 9\left[n^2\frac{d^2}{dn^2}(\frac{\epsilon}{n}) + 2n\frac{d}{dn}(\frac{\epsilon}{n})\right].
\end{aligned} \tag{11.21}$$

We may model the relation and find appropriate coefficient from the constraints,

$$\frac{\epsilon(n)}{n} = m_N + \frac{3}{5}\frac{\hbar^2 k_F^2}{2m_N} + \frac{A}{2}(\frac{n}{n_0}) + \frac{B}{\sigma+1}(\frac{n}{n_0})^\sigma. \tag{11.22}$$

Then, pressure

$$p(n) = n^2\frac{d}{dn}(\frac{\epsilon}{n}). \tag{11.23}$$

For asymmetric nuclear matter, introduce $\alpha = \frac{n_n - n_p}{n} = \frac{N-Z}{A}$, or $x = \frac{n_p}{n} = \frac{1-\alpha}{2}$. One can first have kinectic energy difference from symmetric matter,

$$\Delta\epsilon(n,\alpha) = \epsilon_{KE}(n,\alpha) - \epsilon(n,0) \simeq nE_F\frac{\alpha^3}{3}(1 + \frac{\alpha^2}{27} + \cdots). \tag{11.24}$$

Potential energy contribution may be modeled with symmetry energy model $S(n)$,

$$E(n,\alpha) = E(n,0) + \alpha^2 S(n) \tag{11.25}$$

In a similar way, one can get the pressure.

One also can compute the speed of sound from bulk modulus

$$(\frac{c_s}{c})^2 = \frac{B}{\rho c^2} = \frac{dp}{d\epsilon} = \frac{dp/dn}{d\epsilon/dn} \tag{11.26}$$

11.1.5 Numerical method

For numerical calculation, because TOV involves very different mass scales, it is better to construct dimensionless equations by using some pre-defined mass units.

Non-relativistic form,

$$\begin{aligned}
\frac{dm(r)}{dr} &= \frac{4\pi r^2\epsilon(r)}{c^2}, \\
\frac{dp(r)}{dr} &= -\frac{G\epsilon(r)m(r)}{r^2c^2}
\end{aligned} \tag{11.27}$$

can be re-written as

$$\frac{d\bar{m}}{d\bar{r}} = \bar{r}^2\bar{\rho}, \quad \frac{d\bar{P}}{d\bar{r}} = -\frac{\bar{m}\bar{\rho}}{\bar{r}^2} \tag{11.28}$$

with

$$\begin{aligned}
\bar{r} &= \frac{r}{R_0}, \quad \bar{\rho} = \frac{\rho}{\rho_s}, \quad \bar{P} = \frac{P}{\rho_s}, \quad \bar{m} = \frac{m}{M_0}. \\
R_0 &= \frac{1}{\sqrt{\rho_s G 4\pi}}, \quad M_0 = \frac{4\pi\rho_s}{(\sqrt{\rho_s G 4\pi})^3}.
\end{aligned} \tag{11.29}$$

Further, we want to express r in units of 10 km and M_0 in units of solar mass. where ρ_s, n_s is a central energy density and central density at the starting radius.

Chapter 12

From here on are old notes

Chapter 13

Shell Model

13.1 Field operators in the coordinate space

Each occupied state corresponds to many-body wave function, [1]

$$\begin{aligned} |i\rangle &= c_i^\dagger|-\rangle \leftrightarrow \phi_i(\boldsymbol{x}), \\ |ij\rangle &= c_j^\dagger c_i^\dagger|-\rangle \leftrightarrow \frac{1}{\sqrt{2}}\left(\phi_i(r_1)\phi_j(r_2) - \phi_j(r_1)\phi_i(r_2)\right), \\ |i_i i_2..i_A\rangle &= \prod_i c_i^\dagger|-\rangle \leftrightarrow \frac{1}{\sqrt{A!}}\det(\phi_{i_i}(r_j)) \end{aligned} \tag{13.1}$$

(여기서 factor $1/\sqrt{A!}$이 creation operator로 나타낼때는 없음에 유의. $|ab\rangle = c_a^\dagger c_b^\dagger|0\rangle$ 는 이미 anti-symmetrization과 normalization을 만족시킨다. $\langle ab|cd\rangle = \delta_{ac}\delta_{bd} - \delta_{ad}\delta_{bc}$)

In fact, one have to use occupation number representation $|n_{s1}n_{s2}\ldots\rangle$, where n_s is a occupation number for state s. However, since occupation number of fermion is either 0 or 1, we can equivalently express $|s1, s2\ldots\rangle$ for occupied states.

In a more formal way, let us define coordinate space operators,

$$a(\boldsymbol{r}, s) = \sum_\nu \phi_\nu(\boldsymbol{r}, s)a_\nu, \quad a^\dagger(\boldsymbol{r}, s) = \sum_\nu \phi_\nu^*(\boldsymbol{r}, s)a_\nu^\dagger, \tag{13.2}$$

where $a_\nu, a_\nu^\dagger$ are operators for a single particle state ν and corresponding single particle wave functions $\phi_\nu(\boldsymbol{r})$. Note that $a(\boldsymbol{r}, s), a^\dagger(\boldsymbol{r}, s)$ are operators acting on space and does not have specific single particle state index. [2] Inversion is

$$a_\nu = \sum_s \int d^3\boldsymbol{r}\phi_\nu^*(\boldsymbol{r}, s)a(\boldsymbol{r}, s), \quad a_\nu^\dagger = \sum_s \int d^3\boldsymbol{r}\phi_\nu(\boldsymbol{r}, s)a^\dagger(\boldsymbol{r}, s). \tag{13.4}$$

[1] 헷갈리는 점. $|ab\rangle$ 는 $c_a^\dagger c_b^\dagger|\rangle$ 인가, $c_b^\dagger c_a^\dagger|\rangle$ 인가? 어느 정의를 사용하건, matrix element는 항상 양쪽에 bra-ket이 나타나므로, 어느쪽을 쓰건 상관 없다. 다만,

$$\begin{aligned} \text{if } |m_1m_2\rangle &= c_{m_1}^\dagger c_{m_2}^\dagger|\rangle \to \langle m_1m_2| = \langle|c_{m_2}c_{m_1}, \\ \text{if } |m_1m_2\rangle &= c_{m_2}^\dagger c_{m_1}^\dagger|\rangle \to \langle m_1m_2| = \langle|c_{m_1}c_{m_2}, \end{aligned}$$

와 같이 bra-ket에서 operator의 순서가 바뀌어야한다. 즉, $(xyz)^\dagger = z^\dagger y^\dagger x^\dagger$ 와 같은 relation이 성립해야한다.

만약 위와 같이 쓰지않으면 $\langle m_1m_2|m_1m_2\rangle = 1$ 이라는 관계가 성립하지 않게 된다. 이 노트에서는 P. Ring의 convention을 따라서, $|ab\rangle = c_b^\dagger c_a^\dagger|-\rangle$ 를 사용한다.

[2] This is a analogue of plane wave expansion in momentum,

$$\psi(\boldsymbol{x}) = \int d^3\boldsymbol{p}\phi_{\boldsymbol{p}}(\boldsymbol{x})a_{\boldsymbol{p}}, \quad \phi_{\boldsymbol{p}}(\boldsymbol{x}) = e^{i\boldsymbol{p}\cdot\boldsymbol{x}} \tag{13.3}$$

Commutation relations are

$$\begin{aligned}\{a(\boldsymbol{r},s),a^\dagger(\boldsymbol{r}',s')\} &= \sum_{\nu\nu'}\phi_\nu(\boldsymbol{r},s)\phi^*_{\nu'}(\boldsymbol{r}',s')\{a_\nu,a^\dagger_{\nu'}\}=\delta_{ss'}\delta(\boldsymbol{r}-\boldsymbol{r}')\\ \{a(\boldsymbol{r},s),a(\boldsymbol{r},s')\} &= \{a^\dagger(\boldsymbol{r},s),a^\dagger(\boldsymbol{r},s')\}=0\end{aligned} \tag{13.5}$$

Then, many-body wave function can be expressed

$$\Phi_{\{n_\nu\}}(1\ldots N)=\frac{1}{\sqrt{N!}}\langle-|a(N)\ldots a(1)|n_1n_2\ldots n_\nu\ldots\rangle=\frac{1}{\sqrt{N!}}\langle-|a(N)\ldots a(1)|\Phi_{\{n_\nu\}}\rangle \tag{13.6}$$

and (Here $a(i)$ means coordinate operator $a(\boldsymbol{r}_i,s_i)$.)

$$|\Phi\rangle=|n_1n_2\ldots n_\nu\ldots\rangle=\int d1\ldots dN\frac{1}{\sqrt{N!}}\Phi_{\{n_\nu\}}(1\ldots N)a^\dagger(1)\ldots a^\dagger(N)|-\rangle \tag{13.7}$$

For example,

$$\begin{aligned}&a(\boldsymbol{r}_i,s_i)|1_j\rangle=\phi_j(\boldsymbol{r}_i,s_i)|-\rangle\\ &a(\boldsymbol{r}_1,s_1)a(\boldsymbol{r}_2,s_2)|1_i,1_j\rangle=\sum_{\nu\nu'}\phi_\nu(1)\phi_{\nu'}(2)a_\nu a_{\nu'}a^\dagger_ja^\dagger_i|-\rangle\\ &\quad=\sum_{\nu\nu'}\phi_\nu(1)\phi_{\nu'}(2)(\delta_{\nu i}\delta_{\nu' j}-\delta_{\nu j}\delta_{\nu' i})|-\rangle=(\phi_i(1)\phi_j(2)-\phi_j(1)\phi_i(2))\,|-\rangle\end{aligned} \tag{13.8}$$

We may also use a notation,

$$|1\ldots N\rangle=\frac{1}{\sqrt{N!}}a^\dagger(1)\ldots a^\dagger(N)|-\rangle \tag{13.9}$$

such that

$$\Phi_{\{n_\nu\}}(1\ldots N)=\langle 1\ldots N|\Phi_{\{n_\nu\}}\rangle \tag{13.10}$$

13.1.1 Representation of Operators

If the basis is complete and any many-body state can be expressed by combining single particle basis states, for many-body state space, the original Hamiltonian can be equivalently expressed in terms of creation and annihilation operators and matrix elements.

One-body operator in coordinate space of N-body system is (operator $\hat{f}_i$ only acts on coordinate r_i.)

$$\begin{aligned}\hat{F} &= \sum_{i=1}^N\hat{f}_i,\\ f_{\nu\nu'} &\equiv (\nu|\hat{f}|\nu')\ \leftrightarrow\ \hat{f}_i\phi_\nu(i)=\sum_{\nu'}f_{\nu\nu'}\phi_{\nu'}(i).\end{aligned} \tag{13.11}$$

We can show that the same operator can be expressed in basis operators for many-particle state $|\Phi\rangle$,

$$\hat{F} = \sum_{\nu\nu'}f_{\nu\nu'}a^\dagger_\nu a_{\nu'}, \tag{13.12}$$

or in terms of coordinate operators,

$$\hat{F} = \sum_s\int d\boldsymbol{r}a^\dagger(\boldsymbol{r},s)\hat{f}(\boldsymbol{r})a(\boldsymbol{r},s). \tag{13.13}$$

In other words,

$$\sum_i \hat{f}_i \Phi(1,\dots N) = \langle 1\dots N| \left(\sum_{\nu\nu'} f_{\nu\nu'} a^\dagger_\nu a_{\nu'} \right) |\Phi\rangle \tag{13.14}$$

This can be shown

$$\begin{aligned}
(l.h.s) &= \sum_i \hat{f}_i \Phi(1,\dots N) \\
&= \sum_i \hat{f}_i \frac{1}{\sqrt{N!}} \sum_{\nu_1\nu_2\dots} \phi_{\nu_1}(1)\dots\phi_{\nu_N}(N)\langle -|a_{\nu_N}\dots a_{\nu_1}|\Phi\rangle \\
&= \frac{1}{\sqrt{N!}} \sum_i \sum_{\nu_1\nu_2\dots} \phi_{\nu_1}(1)\dots \left(\sum_{\nu'} f_{\nu_i\nu'}\phi_{\nu'}(i) \right) \dots \phi_{\nu_N}(N)\langle -|a_{\nu_N}\dots a_{\nu_1}|\Phi\rangle. \qquad (13.15)
\end{aligned}$$

$$\begin{aligned}
(r.h.s) &= \langle 1\dots N| \left(\sum_{\nu\nu'} f_{\nu\nu'} a^\dagger_\nu a_{\nu'} \right) |\Phi\rangle \\
&= \frac{1}{\sqrt{N!}} \langle -|a(N)\dots a(1) \left(\sum_{\nu\nu'} f_{\nu\nu'} a^\dagger_\nu a_{\nu'} \right) |\Phi\rangle \\
&= \frac{1}{\sqrt{N!}} \sum_{\nu\nu'} f_{\nu\nu'} \sum_{\nu_1\nu_2\dots} \phi_{\nu_N}(N)\dots\phi_{\nu_1}(1)\langle -|a_{\nu_N}\dots a_{\nu_1} a^\dagger_\nu a_{\nu'}|\Phi\rangle \\
&= \frac{1}{\sqrt{N!}} \sum_i \sum_{\nu'} \sum_{\nu_1\nu_2\dots} f_{\nu'\nu_i}\phi_{\nu_N}(N)\dots\phi_{\nu'}(i)\dots\phi_{\nu_1}(1)\langle -|a_{\nu_N}\dots a_{\nu_1}|\Phi\rangle \qquad (13.16)
\end{aligned}$$

In last term, we can move $a^\dagger_\nu a_{\nu'}$ to left side and the matrix element is non-zero only when ν is in $\{\nu_i\}$ sets (if not, it will gives zero because $\langle -|a^\dagger_\nu = 0$) and ν' is not in $\{\nu_i\}$ sets (if not, it will gives zero because $\langle -|a_{\nu'}a_{\nu'} = 0$). Thus in effect, it is the same as replacing one of a_{ν_i} into $a_{\nu'}$ and $\phi_{\nu_i}(i) = \phi_\nu(i)$ when $\nu_i = \nu$. Thus, adding all cases $\nu = \nu_i$, and rename $\nu' \to \nu_i$ and $\nu_i \to \nu'$ we get last line. (어라 ? $f_{\nu_i\nu'} = f_{\nu'\nu_i}$? 이상함...)

For example,

$$\begin{aligned}
&\text{(kinetic energy)} \qquad \hat{T} = \sum_i \frac{-\hbar^2}{2m}\Delta_i = \sum_{\nu\nu'} \langle\nu|\frac{-\hbar^2}{2m}\Delta|\nu'\rangle a^\dagger_{\nu'}a_\nu \\
&\qquad\qquad = \sum_s \int d^3\boldsymbol{r} a^\dagger(\boldsymbol{r},s)\frac{-\hbar^2}{2m}\Delta a(\boldsymbol{r},s) \\
&\text{(s.p. density)} \qquad \hat{\rho}(\boldsymbol{r}) = \sum_{i=1}^N \delta(\boldsymbol{r}-\boldsymbol{r}_i) = \sum_{\nu\nu'}\sum_s \int d^3r' \phi^*_\nu(\boldsymbol{r}',s)\delta(\boldsymbol{r}-\boldsymbol{r}')\phi_{\nu'}(\boldsymbol{r}',s)a^\dagger_\nu a_{\nu'} \\
&\qquad\qquad = \sum_s a^\dagger(\boldsymbol{r},s)a(\boldsymbol{r},s) \\
&\text{(particle number)} \qquad \hat{N} = \sum_\nu a^\dagger_\nu a_\nu = \sum_\nu \sum_{ss'} \int d^3r d^3r' \phi_\nu(\boldsymbol{r},s)\phi^*_\nu(\boldsymbol{r}',s')a^\dagger(\boldsymbol{r},s)a(\boldsymbol{r}',s) \\
&\qquad\qquad = \int \hat{\rho}(\boldsymbol{r})d^3r, \\
&\text{(non-local 1B)} \qquad \hat{f}\phi(\boldsymbol{r},s) = \sum_{s'} \int d^3r' f_{ss'}(\boldsymbol{r},\boldsymbol{r}')\phi(\boldsymbol{r}',s'). \qquad (13.17)
\end{aligned}$$

In case of two-body operators,

$$\hat{V} = \sum_{i<j} v_{ij} = \frac{1}{2}\sum_{i\neq j} v_{ij} \tag{13.18}$$

Two-body operator can be local $v_{ij} = v(\boldsymbol{r}_i, \boldsymbol{r}_j)$ or non-local $v_{ij} = v(\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{r}'_i, \boldsymbol{r}'_j)$.

In general matrix elements of two-body operator can be written in terms of

$$v_{\mu\nu\mu'\nu'} = (\mu\nu|v|\mu'\nu') = \int d1d2d3d4\phi^*_\mu(1)\phi^*_\nu(2)v(1,2,3,4)\phi_{\mu'}(3)\phi_{\nu'}(4). \tag{13.19}$$

In a similar way as one-body, two-body operators can be written as

$$\hat{V} = \frac{1}{2}\sum_{\mu\nu\mu'\nu'} v_{\mu\nu\mu'\nu'} a^\dagger_\mu a^\dagger_\nu a_{\nu'} a_{\mu'} = \frac{1}{4}\sum_{\mu\nu\mu'\nu'} \bar{v}_{\mu\nu\mu'\nu'} a^\dagger_\mu a^\dagger_\nu a_{\nu'} a_{\mu'} \tag{13.20}$$

(즉, matrix-element를 simple product state에 대해 쓰면 $\frac{1}{2}$ factor, anti-symmetrized state에 대해 쓰면 $\frac{1}{4}$이 필요하다.) where anti-symmetrized matrix element is [3]

$$\bar{v}_{\mu\nu\mu'\nu'} = (\mu\nu|v|\mu'\nu' - \nu'\mu') = \langle\mu\nu|v|\mu'\nu'\rangle, \tag{13.23}$$

즉, normalized anti-symmetrized state에 대한 matrix element는 simple product matrix element의 sum으로 나타낼 수 있다.

In other words,

$$\frac{1}{2}\sum_{i\neq j} v_{ij}\Phi(1\ldots N) = \langle 1\ldots N|\frac{1}{2}\sum_{\mu\nu\mu'\nu'} v_{\mu\nu\mu'\nu'} a^\dagger_\mu a^\dagger_\nu a_{\nu'} a_{\mu'}|\Phi\rangle \tag{13.24}$$

The proof is **to be added...**

13.2 Diagonalization

Suppose we contructed many-body wave function of good (J,T) values from the single particle wave functions. Then we have

$$\hat{H}^{(0)}\Phi_{JT,k}(1,2\ldots,A) = E^{(0)}_{JT,k}(1,2\ldots,A), \quad E^{(0)}_{JT,k} = \sum_i^A \epsilon_i \tag{13.25}$$

with $k = 1\ldots, d$ with model space dimension d. Then, the solution of problem,

$$\hat{H}|\Psi_p\rangle = E_p|\Psi_p\rangle, \quad |\Psi_p\rangle = \sum_{k=1}^d a_{kp}|\Phi_k\rangle, \quad \sum_k |a_{kp}|^2 = 1. \tag{13.26}$$

is a linear combination of such basis states. (Note that in J-scheme, the basis is already constructed to have good quantum numbers and thus for given J,T only basis states with J,T can mix. On the other

[3] where additional $\frac{1}{2}$ factor comes from

$$\begin{aligned}
\sum_{ijkl}\bar{v}_{ijkl}a^\dagger_i a^\dagger_j a_l a_k &= \sum_{ijkl}(v_{ijkl} - v_{ijlk})a^\dagger_i a^\dagger_j a_l a_k \\
&= \sum_{ijkl} v_{ijkl}(a^\dagger_i a^\dagger_j a_l a_k - a^\dagger_i a^\dagger_j a_k a_l) \\
&= 2\sum_{ijkl} v_{ijkl} a^\dagger_i a^\dagger_j a_l a_k
\end{aligned} \tag{13.21}$$

Also, computing matrix elements for normalzied anti-symmetrized states $|pq\rangle$,

$$\begin{aligned}
\langle pq|\hat{V}|rs\rangle &= \frac{1}{2}\sum_{\mu\nu\mu'\nu'} v_{\mu\nu\mu'\nu'}\langle pq|a^\dagger_\mu a^\dagger_\nu a_{\nu'} a_{\mu'}|rs\rangle = \frac{1}{2}\sum_{\mu\nu\mu'\nu'} v_{\mu\nu\mu'\nu'}\frac{1}{2}\langle 0|a_q a_p a^\dagger_\mu a^\dagger_\nu a_{\nu'} a_{\mu'} a^\dagger_r a^\dagger_s|0\rangle \\
&= \frac{1}{4}\left(v_{pqrs} - v_{qprs} - v_{pqsr} + v_{qpsr}\right) = v_{pqrs}
\end{aligned} \tag{13.22}$$

hand, m-scheme basis may mix in more larger model space.) To solve this, we need matrix elements of $H_{lk} = \langle\Phi_l|\hat{H}|\Phi_k\rangle$. There exist different numerical algorithms for matrix diagonalization: the Jacobi method for small matrices (d<50), the Householder method for matrices with $50 < d < 200$, the Lanczos method for dimensions d >200 and for giant matrices.

basis dimension grows quickly (c is available valence states, N is valence nucleon number),

$$dim \simeq \left(\begin{array}{c} Z_c \\ N_\pi \end{array} \right) \left(\begin{array}{c} N_c \\ N_\nu \end{array} \right) \tag{13.27}$$

General Shell Model Scheme:

- Construct Basis $|\Phi_k\rangle$: Note that the basis is for A-body wave function, not just a single particle.
- Expand the wave function, $|\Psi_p\rangle = \sum_k a_{pk}|\Phi_k\rangle$ and construct Hamiltonian H_{lk}. In fact, the many-body matrix element H_{lk} can be decomposed into a few-body matrix elements(one-body, two-body and three-body). Thus, the input of shell model code are few-body matrix elements.
- diagonalization of Hamiltonian, get eigen values E_p and eigen solution a_{pk}
- calculate matrix elements of interested operators, $\langle\Psi_f|\hat{O}|\Psi_i\rangle$

13.2.1 Representation of potential

We may express the general potential in terms of projection operators

$$V = \sum_{\nu,T} U_\nu^T(r) W_\nu P_T. \tag{13.28}$$

Because of $L + S + T = odd$ relation, we may represent spin state (singlet,triplet) and parity of orbital (even, odd) to represent the acts on spin and isospin.

Central potential

A local Central potential can be expressed in several different ways

$$\begin{aligned} V_C(1,2) &= V_0(r) + V_\sigma(r)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + V_\tau(r)\tau_1\cdot\tau_2 + V_{\sigma\tau}(r)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\tau_1\cdot\tau_2, \\ &= V_W(r) + V_M(r)P^r + V_B(r)P^\sigma + V_H(r)P^rP^\sigma, \quad P^\sigma = \frac{1+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{2}, \ldots, \\ &= V_{SE}(r)W_{S=0}P_{T=1} + V_{TO}(r)W_{S=1}P_{T=1} + V_{SO}(r)W_{S=0}P_{T=0} + V_{TE}(r)W_{S=1}P_{T=0} \end{aligned}$$

with

$$\begin{aligned} W_{S=0} &= \frac{1}{4}(1-\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2), \quad W_{S=1} = \frac{1}{4}(3+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2), \\ P_{T=0} &= \frac{1}{4}(1-\tau_1\cdot\tau_2), \quad P_{T=1} = \frac{1}{4}(3+\tau_1\cdot\tau_2). \end{aligned} \tag{13.29}$$

Here $S(T)$ means spin singlet(triplet) and $E(O)$ means even(odd) orbital parity.

The relation between different expression can be worked out.

For example, $V_0(r)$ can be changed into $V_{SE}(r) = V_{TO}(r) = V_{SO}(r) = V_{TE}(r) = V_0(r)$.

For example of delta potential, $V_0\delta^{(3)}(\boldsymbol{r}) = V_0\frac{\delta(r)}{r^2}\delta(\cos\theta)\delta(\phi)$ is only for even-parity states. It's matrix element has radial part contribution and angular part $\langle Y_{lm}|\delta(\cos\theta)\delta(\phi)|Y_{l'm'}\rangle = \delta_{l0}\delta_{l'0}\delta_{mm'}\delta_{m0}\frac{1}{4\pi}$.

spin-orbit potential

Spin-orbit component (because it only acts on spin triplet $S = 1$)

$$V_{LS} = U_{LSO}(r)P^{LSO} + U_{LSE}(r)P^{LSE}, \tag{13.30}$$

with

$$\begin{aligned} W_{LS} &= l \cdot s = \frac{1}{2} l \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2), \\ P^{LSO} &= W_{LS} P_{T=1}, \quad P^{LSE} = W_{LS} P_{T=0} \end{aligned} \tag{13.31}$$

tensor potential

tensor force can be expressed as (because it only acts on spin triplet $S = 1$)

$$\begin{aligned} V_{TN}(1,2) &= V_{TN}(r)(v_{t0} + v_{tt}\tau_1 \cdot \tau_2)(\frac{(\boldsymbol{\sigma}_1 \cdot \boldsymbol{r})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{r})}{r^2} - \frac{1}{3}\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \\ &= V_{TN}(r)(v_{t0} + v_{tt}\tau_1 \cdot \tau_2)[\boldsymbol{r} \times \boldsymbol{r}]^{(2)} \cdot [\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2]^{(2)}, \\ &= U_{TNO}(r)P^{TNO} + U_{TNE}(r)P^{TNE}, \\ P^{TNO} &= W_{TN} P_{T=1}, \quad P^{TNE} = W_{TN} P_{T=0}, \\ W_{TN} &= \frac{3}{r^2}(\boldsymbol{\sigma}_1 \cdot \boldsymbol{r})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{r}) - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2. \end{aligned} \tag{13.32}$$

13.2.2 Commonly used operators

$$\begin{aligned} \hat{O}(E, LM) &= \sum_{k=1}^{A} e_k r_k^L Y_{LM}(\hat{r}_k), \\ \hat{O}(M, 1M) &= \sum_{k=1}^{A} \mu_n \left(g_s(k)\vec{s}_k + g_l(k)\vec{l}_k \right), \\ \hat{O}(F) &= \sum_{k=1}^{A} \tau_k^{\pm}, \quad \hat{O}(GT) = \sum_{k=1}^{A} \vec{\sigma}_k \tau_k^{\pm} \end{aligned} \tag{13.33}$$

13.3 Effective Interaction

The most fundamental way to get the two-nucleon interaction to be exploited in the many-body calculations is to derive it from a bare NN potential for free nucleons in a vacuum, by taking into account medium effects, the Pauli principle and truncated model space. This is why such an interaction is called an **effective interaction**.

13.3.1 Many-body perturbation theory and G-matrix

Instead of solving

$$\hat{H}\Psi = E\Psi \tag{13.34}$$

in a full Hilbert space, we may want to solve in a smaller model space such that

$$\hat{H}_{eff}\Psi^M = (\hat{H}^{(0)} + \hat{V}_{eff})\Psi^M = E\Psi^M. \tag{13.35}$$

how one can have such $\hat{V}_{eff}$?. By introducing some model space projection operators $\hat{P}$ and $\hat{Q}$,

$$\hat{P} = \sum_{k\in M} |\Phi_k\rangle\langle\Phi_k|, \quad \hat{Q} = \sum_{k\notin M} |\Phi_k\rangle\langle\Phi_k| \tag{13.36}$$

we get

$$\begin{aligned} \hat{V}_{eff} &= \hat{V} + \hat{V}\frac{\hat{Q}}{E-\hat{H}^{(0)}}\hat{V}_{eff}, \\ \Psi &= \Psi^M + \frac{\hat{Q}}{E-\hat{H}^{(0)}}\hat{V}\Psi \end{aligned} \tag{13.37}$$

However, because equation depends on the exact energy E, which is unknown, it is not so useful. But, then by rewriting $E = E_c^{(0)} + \Delta E_c + E_v^{(0)} + \Delta E_{cv}$, where $E_c^{(0)}$ is an unperturbed core energy, $E_c^{(0)} + \Delta E_c$ is true core energy, $E_v^{(0)}$ is unperturbed valence energy and ΔE_{cv} is the rest, the equation can be re-written for valence nucleons as

$$\begin{aligned} \hat{V}_{eff} &= \hat{V} + \hat{V}\frac{\hat{Q}}{E_v-\hat{H}_v^{(0)}}\hat{V}_{eff} \\ &= \hat{V} + \hat{V}\frac{\hat{Q}}{E_v-\hat{H}_v^{(0)}}\hat{V} + \hat{V}\frac{\hat{Q}}{E_v-\hat{H}_v^{(0)}}\hat{V}\frac{\hat{Q}}{E_v-\hat{H}_v^{(0)}}\hat{V} + \ldots, \end{aligned} \tag{13.38}$$

where $\hat{H}_v^{(0)}$ is an unperturbed Hamiltonian for valence particles. These series can be evaluated by using a diagrammatic technique. The summations include only the special class of diagrams, linked and folded diagrams

The standard approach to this equation was to sum first an infinite class of diagrams, called ladder diagrams which result in the Br¨uckner's reaction G-matrix, solution of the Bethe-Goldstone equation

$$\hat{G}(\omega) = \hat{V} + \hat{V}\frac{\hat{Q}_{2p}}{\omega-\hat{H}_{2p}^{(0)}}\hat{G}(\omega), \tag{13.39}$$

where, $\hat{H}_{2p}^{(0)}$ is an unperturbed Hamiltonian of the intermediate two-particle, the Pauli operator $\hat{Q}_{2p}$ produces a non-vanishing result only if it acts on a pair of particles, both of which are beyond the Fermi level. The parameter ω represents the so-called starting energy at which G-matrix is evaluated. It is considered as a softer interaction compared to the bare NN potential. Then, in the second step , the G-matrix is used to calculate the effective interaction for the model space to be used in the shell model calculations

$$\begin{aligned} \hat{V}_{eff} &= \hat{G} + \hat{G}\frac{\hat{Q}'}{E_v-\hat{H}_v^{(0)}}\hat{V}_{eff} \\ &= \hat{G} + \hat{G}\frac{\hat{Q}'}{E_v-\hat{H}_v^{(0)}}\hat{G} + \hat{G}\frac{\hat{Q}'}{E_v-\hat{H}_v^{(0)}}\hat{G}\frac{\hat{Q}'}{E_v-\hat{H}_v^{(0)}}\hat{G} + \ldots \end{aligned} \tag{13.40}$$

where the primed projection operator $\hat{Q}'$ indicates that the ladder diagrams are excluded. But, the finite cuclei requires beyond leading order approximation of $\hat{V}_{eff} \simeq \hat{G}$. However, this is too difficult to get effective interaction in this way.

13.4 Hamiltonian in second quantized form

Let us consider Hamiltonian in second quantized form for the particle operators $c_n^\dagger$ and c_n with particle vacuum $c_n|0\rangle = 0$.

$$H = \sum_{n_1 n_2} e_{n_1 n_2} c_{n_1}^\dagger c_{n_2} + \frac{1}{4}\sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} c_{n_1}^\dagger c_{n_2}^\dagger c_{n_4} c_{n_3}, \tag{13.41}$$

where

$$\bar{v}_{n_1n_2n_3n_4} = \langle n_1n_2|V|n_3n_4 - n_4n_3\rangle. \tag{13.42}$$

We will express the Hamiltonian in terms of density matrix defined as

$$\rho_{ll'} \equiv \langle\Phi|c^\dagger_{l'}c_l|\Phi\rangle, \quad \kappa_{ll'} \equiv \langle\Phi|c_{l'}c_l|\Phi\rangle. \tag{13.43}$$

Minimization?: Schematically above expression is like, $H = H_0 + H^{20}_{\alpha\beta}N(c^\dagger_\alpha c_\beta) + (residual)$. Because here normal ordering is defined such that $\langle\Phi|N(O)|\Phi\rangle = 0$, the energy expectation value is $H_0 = \langle\Phi|H|\Phi\rangle$. According to book, it looks like to find an diagonalizing transformation(or new basis) such that the second term becomes $H^{20}_{\alpha\beta}N(c^\dagger_\alpha c_\beta) \to E_\alpha N(\beta^\dagger_\alpha\beta_\alpha)$ is equivalent to minimize H_0... But how?

13.4.1 angular momentum coupling

A state of two fermion coupled to a certain J can be expressed in the second quantization as

$$|ab;JM\rangle \quad = \quad |(n_al_aj_a)(n_bl_bj_b);JM\rangle = -\frac{1}{\sqrt{1+\delta_{ab}}}\left[a^\dagger_a \otimes a^\dagger_b\right]^J_M|0\rangle \tag{13.44}$$

here $\delta_{ab} = \delta_{n_an_b}\delta_{l_al_b}\delta_{j_aj_b}$.

The particle-particle form of residual interaction,

$$\hat{V} = -\frac{1}{4}\sum_{abcd,J}\langle ab;JM|\hat{V}|cd;JM\rangle\sqrt{2J+1}\sqrt{(1+\delta_{ab})(1+\delta_{cd})}\left[\left[a^\dagger_a \otimes a^\dagger_b\right]^{(J)} \otimes [\tilde{a}_c \otimes \tilde{a}_d]^{(J)}\right]^{(0)}_0 \tag{13.45}$$

where $\tilde{a}_{cm_c} = (-1)^{j_c+m_c}a_{c,-m_c}$.

It is possible to get particle-hole form of interaction. Let us simply refer the reference, N.A. Smirnova, "Shell structure evolution and effective in-medium NN interaction".

13.5 Matrix elements in shell model

Let us consider a matrix elements in shell model. Basically, many-body wave function $\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2\cdots\boldsymbol{r}_A)$ can be written in terms of many-body basis states $\Phi_\alpha(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_A)$ which can be considered as a slater determinant of single particle basis orbits.

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2\cdots\boldsymbol{r}_A) = \sum_\beta c_\alpha\Phi_\alpha(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_A) \tag{13.46}$$

Thus, in the shell model, one have to prepare appropriate model space of many-body basis states and their matrix elements $\langle\Phi_\alpha|\hat{H}|\Phi_\beta\rangle$. The Hamiltonian is a sum of few-body operators and their matrix elements can be reduced to sums of matrix elements of few-body states. Thus, what one needs only matrix elements of few-body operators in few-body basis states. The full many-body matrix elements can be calculated easily in occupation number representation. In this case, all one needs is to represent Hamiltonian in second quantized form which requires coefficients.

$$\hat{H} = \sum_\alpha h_{\alpha\beta}\hat{a}^\dagger_\alpha a_\beta + \sum_{abcd} h_{ab;cd}\hat{a}^\dagger_\alpha\hat{a}^\dagger_\beta\hat{a}_d\hat{a}_c \tag{13.47}$$

For a two-body potential V_{ij},

$$\begin{aligned} h_{ab;cd} &= \frac{1}{2}v_{ab;cd} = \frac{1}{2}\langle ab|V|cd\rangle \\ &= \frac{1}{4}\bar{v}_{ab;cd} = \frac{1}{4}\langle ab|V|cd-dc\rangle \\ \langle ab|V|cd-dc\rangle &= \int d\boldsymbol{r}_1 d\boldsymbol{r}_2\phi^\dagger_a(\boldsymbol{r}_1)\phi^\dagger_b(\boldsymbol{r}_2)V(\boldsymbol{r}_1,\boldsymbol{r}_2)\left(\phi_c(\boldsymbol{r}_1)\phi_d(\boldsymbol{r}_2) - \phi_d(\boldsymbol{r}_1)\phi_c(\boldsymbol{r}_2)\right) \end{aligned} \tag{13.48}$$

The angular momentum is not considered here yet. If we consider angular momentum, two-body operator actually can be re-expressed in terms of specific angular momentum operators.

13.6 Two-body matrix elements(TBME)

In the shell model, all the information of Hamiltonian is expressed in terms of matrix elements of the Hamiltonian in certain basis.

Because of scalar potential, the TBME does not depend on M-value. Thus, one can use M-independent expression(instead of reduced matrix elements.)

$$\langle (ab)JM|V|(cd)JM\rangle_{nas} = \langle (ab)J|V|(cd)J\rangle_{nas} = \frac{1}{\sqrt{2J+1}}\langle (ab)J||V||(cd)J\rangle_{nas} \tag{13.49}$$

Note: TBME of $\langle (ab)J|V|(cd)J\rangle$ for given two-body interaction V is for $|ab;JM\rangle_{nas}$(normalized anti-symmetrized state), not for for $|ab;JM\rangle_p$(a simple product).

$$\begin{aligned}
|j_a m_a, j_b m_b\rangle_{nas} &= \frac{1}{\sqrt{2}}(|j_a m_a, j_b m_b\rangle_p - |j_b m_b, j_a m_a\rangle_p) \\
|(ab)JM\rangle_p &= \sum_{m_a m_b} \langle j_a m_a, j_b m_b|JM\rangle |j_a m_a, j_b m_b\rangle_p \\
|(ab)JM\rangle_{nas} &= \frac{1}{\sqrt{1+\delta_{ab}}} \sum_{m_a m_b} \langle j_a m_a, j_b m_b|JM\rangle |j_a m_a, j_b m_b\rangle_{nas} \\
&= \frac{1}{\sqrt{1+\delta_{ab}}}\frac{1}{\sqrt{2}}\Big[|(ab)JM\rangle_p - (-1)^{j_a+j_b-J}|(ba)JM\rangle_p\Big]
\end{aligned} \tag{13.50}$$

[4] Inverse gives

$$|k_1 m_1 k_2 m_2\rangle_{nas} = \sqrt{1+\delta_{j_1 j_2}} \sum_{JM} \langle JM|j_1 m_1 j_2 m_2\rangle |k_1 k_2 JM\rangle_{nas} \tag{13.54}$$

However, one have to be careful to distinguish $|\rangle_{nas}$ and $|\rangle_p$,

$$|k_2 k_1; JM\rangle_{nas} = (-1)^{j_1+j_2-J+1}|k_1 k_2; JM\rangle_{nas}, \tag{13.55}$$

$$\begin{aligned}
&|k_2 k_1; JM\rangle_p \propto \sum_{m2,m1} C^{JM}_{m2,m1} R_{k2}(r_1) R_{k1}(r_2) \\
\neq\ & (-1)^{j_1+j_2-J+1}|k_1 k_2; JM\rangle_p \propto (-1)^{j_1+j_2-J+1} \sum_{m1,m2} C^{JM}_{m1,m2} R_{k1}(r_1) R_{k2}(r_2).
\end{aligned} \tag{13.56}$$

---

[4] If $a \neq b$,

$$\begin{aligned}
|(ab)JM\rangle_{nas} &= \frac{1}{2}\sum_{m_a m_b} \langle j_a m_a, j_b m_b|JM\rangle \Big(|j_a m_a\rangle \otimes |j_b m_b\rangle - |j_b m_b\rangle \otimes |j_a m_a\rangle\Big) \\
&= \frac{1}{\sqrt{2}}\Big[|(ab)JM\rangle - (-1)^{j_a+j_b-J}|(ba)JM\rangle\Big] \quad a \neq b.
\end{aligned} \tag{13.51}$$

If $a = b$, (implies J of two identical states should always be even integer.)

$$\begin{aligned}
|(aa)JM\rangle_{nas} &= \frac{1-(-1)^{2j_a-J}}{2} \sum_{m_1 m_2} \langle j_a m_1 j_a m_2|JM\rangle |j_a m_1\rangle \otimes |j_a m_2\rangle \\
&= \frac{1-(-1)^{2j_a-J}}{2}|(j_a j_a)JM\rangle
\end{aligned} \tag{13.52}$$

These two case can be combined as

$$|(ab)JM\rangle_{nas} = \frac{1}{\sqrt{(1+\delta_{ab})}}\Big[|(ab)JM\rangle_p - (-1)^{j_a+j_b-J}|(ba)JM\rangle_p\Big] \tag{13.53}$$

• TBME for nas states becomes

$$
\begin{aligned}
&{}_{nas}\langle k_1k_2;J|V|k_3k_4;J\rangle_{nas} = {}_{nas}\langle k_1k_2;JM|V|k_3k_4;JM\rangle_{nas} \\
= \;& N_{12}N_{34}\sum_{m_i} C^{JM}_{j_1m_1j_2m_2}C^{JM}_{j_3m_3j_4m_4}{}_{nas}\langle k_1m_1k_2m_2|V|k_3m_3k_4m_4\rangle_{nas} \\
= \;& N_{12}N_{34}\sum_{m_i} C^{JM}_{j_1m_1j_2m_2}C^{JM}_{j_3m_3j_4m_4} \\
& \times(\frac{1}{\sqrt{2}})^2\Big(\langle k_1m_1k_2m_2|V|k_3m_3k_4m_4\rangle_p - \langle k_1m_1k_2m_2|V|k_4m_4k_3m_3\rangle_p \\
& -\langle k_2m_2k_1m_1|V|k_3m_3k_4m_4\rangle_p + \langle k_2m_2k_1m_1|V|k_4m_4k_3m_3\rangle_p\Big) \\
= \;& N_{12}N_{34}\sum_{m_i} C^{JM}_{j_1m_1j_2m_2}C^{JM}_{j_3m_3j_4m_4}(\langle k_1m_1k_2m_2|V|k_3m_3k_4m_4\rangle_p - \langle k_1m_1k_2m_2|V|k_4m_4k_3m_3\rangle_p) \\
= \;& \frac{1}{\sqrt{(1+\delta_{k_1k_2})(1+\delta_{k_3k_4})}} \\
& \times\left[{}_p\langle k_1k_2;JM|V|k_3k_4;JM\rangle_p - (-1)^{j_3+j_4-J}{}_p\langle k_1k_2;JM|V|k_4k_3;JM\rangle_p\right]
\end{aligned}
\tag{13.57}
$$

For example,

$$
{}_{nas}\langle (j_a)^2;JM|V|(j_a)^2;JM\rangle_{nas} = \langle (j_a)^2;JM|V|(j_a)^2;JM\rangle, \quad \text{for even J .} \tag{13.58}
$$

From symmetry,

$$
\begin{aligned}
\langle k_3k_4J|V|k_1k_2J\rangle_{nas} &= \langle k_1k_2J|V|k_3k_4J\rangle_{nas}, \\
\langle k_1k_2J|V|k_4k_3J\rangle_{nas} &= -(-1)^{j_3+j_4-J}\langle k_1k_2J|V|k_3k_4J\rangle_{nas}, \\
\langle k_2k_1J|V|k_3k_4J\rangle_{nas} &= -(-1)^{j_1+j_2-J}\langle k_1k_2J|V|k_3k_4J\rangle_{nas},
\end{aligned}
\tag{13.59}
$$

we need only one order of $\langle k_1k_2J|V|k_3k_4J\rangle_{nas}$ TBME.

• If we consider isospin, one also have to consider similar relations in isospin. Including isospin in state index

$$
\begin{aligned}
&{}_{nas}\langle k_1k_2;JT|V|k_3k_4;JT\rangle_{nas} = {}_{nas}\langle k_1k_2;JMTT_z|V|k_3k_4;JMTT_z\rangle_{nas} \\
= \;& \frac{1}{\sqrt{(1+\delta_{k_1k_2})}}\frac{1}{\sqrt{(1+\delta_{k_3k_4})}}\left[{}_p\langle k_1k_2JT|V|k_3k_4JT\rangle_p - (-1)^{j_3+j_4-J+1-T}{}_p\langle k_1k_2JT|V|k_4k_3JT\rangle_p\right]
\end{aligned}
\tag{13.60}
$$

Now the previous symmetry relations holds including additional $(-1)^{1-T}$ factors.

• If one does not use iso-spin for nas states, one may use proton and neutron states. Another convention dependence comes from normalized(xpn) and unnormalized(upn) pn state.

$$
V^{xpn}_J(a_\pi b_\nu, c_\pi d_\nu) = \frac{2}{\sqrt{(1+\delta_{ab})(1+\delta_{cd})}}V^{upn}_J(a_\pi b_\nu, c_\pi d_\nu) \tag{13.61}
$$

where δ_{ab} only considers n,l,j not isospin. (For example, for state index proton $1(0d_{3/2})$, neutron $6(1s_{1/2})$, proton $2(0d_{5/2})$, neutron $5(0d_{5/2})$ $V^{xpn}_J(16,25) = \sqrt{2}V^{upn}_J(16,25)$.)

The factor is related with the convention of normalized p-n wave function. In normalized p-n wave function,

$$
V^{xpn}_J(ab,cd) = \frac{\sqrt{(1+\delta_{ab})(1+\delta_{cd})}}{2}[V^{iso}_{J,T=0}(ab,cd) + V^{iso}_{J,T=1}(ab,cd)]. \tag{13.62}
$$

In unnormalized p-n wave function,

$$
V^{upn}_J(ab,cd) = [V^{iso}_{J,T=0}(ab,cd) + V^{iso}_{J,T=1}(ab,cd)]. \tag{13.63}
$$

13.7 No core shell model

Simple single particle form of Hamiltonian($\boldsymbol{r}_i$들로 표현되는 Hamiltonian은 total center of mass energy를 가지고, 따라서, intrinsic part를 분리해야한다.) 이것을 **translational-invariant Hamiltonian**으로 쓰면,

$$\hat{H} = \frac{1}{2mA}\sum_{i<j=1}^{A}(\boldsymbol{p}_i - \boldsymbol{p}_j)^2 + \sum_{i<j=1}^{A} W(\boldsymbol{r}_i - \boldsymbol{r}_j) \tag{13.64}$$

이고, 이것이 실제 intrinsic motion을 기술하며 풀어야하는 Hamiltonian. (W can include Coulomb interaction.)

특별히 Harmonic Oscillator의 경우, 다음과 같은 식이 성립한다. [5]

$$\begin{aligned}
\sum_{i=1}^{A}\frac{\boldsymbol{p}_i^2}{2m} &= \frac{1}{2mA}\sum_{i<j=1}^{A}(\boldsymbol{p}_i - \boldsymbol{p}_j)^2 + \frac{\boldsymbol{P}^2}{2(mA)} = \frac{1}{4mA}\sum_{i\neq j}^{A}(\boldsymbol{p}_i - \boldsymbol{p}_j)^2 + \frac{\boldsymbol{P}^2}{2(mA)} \\
\sum_{i=1}^{A}\frac{m}{2}\Omega^2\boldsymbol{r}_i^2 &= \frac{m\Omega^2}{2A}\sum_{i<j=1}^{A}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 + \frac{(mA)\Omega^2}{2}\boldsymbol{R}^2
\end{aligned} \tag{13.66}$$

Let us define some conventions:

$$\begin{aligned}
\hat{T}_{rel} &= \frac{1}{2mA}\sum_{i<j=1}^{A}(\boldsymbol{p}_i - \boldsymbol{p}_j)^2, \\
\hat{U}_{rel} &= \frac{m\Omega^2}{2A}\sum_{i<j=1}^{A}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2, \\
\hat{H}_{rel} &= \hat{T}_{rel} + \hat{U}_{rel}, \\
\hat{H}_{cm} &= \frac{\boldsymbol{P}^2}{2mA} + \frac{mA\Omega^2}{2}\boldsymbol{R}^2 \\
\hat{H}_{osc} &= \sum_{i=1}^{A}\left[\frac{\boldsymbol{p}_i^2}{2m} + \frac{m}{2}\Omega^2\boldsymbol{r}_i^2\right] = \hat{H}_{rel} + \hat{H}_{cm}.
\end{aligned} \tag{13.67}$$

Translation invariant Hamiltonian for A-body is

$$\begin{aligned}
\hat{H} &= \hat{T}_{rel} + \hat{V}_{pot} + \hat{V}_{coul} \\
&= \sum_{i=1}^{A}\left[\frac{\boldsymbol{p}_i^2}{2m} + \frac{m}{2}\Omega^2\boldsymbol{r}_i^2\right] - \frac{\boldsymbol{P}^2}{2mA} + \sum_{i<j=1}^{A} W(\boldsymbol{r}_i - \boldsymbol{r}_j) - \sum_{i=1}^{A}\frac{m}{2}\Omega^2\boldsymbol{r}_i^2 + \hat{V}_{coul} \\
&= \sum_{i=1}^{A}\left[\frac{\boldsymbol{p}_i^2}{2m} + \frac{m}{2}\Omega^2\boldsymbol{r}_i^2\right] + \sum_{i<j=1}^{A}\left[W(\boldsymbol{r}_i - \boldsymbol{r}_j) - \frac{m\Omega^2}{2A}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2\right] - \hat{H}_{cm} + \hat{V}_{coul} \\
&= \hat{H}_{osc} + \hat{V}_{pot} - \hat{U}_{rel} + \hat{V}_{coul} - \hat{H}_{cm}
\end{aligned} \tag{13.68}$$

으로 쓸 수 있다. 단, 주의할 것은 이것은 어디까지나, original translation invariant Hamiltonian을 다시 쓴 것이므로 Ω에 대한 dependence는 $\hat{H}$에는 없다.

It is still confusing what is the exact no-core shell model Hamiltotnian.

[5] Let $\boldsymbol{R} = \frac{1}{A}\sum_i \boldsymbol{r}_i$, then (Similarly $\boldsymbol{P} = \sum_i \boldsymbol{p}_i$)

$$(A\boldsymbol{R})^2 + \sum_{i<j=1}^{A}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 = A\sum_{i=1}^{A}\boldsymbol{r}_i^2, \quad \boldsymbol{P}^2 + \sum_{i<j=1}^{A}(\boldsymbol{p}_i - \boldsymbol{p}_j)^2 = A\sum_{i=1}^{A}\boldsymbol{p}_i^2. \tag{13.65}$$

In one reference, it says (Coulomb seems to be omitted)

$$\begin{aligned} H_\Omega^{[A]} &= H + H_{CM}^{HO} = H + \frac{\boldsymbol{P}^2}{2mA} + \frac{mA\Omega^2}{2}\boldsymbol{R}^2 \\ &= \sum_{i=1}^{A}\left[\frac{\boldsymbol{p}_i^2}{2m} + \frac{m}{2}\Omega^2\boldsymbol{r}_i^2\right] + \sum_{i<j=1}^{A}\left[W(\boldsymbol{r}_i-\boldsymbol{r}_j) - \frac{m\Omega^2}{2A}(\boldsymbol{r}_i-\boldsymbol{r}_j)^2\right] \\ &= \sum_{i=1}^{A} h_i^{HO} + \sum_{i<j}^{A}\tilde{V}_{ij} \end{aligned} \tag{13.69}$$

This $H_\Omega^{[A]}$ is not translation invariant. ($H = H_\Omega^{[A]} - H_{COM}$) The $\tilde{V}_{ij}$ is a modified interaction depends on both HO frequency Ω and nuclear system A. Then, the ground state energy of H is obtained by subtraction of the CM g.s. energy $\frac{3}{2}\Omega$ from the $E_\Omega^{[A]}$ of $H_\Omega^{[A]}$.

The calculation is done in model space P_A (of A-body Slater determinants) with $\tilde{V}_{ij}$. However, the convergence is very slow and one can speed it up by using $\tilde{V}^{(2,eff)}$ which is obtained via SL procedure to a two-body internal Hamiltonian by restricting the sums to two nucleons only, however keeping the original mass number A in the ineraction term $\tilde{V}$.

$$H_\Omega^{(2)} = \left[\frac{\pi^2}{2m} + \frac{1}{2}m\Omega^2\eta^2\right] + \tilde{V}_{A(A-1)} = H_{HO}^{(2)} + \tilde{V}_{A(A-1)} \tag{13.70}$$

The effective Hamiltonian $H_{eff}^{(2)}$ is determined in the P_2 space, a subspace of P, via the two-body transformation operator $S^{(2)} = Q_2 S^{(2)} P_2$. Then by subtracting $H_{HO}^{(2)}$ from $H_{eff}^{(2)}$ thw two-body effective interaction is obtained,

$$\tilde{V}_{12}^{(2,eff)} = H_{eff}^{(2)} - H_{HO}^{(2)} \tag{13.71}$$

Then, this $\tilde{V}^{(2,eff)}$ is used instead of $\tilde{V}$.

In another reference, 여기에 새로이 additional C.M. term을 더하여 새로운 Hamiltonian $\hat{H}^\Omega$를 정의한다.

$$\begin{aligned} \hat{H}_\Omega^{[A]} &= \hat{H} + \beta'(\hat{H}_{cm} - \frac{3}{2}\hbar\Omega) \\ &= \hat{H}_{osc} + \hat{V}_{pot} - \hat{U}_{rel} + \hat{V}_{coul} - \hat{H}_{cm} + \beta'(\hat{H}_{cm} - \frac{3}{2}\hbar\Omega) \\ &= \hat{H}_{rel} + \hat{V}_{pot} - \hat{U}_{rel} + \hat{V}_{coul} + \beta'\hat{H}_{cm} - \beta'\frac{3}{2}\hbar\Omega \\ &= (1-\beta')\hat{H}_{rel} + \hat{V}_{pot} - \hat{U}_{rel} + V_{coul} + \beta'\hat{H}_{osc} - \beta'\frac{3}{2}\hbar\Omega \\ &= \hat{T}_{rel} - \beta'\hat{H}_{rel}^\Omega + \hat{V}_{pot} + V_{coul} + \beta'\hat{H}_{osc}^\Omega - \beta'\frac{3}{2}\hbar\Omega \end{aligned} \tag{13.72}$$

으로 두고 $\hat{H}^\Omega$의 eigenvalue를 구하면, 이것은 $E_{int} + \beta' N\hbar\Omega$ 꼴이 될 것으로 생각할 수 있고, 따라서, 원하는 internal state E_{int}에 대한 정보를 얻을 수 있다.

(Note that the last form does not contain $\hat{H}_{cm}$ explicitly. Thus, it can be calculated in terms of $\boldsymbol{r}_i$'s. Since there is a relation between $(H,T,U)_{rel}$, one only have to provide two of them.)

주의: NCSM Hamiltonian depends on A. One can use $H_\Omega^{[2]}$ to obtain part of $H_\Omega^{[A]}$.

(이 아래 내용도 정리가 필요한 것 같다.) One can obtain matrix element of H_{osc} analytically. For relative part of Hamiltonian can be scaled from A=2 TBME of $T_{rel}^{(2B)}$ and $H_{rel}^{(2B)}$ in $\hbar\Omega$ units. Then, the total A-body Hamiltonian matrix which involving two-body interaction $\hat{H}^\Omega = \hat{H}_{1B}^\Omega + \hat{H}_{2B}^\Omega + \cdots$,

$$\hat{H}_2^\Omega = \frac{2\hbar\Omega}{A}T_{rel}^{(2)} - \frac{2\hbar\Omega}{A}\lambda\hat{H}_{rel}^{(2)} + \hat{V}_{pot}^{(2)} + V_{coul}^{(2)} + \lambda\frac{\hbar\Omega}{A-1}(2n_a + l_a + 2n_b + l_b + 3) - \lambda\frac{3\hbar\Omega}{A(A-1)} \tag{13.73}$$

where $T^{(2)}_{rel} = \frac{1}{2m*2}(\boldsymbol{p}_1 - \boldsymbol{p}_2)^2$, $H^{(2)}_{rel} = \frac{m\Omega^2}{2*2}(\boldsymbol{r}_1 - \boldsymbol{r}_2)^2$ (?)

Ordering of single particle H.O. orbits (n, l, j) can be done as follows:

(1) For given maximum ip value, change N$(= 2n + l)$ from 0 to ip.

(2) For given N, n value can change from $[N/2]$ to 0. This fix the value of $l = N - 2n$.

(3) For given N and n value, $2 * j$ can change from $(2l - 1)$ to $2l + 1$ as long as it is positive.

Shell model terms: Seniority

Shell model에서 Seniority 라는 용어는 두 nucleon이 $J = 0$인 pair를 만드는 pairing interaction과 관련하여 사용한다. 일반적으로 이러한 paring interaction은 even-even nuclei의 ground state를 $J = 0$으로 만드는 역할을 한다. 핵자간의 힘 중 $J = 0$을 이루는 힘이 가장 중요하다고 보고, 이것을 local contact potential로 생각하면, $J = 0$ pair를 이루지 않은 쌍이 많을 수록 energy가 높아질 것이다. Seniority는 j-shell 에 있는 핵자중 $J = 0$ pairing 을 하지 않은 핵자의 수를 말한다. 따라서, Seniority $\nu = 0$ 인 상태는 $J = 0$ 이고 가장 낮은 에너지 상태가된다. $\nu = 2$ 라면, j^2 로 만들 수 있는 $J = 2, 4...$ 을 줄 수 있다.

13.8 Harmonic Oscillator basis

For

$$U(r) = \frac{1}{2}m\omega^2 r^2, \quad \nu = \frac{m\omega}{2\hbar} = \frac{1}{2b^2}, \tag{13.74}$$

Schrodinger equation solution

$$(-\frac{\hbar^2}{2m}\nabla^2 + U(r))\psi_{nlm}(\boldsymbol{r}) = E_{nl}\psi_{nlm}(\boldsymbol{r}), \tag{13.75}$$

is

$$\begin{aligned} E_{kl} &= \hbar\omega(n + \frac{3}{2}) = \hbar\omega(2k + l + \frac{3}{2}), \quad n \geq 0,\ k = (n - l)/2 \geq 0 \\ \psi_{nlm}(\boldsymbol{r}) &= \frac{u_{nl}(r)}{r}Y_{lm}(\hat{\boldsymbol{r}}) \end{aligned} \tag{13.76}$$

Be careful to distinguish n and k.

$$\begin{aligned} \frac{u_{kl}(r)}{r} &= \sqrt{\frac{2(2\nu)^{l+3/2}(k!)}{\Gamma(k + l + 3/2)}}r^l e^{-\nu r^2}L_k^{(l+1/2)}(2\nu r^2) \\ &= \sqrt{\frac{2(k!)}{b^3\Gamma(k + l + 3/2)}}(\frac{r}{b})^l e^{-\frac{1}{2}(\frac{r}{b})^2}L_k^{(l+1/2)}((\frac{r}{b})^2), \quad 2\nu = \frac{1}{b^2} \end{aligned} \tag{13.77}$$

Where we used, for associated Laguerre polynomial

$$\int_0^\infty dx L_n^{(\alpha)}(x)L_m^{(\alpha)}(x)e^{-x}x^\alpha = \frac{\Gamma(n + \alpha + 1)}{n!}\delta_{nm}. \tag{13.78}$$

Note that the de-shalit book has typo on normalization. Also, normalization can be expressed using double factorial (instead of Gamma function $\Gamma(j + 1/2) = \sqrt{\pi}\frac{(2j-1)!!}{2^j}$) such as

$$N_{nl} = \sqrt{\sqrt{\frac{2\nu^3}{\pi}}\frac{2^{k+2l+3}(k!)\nu^l}{(2k + 2l + 1)!!}}, \ n = 2k + l. \tag{13.79}$$

Note that one can express Laguerre polynomial as

$$L_n^{l+1/2}(x) = \sum_{m=0}^{n}(-1)^m\frac{1}{m!}\frac{(2n + 2l + 1)!!}{2^{n-m}(n - m)!(2m + 2l + 1)!!}x^m \tag{13.80}$$

$$L_n^{(\alpha)}(x) = L_n^{(\alpha+1)}(x) - L_{n-1}^{(\alpha+1)}(x),$$
$$xL_n^{(\alpha+1)}(x) = -(n+1)L_{n+1}^{(\alpha)}(x) + (n+\alpha+1)L_n^{(\alpha)}(x). \tag{13.81}$$

Special value

$$L_n^{(1/2)}(0) = \frac{2\Gamma(n+3/2)}{\sqrt{\pi}\Gamma(n+1)}. \tag{13.82}$$

Note that in this convention, **the radial wave function is positive at and near the origin**.

Each single particle wave function can have $k = (n_r, l, j)$ quantum numbers and each j value has $(2j+1)$ m-states. The single particle wave fuction can be labeld as $\alpha = (km)$. We may assign a number to s.p. states such as

$$(\text{k-index}) = \frac{1}{2}[(2n+l)(2n+l+3) - 2j + 3] \tag{13.83}$$

This means $(k - index) = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, \ldots$ for sequence, $0s_{1/2}$, $0p_{3/2}$, $0p_{1/2}$, $0d_{5/2}$, $0d_{3/2}$, $1s_{1/2}$, $0f_{7/2}$, $0f_{5/2}$, $1p_{3/2}$, $1p_{1/2}$, ...

It can be more convenient to use r in a unit of $b = \frac{1}{\sqrt{2\nu}} = \sqrt{\frac{\hbar}{m\omega}}$ fm. In other words, by using $\tilde{r} = \sqrt{2\nu}r$(dimensionless),

$$\frac{u_{nl}(r;\nu)}{r} \to (2\nu)^{3/4}\frac{u_{nl}(\tilde{r})}{\tilde{r}} = (2\nu)^{3/4}\sqrt{\frac{2(k!)}{\Gamma(k+l+3/2)}}\tilde{r}^l e^{-\frac{1}{2}\tilde{r}^2} L_k^{(l+1/2)}(\tilde{r}^2) \tag{13.84}$$

where factor $(2\nu)^{3/4}$ is from the dimension of original wave function $[MeV^{3/2}]$, which will cancel with dimensional factor of integral $\int drr^2$ in normalization.

Now the dimensionless radial wave function can be written as(r is now dimensionless)

$$\begin{aligned} \mathcal{R}_{nl}(r) &= \frac{u_{nl}(\tilde{r})}{\tilde{r}} = r^l \exp(-\frac{1}{2}r^2)\sum_{k=0}^{n} a_{nlk} r^{2k}, \\ a_{nlk} &= \left[\frac{2(n!)}{\Gamma(n+l+3/2)}\right]^{\frac{1}{2}} \begin{pmatrix} n+l+\frac{1}{2} \\ n-k \end{pmatrix} \frac{(-1)^k}{k!} \end{aligned} \tag{13.85}$$

At $r = 0$, only $l = 0$ is non-zero,

$$\begin{aligned} R_{kl}(0) &= \frac{1}{b^{3/2}}\mathcal{R}_{kl}(0) = \frac{1}{b^{3/2}}\sqrt{\frac{2(k!)}{\Gamma(k+3/2)}}\frac{2\Gamma(k+3/2)}{\sqrt{\pi}\Gamma(k+1)} \\ &= \frac{1}{2^{n-1}n!}\sqrt{\frac{(2n+1)!}{\sqrt{\pi}}} \end{aligned} \tag{13.86}$$

$$\Gamma(n+\frac{3}{2}) = (n+\frac{1}{2})! = \frac{\sqrt{\pi}(2n+1)!}{2^{2n+1}n!} \tag{13.87}$$

Radial integrals for H.O. wave functions can be obtained by

$$\begin{aligned} &\langle n, l+1|r|n, l\rangle = b\sqrt{n+l+3/2}, \\ &\langle n-1, l+1|r|n, l\rangle = -b\sqrt{n} \end{aligned} \tag{13.88}$$

$$
\begin{aligned}
&\langle n,l|r^2|nl\rangle = b^2(2n+l+3/2),\\
&\langle n-1,l+2|r^2|nl\rangle = -b^2\sqrt{2n(2n+2l+3)},\\
&\langle n,l+2|r^2|nl\rangle = b^2\sqrt{(n+l+3/2)(n+l+5/2)},\\
&\langle n+1,l|r^2|nl\rangle = -b^2\sqrt{(n+1)(n+l+3/2)},\\
&\langle n,l|p^2|n,l\rangle = \frac{\hbar^2}{b^2}(2n+l+3/2),\\
&\langle n-1,l+2|p^2|n,l\rangle = \frac{\hbar^2}{b^2}\sqrt{2n(2n+2l+3)},\\
&\langle n,l+2|p^2|n,l\rangle = -\frac{\hbar^2}{b^2}\sqrt{(n+l+3/2)(n+l+5/2)},\\
&\langle n+1,l|p^2|n,l\rangle = \frac{\hbar^2}{b^2}\sqrt{(n+1)(n+l+3/2)}.
\end{aligned}
\tag{13.89}
$$

13.9 CM motion

Many particles within Harmonic oscillator potential,

$$
H_{osc} = \sum_{i=1}^{A}\frac{p_i^2}{2m} + \sum_{i=1}^{A}\frac{1}{2}m\omega^2 r_i^2 \tag{13.90}
$$

The eigen state of this Hamiltonian is simply a Slater determinant of H.O. basis wave functions. $|\alpha_1,\alpha_2,\ldots\alpha_A$ with $(\alpha_i) = |n_i,l_i\rangle$ with H.O. frequency ω. Thus, energy of the system is $E = \hbar\omega((\sum_{i=1}^{A} 2n_i + l_i) + A\frac{3}{2})$. This contains center of mass motion. We want only energy of the system without CM kinetic energy. How can we extract it? Obviously, we can separate Hamiltonian into

$$
\begin{aligned}
\hat{H}_{osc} &= \sum_{i=1}^{A}\left[\frac{\boldsymbol{p}_i^2}{2m} + \frac{m}{2}\Omega^2\boldsymbol{r}_i^2\right] = \hat{H}_{rel} + \hat{H}_{cm},\\
\hat{T}_{rel} &= \frac{1}{2mA}\sum_{i<j=1}^{A}(\boldsymbol{p}_i - \boldsymbol{p}_j)^2,\\
\hat{U}_{rel} &= \frac{m\Omega^2}{2A}\sum_{i<j=1}^{A}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2,\\
\hat{H}_{rel} &= \hat{T}_{rel} + \hat{U}_{rel},\\
\hat{H}_{cm} &= \frac{\boldsymbol{P}^2}{2mA} + \frac{mA\Omega^2}{2}\boldsymbol{R}^2.
\end{aligned}
\tag{13.91}
$$

This implies that one can change $|n_1l_1,n_2l_2,\ldots n_Al_A\rangle$ into $|(relative),N\Lambda\rangle$ with CM energy $E_{cm} = \hbar\omega(2N+\Lambda+\frac{3}{2})$. Can we determine N and Λ for given (n_i,l_i)'s ?

13.10 Moshinsky transformation

In shell model or HF calculation, the full matrix elements of Hamiltonian for slater-determinant states can be written in terms of one-body and two-body matrix elements, $\langle i|\hat{F}|j\rangle$ and $\langle ij|\hat{V}|kl\rangle_{AS}$. Thus, usually these matrix elements are input to the shell model code.

To obtain TBME (note for normalized-anti-symmetrized two-particle states), One can simply to the multi-dimensional integration over $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ with four single particle basis wave wave functions directly.

On the other hand, because of center of mass motion is conserved, one should be able to obatin TBME from the integration of wave function for relative motion. This can be done by using Moshinsky transformation, in case of H.O. basis.

• One way to express TBME is to transform two nucleon states into relative part and center of mass part by using Moshinsky transformation. This method is valid only for H.O. basis.

$$\begin{aligned} H &= \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m\omega^2 r_1^2 + \frac{1}{2}m\omega^2 r_2^2 \\ &= \frac{Q^2}{2M} + \frac{1}{2}M\omega^2 R^2 + \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2 r^2. \end{aligned} \tag{13.92}$$

where $M = 2m$, $\mu = m/2$. Thus total wave function can be written in terms of $R_{N\Lambda}(R; \nu = \frac{M\omega}{2\hbar})$ and $R_{n\lambda}(r; \nu = \frac{\mu\omega}{2\hbar})$. In other words, energy becomes

$$\hbar\omega(2n_1 + l_1 + 2n_2 + l_2 + 3) = \hbar\omega(2n + l + 2N + \Lambda + 3). \tag{13.93}$$

Note that though ν of wave functions are different, ω are the same.

For example, in case of $(0s)^2$ waves,

$$\begin{aligned} R_{00}(r_1)R_{00}(r_2)Y_{00}(\hat{r}_1)Y_{00}(\hat{r}_2) &= (2\nu)^3(\frac{2^2}{\sqrt{\pi}})^2 r_1 r_2 e^{-\nu(r_1^2+r_2^2)} Y_{00}(\hat{r}_1)Y_{00}(\hat{r}_2) \\ &= (2\nu)^3(\frac{2^2}{\sqrt{\pi}})^2 r_1 r_2 e^{-\nu(\frac{1}{2}r^2+2R^2)} Y_{00}(\hat{r}_1)Y_{00}(\hat{r}_2) \\ &= \left(\frac{r_1 r_2}{rR} Y_{00}(\hat{r})Y_{00}(\hat{R})\right) R_{00}(r; \nu' = \frac{\mu\omega}{2\hbar}) R_{00}(R; \nu' = \frac{M\omega}{2\hbar}) \end{aligned} \tag{13.94}$$

where integration over angle of first term gives Talmi-Moshinsky bracket.

Alternatively, one may redefine $\boldsymbol{R}' = \frac{(\boldsymbol{r}_1+\boldsymbol{r}_2)}{\sqrt{2}}$ and $\boldsymbol{r}' = \frac{(\boldsymbol{r}_1-\boldsymbol{r}_2)}{\sqrt{2}}$ and use radial wave functions $R_{N\Lambda}(R' = \frac{R}{\sqrt{2}}; \nu = \frac{m\omega}{2\hbar})$ and $R_{n\lambda}(r' = \frac{r}{\sqrt{2}}; \nu = \frac{m\omega}{2\hbar})$.

In this case, potential becomes $V(|\boldsymbol{r}_1 - \boldsymbol{r}_2| = \sqrt{2}r')$.

In other words, for $\boldsymbol{r}_0 = \boldsymbol{r}_1 - \boldsymbol{r}_2$, $b_0 = \sqrt{\frac{\hbar}{m\omega}}$, different convention corresponds to

$$R_{nl}(\frac{r_0}{\sqrt{2}}; b = b_0) = \frac{1}{\sqrt{b_0^3}}\mathcal{R}_{nl}(\frac{r_0}{\sqrt{2}b_0}) = 2^{3/4}R_{nl}(r_0; b = \sqrt{2}b_0) \tag{13.95}$$

Thus radial integration with relative wave function can be re-written as dimensionless wave function,

$$\int dr_0 r_0^2 R_{nl}(r_0; \sqrt{2}b_0)V(r_0)R_{n'l'}(r_0; \sqrt{2}b_0) = \int dR R^2 \mathcal{R}_{nl}(R)V(r_0)\mathcal{R}_{n'l'}(R), \quad R = \frac{r_0}{\sqrt{2}b_0} \tag{13.96}$$

One can transform the product of two H.O. basis into relative and center of mass coordinates. (This is a special property of H.O. basis)

$$|(n_1 l_1, n_2 l_2)LM\rangle = \sum_{n,l,N,\Lambda} \langle nl, N\Lambda; L|n_1 l_1 n_2 l_2; L\rangle |(nl, N\Lambda)LM\rangle \tag{13.97}$$

Here the conversion is called **Talmi-Moshinsky transformation** and it is determined by coefficients $\langle nl, N\Lambda; L|n_1 l_1 n_2 l_2; L\rangle$, called **Talmi-Moshinsky transformation brackets**. Obviously, there are constraints on possible n, l, N, Λ values by

$$\begin{aligned} &\boldsymbol{L} = \boldsymbol{l}_1 + \boldsymbol{l}_2 = \boldsymbol{l} + \boldsymbol{\Lambda}, \\ &\rho = 2n_1 + l_1 + 2n_2 + l_2 = 2n + l + 2N + \Lambda. \end{aligned} \tag{13.98}$$

where all numbers are non-negative integers. (Also, conservation of parity, $(-1)^{l_1+l_2} = (-1)^{l+L}$)

• Reduction of spatial reduced matrix elements of operators in relative coordinates,

$$\langle k_A k_B L||U^{(q)}||k_C k_D L'\rangle = \sum_{nln'l'N\Lambda N'\Lambda'} \langle nlN\Lambda|k_A k_B L\rangle\langle n'l'N'\Lambda'|k_C k_D L'\rangle\langle nlN\Lambda; L||U^{(q)}(\boldsymbol{r})||n'l'N'\Lambda'; L'\rangle \quad (13.99)$$

We can further reduce in relative coordinates,

$$\begin{aligned}\langle nlN\Lambda; L||U^{(q)}(\boldsymbol{r})||n'l'N'\Lambda'; L'\rangle &= (-1)^{l+\Lambda+L'+q}\sqrt{(2L+1)(2L'+1)}\begin{Bmatrix} l & l' & q \\ L' & L & \Lambda \end{Bmatrix} \\ &\times\langle nl||U^{(q)}(\boldsymbol{r})||n'l'\rangle\delta_{NN'}\delta_{\Lambda\Lambda'} \end{aligned} \quad (13.100)$$

Be careful that the last reduced matrix element does not contain angular integral! In other words, the angular integration is already implied in the Moshinsky brakets and the final reduced matrix element is purely radial integral. Thus, it is possible that $l \neq l'$ for $\langle nl|V(r)|v'l'\rangle$ for scalar function $V(r)$. Note the $\langle N\Lambda|N'\Lambda'\rangle = \delta_{NN'}\delta_{\Lambda\Lambda'}$ comes from orthogonal relation of radial function of H.O. (Not from relation of spherical Harmonics.)

• Two-body matrix elements in ll-coupled basis : Once Moshinsky transformation is done, we can compute the matrix elements.

For potential $V(\boldsymbol{r})$,

$$\begin{aligned} M &= \langle n_1 l_1, n_2 l_2; LM|V(\boldsymbol{r})|n_1' l_1', n_2' l_2'; LM\rangle_p \\ &= \sum_{n,n'}\sum_{l,l'}\sum_{N,\Lambda}\langle n_1 l_1, n_2 l_2; L|nl, N\Lambda; L\rangle\langle n_1' l_1', n_2' l_2'; L|n'l', N\Lambda; L\rangle\langle nl|V(\boldsymbol{r})|n'l'\rangle. \end{aligned} \quad (13.101)$$

where the conservation of l is only valid for central potential and[6]

$$\langle nl|V(\boldsymbol{r})|n'l'\rangle = \int d^3\boldsymbol{R}\mathcal{R}_{nl}(R)Y_l^* V(\boldsymbol{r})\mathcal{R}_{n'l'}(R)Y_l, \quad (13.102)$$

Note: The wave function is written in dimensionless $R = \frac{r_0}{\sqrt{2}b_0}$. ($b_0 = \sqrt{\frac{\hbar}{m\omega}}$[fm]) while potential is written in conventional definition $\boldsymbol{r}_0 = \boldsymbol{r}_1 - \boldsymbol{r}_2$.

Note, n and n' is not independent and are related by $n' - n = n_1' - n_1 + n_2' - n_2 + \frac{1}{2}(l_1' + l_2' - l_1 - l_2)$. Thus, one can remove the sum over n'.

Let us use $\rho = 2n_1 + l_1 + 2n_2 + l_2$, then non-trivial value of $\langle nlN\Lambda|n_1 l_1 n_2 l_2\rangle_L$ is when,

- $0 \leq \Lambda \leq \rho$ Careful: $\boldsymbol{l} + \boldsymbol{\Lambda} = \boldsymbol{L}$ does not imply $\Lambda \leq L$.
- for given Λ, $|L - \Lambda| \leq l \leq L + \Lambda$ and $l + \Lambda$ should have the same parity with $l_1 + l_2$. Also, it have to satisfy $l \leq (\rho - \Lambda)$.
- for given Λ and l, $0 \leq N \leq \frac{1}{2}(\rho - l - \Lambda)$
- for given Λ,l,N, $n = \frac{\rho - l - \Lambda - 2N}{2} \geq 0$

This radial integral can be expressed in terms of Talmi integrals with explicit expansion of Laguerre polynomials,

$$I_p = \frac{2}{\Gamma(p + 3/2)}\int_0^\infty r^{2p}\exp(-r^2)V(r)r^2 dr, \quad (13.103)$$

so that

$$\langle nl|V(r)|n'l'\rangle = \sum_p B(nl, n'l', p)I_p. \quad (13.104)$$

[6]Sometimes it is written as reduced matrix elements $\langle nl||V(r)||n'l'\rangle$.

Be careful that above expression use $\boldsymbol{r} = \frac{\boldsymbol{r}_1 - \boldsymbol{r}_2}{\sqrt{2}}$ in units of b. To restore usual definition of $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$ in fm units, Talmi-integral becomes

$$\begin{aligned} I_p^b &= \frac{\sqrt{2}}{b\Gamma(p+\frac{3}{2})} \int (\frac{r^2}{2b^2})^{p+1} V(r) e^{-\frac{r^2}{2b^2}} dr \\ &= \frac{2}{\Gamma(p+3/2)} \int R^{2p+2} V(r) e^{-R^2} dR \end{aligned} \tag{13.105}$$

with $R = r/\sqrt{2}b$ and $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$.

• TBME for central potential with isospin in LS-scheme:

For the central potential, including isospin

$$\begin{aligned} & \langle k_a k_B LSJT | f(r) | k_c k_d L'S'JT \rangle_p \\ = & \sum_{n\lambda n'\lambda' N\Lambda N'\Lambda'} \langle n\lambda N\Lambda | k_A k_B L \rangle \langle n'\lambda' N'\Lambda' | k_C k_D L' \rangle \\ & \times \langle n\lambda | f(r) | n'\lambda' \rangle \delta_{NN'} \delta_{\Lambda\Lambda'} \delta_{LL'} \delta_{SS'} \end{aligned} \tag{13.106}$$

(Note that this is not the reduced matrix element. And $\lambda = \lambda'$.)

• TBME in jj coupling: We may convert jj coupling into LS coupling first and then use previous expression, if the potential is spin independent central potential,

$$\begin{aligned} & \langle (n_1 l_1 j_1, n_2 l_2 j_2) JM | V(r) | (n_1' l_1' j_1', n_2' l_2' j_2') JM \rangle_{nas} \\ = & \sum_{LS} \langle (n_1 l_1 n_2 l_2) LM | V(r) | (n_1' l_1' n_2' l_2') LM \rangle_{nas} \\ & \times \sqrt{(2j_1+1)(2j_2+1)(2L+1)(2S+1)} \sqrt{(2j_1'+1)(2j_2'+1)(2L+1)(2S+1)} \\ & \times \left\{ \begin{array}{ccc} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ L & S & J \end{array} \right\} \left\{ \begin{array}{ccc} l_1' & \frac{1}{2} & j_1' \\ l_2' & \frac{1}{2} & j_2' \\ L & S & J \end{array} \right\} \end{aligned} \tag{13.107}$$

where $\langle (n_1 l_1 n_2 l_2) LM | V(r) | (n_1' l_1' n_2' l_2') LM \rangle$ can be obtained from previous result.

13.10.1 Recurrence relation of braket

Any T-M braket with $n_{1,2} \neq 0$ can be obtained by the recursion relation from $\langle n\lambda, N\Lambda | n_1 = 0, l_1, n_2 = 0 l_2 \rangle$.

One can show the following recurrence relation from the recurrence relation of Larguerre polynomials,

$$\begin{aligned} & \langle n\lambda, N\Lambda; L | n_1+1, l_1, n_2 l_2; L \rangle \\ = & [(n_1+1)(n_1+l_1+\frac{3}{2})]^{-\frac{1}{2}} \langle n\lambda, N\Lambda; LM | -r_1^2 | n_1 l_1, n_2 l_2, LM \rangle \\ = & [(n_1+1)(n_1+l_1+\frac{3}{2})]^{-\frac{1}{2}} \sum_{n'\lambda' N'\Lambda'} \langle n\lambda, N\Lambda; LM | -r_1^2 | n'\lambda', N'\Lambda'; LM \rangle \langle n'\lambda', N'\Lambda'; L | n_1 l_1, n_2 l_2, L \rangle \end{aligned} \tag{13.108}$$

where all two-particle states must in the same energy shell, $\rho = 2n + l + 2N + L = 2(n_1+1) + l_1 + 2n_2 + l_2$.

In a similar way,

$$\begin{aligned} & \langle n\lambda, N\Lambda; L | n_1, l_1, n_2+1, l_2; L \rangle \\ = & [(n_2+1)(n_2+l_1+\frac{3}{2})]^{-\frac{1}{2}} \sum_{n'\lambda' N'\Lambda'} \langle n\lambda, N\Lambda; LM | -r_2^2 | n'\lambda', N'\Lambda'; LM \rangle \langle n'\lambda', N'\Lambda'; L | n_1 l_1, n_2 l_2, L \rangle \end{aligned} \tag{13.109}$$

Thus, one can obtain any n_1, n_2 braket from $n_1 = n_2 = 0$ braket.

The matrix elements of $-r_1^2$ can be tabulated. (matrix elements of $-r_2^2$ can be inferred by changing sign of last four matrix elements in the table.)

n'	l'	N'	L'	$\langle (nl, NL)\lambda \vert - r_1^2 \vert (n'l', N'L')\lambda\rangle$
$n-1$	l	N	L	$\frac{1}{2}[n(n+l+\frac{1}{2})]^{1/2}$
n	l	$N-1$	L	$\frac{1}{2}[N(N+L+\frac{1}{2})]^{1/2}$
$n-1$	$l+1$	$N-1$	$L+1$	$[nN(l+1)(L+1)]^{1/2}(-1)^{\lambda+L+l}W(l,l+1,L,L+1;1\lambda)$
$n-1$	$l+1$	N	$L-1$	$[n(N+L+1/2)(l+1)L]^{1/2}(-1)^{\lambda+L+l}W(l,l+1,L,L-1;1\lambda)$
n	$l-1$	$N-1$	$L+1$	$[(n+l+1/2)Nl(L+1)]^{1/2}(-1)^{\lambda+L+l}W(l,l-1,L,L+1;1\lambda)$
n	$l-1$	N	$L-1$	$[(n+l+1/2)(N+L+1/2)lL]^{1/2}(-1)^{\lambda+L+l}W(l,l-1,L,L-1;1\lambda)$

Orthogonality and symmetry relation

$$\sum_{n_1 l_1 n_2 l_2} \langle (nl, NL)\lambda \vert (n_1 l_1, n_2 l_2)\lambda\rangle \langle (n'l', N'L')\lambda \vert (n_1 l_1, n_2 l_2)\lambda\rangle = \delta_{nn'}\delta_{ll'}\delta_{NN'}\delta_{LL'} \tag{13.110}$$

$$\sum_{nl,NL} \langle (nl, NL)\lambda \vert (n_1 l_1, n_2 l_2)\lambda\rangle \langle (nl, NL)\lambda \vert (n_1' l_1', n_2' l_2')\lambda\rangle = \delta_{n_1 n_1'}\delta_{l_1 l_1'}\delta_{n_2 n_2'}\delta_{l_2 l_2'}. \tag{13.111}$$

$$\begin{aligned} \langle (nl, NL)\lambda \vert (n_1 l_1, n_2 l_2)\lambda\rangle &= (-1)^{L-\lambda}\langle (nl, NL)\lambda \vert (n_2 l_2, n_1 l_1)\lambda\rangle \\ &= (-1)^{l_1-\lambda}\langle (NL, nl)\lambda \vert (n_1 l_1, n_2 l_2)\lambda\rangle \\ &= (-1)^{l_1+l}\langle (NL, nl)\lambda \vert (n_2 l_2, n_1 l_1)\lambda\rangle. \end{aligned} \tag{13.112}$$

13.10.2 $n_1 = 0, n_2 = 0$ braket

$$\begin{aligned} &\langle (nl, NL)\lambda \vert (0l_1, 0l_2)\lambda\rangle \\ = &\left[\frac{l_1! l_2!}{(2l_1)!(2l_2)!}\frac{(2l+1)(2L+1)}{2^{l+L}}\frac{(n+l)!}{n!(2n+2l+1)!}\frac{(N+L)!}{N!(2N+2L+1)!}\right] \\ &\times(-1)^{n+l+L-\lambda}\sum_x (2x+1)A(l_1 l, l_2 L, x)W(lLl_1 l_2; \lambda x) \end{aligned} \tag{13.113}$$

with

$$\begin{aligned} &A(l_1 l, l_2 L, x) \\ = &\left[\frac{(l_1+l+x+1)!(l_1+l-x)!(l_1+x-l)!}{(l+x-l_1)!}\frac{(l_2+L+x+1)!(l_2+L-x)!(l_2+x-L)!}{(L+x-l_2)!}\right]^{\frac{1}{2}} \\ &\times\sum_{q\geq 0}(-1)^{(l+q-l_1)/2}\frac{(l+q-l_1)!}{(\frac{(l+q-l_1)}{2})!(\frac{(l+l_1-q)}{2})!}\frac{1}{(q-x)!(q+x+1)!}\frac{(L+q-l_2)!}{(\frac{L+q-l_2}{2})!(\frac{L+l_2-q}{2})!} \end{aligned} \tag{13.114}$$

13.10.3 Brody Moshinsky Talmi coefficient

The calculation of TBME in H.O. basis can be reduced into computing matrix elements

$$\langle nl \vert V(r) \vert n'l'\rangle = \sum_{p=\frac{1}{2}(l+l')}^{\frac{1}{2}(l+l')+n+n'} B(nl, n'l', p)I_p. \tag{13.115}$$

Talmi-integral is

$$\begin{aligned} I_p &= \frac{\sqrt{2}}{b\Gamma(p+\frac{3}{2})}\int (\frac{r^2}{2b^2})^{p+1}V(r)e^{-\frac{r^2}{2b^2}}dr \\ &= \frac{2}{\Gamma(p+3/2)}\int R^{2p+2}V(r)e^{-R^2}dR \end{aligned} \tag{13.116}$$

with $R = r/\sqrt{2}b$ and $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$.

The Coefficient is given in eq.(23) of Brody-Moshinsky paper.

$$\begin{aligned} B(nl, n'l', p) &= \frac{(-1)^{p-\frac{1}{2}(l+l')}(2p+1)!}{2^{n+n'}p!}\left[\frac{n!n'!(2n+2l+1)!(2n'+2l'+1)!}{(n+l)!(n'+l')!}\right]^{\frac{1}{2}} \\ &\quad \times \sum_{k=\alpha}^{\beta} \frac{(l+k)!(p-\frac{1}{2}(l-l')-k)!}{k!(2l+1+2k)!(n-k)!(2p-l+l'+1-2k)!(n'-p+\frac{1}{2}(l+l')+k)!(p-\frac{1}{2}(l+l')-k)!}, \\ \alpha &= \max[0, (p-\frac{1}{2}(l+l')-n')], \\ \beta &= \min[n, (p-\frac{1}{2}(l+l'))]. \end{aligned} \tag{13.117}$$

For a special case of $V(r) = \frac{\delta(r)}{r^2}$, $I_{p\neq 0} = 0$ and

$$\begin{aligned} B(nl, n'0, 0) &= \frac{\sqrt{(2n+1)!(2n'+1)!}}{2^{n+n'}n!n'!} \\ I_{p=0} &= \frac{\sqrt{2}}{b\Gamma(p+\frac{3}{2})}\int (\frac{r^2}{2b^2})^{p+1}\frac{\delta(r)}{r^2}e^{-\frac{r^2}{2b^2}}dr = \sqrt{\frac{2}{\pi}}\frac{1}{b^3} \end{aligned} \tag{13.118}$$

One can obtain analytic form for $V(r) = r^m \exp(-\lambda^2 r^2)$

$$\int_0^\infty dr r^{2p+2+m}\exp(-(1+\lambda^2)r^2) = \frac{1}{2}(1+\lambda^2)^{-(p+\frac{m+3}{2})}\Gamma\left(p+\frac{3+m}{2}\right). \tag{13.119}$$

for a special case $V(r) = V_0 r^m$,

$$I_p = V_0(\sqrt{2}b)^m\frac{\Gamma(p+\frac{m+3}{2})}{\Gamma(p+3/2)} \tag{13.120}$$

13.11 Slater integral

Another way to express TBME is to use expand the potential into Legendre Polynomials.

$$\begin{aligned} V(\boldsymbol{r}_1 - \boldsymbol{r}_2) &= \sum_{k=0}^{\infty} v_k(r_1, r_2)P_k(\cos\theta_{12}), \\ v_k(r_1, r_2) &= \frac{2k+1}{2}\int V(\boldsymbol{r}_1 - \boldsymbol{r}_2)P_k(\cos\theta_{12})d\cos\theta_{12}. \end{aligned} \tag{13.121}$$

Thus, we can express two-body matrix elements of two particles (not nas),

$$\begin{aligned}
&\langle n_1' l_1' n_2' l_2'; LM | V(\boldsymbol{r}_1 - \boldsymbol{r}_2) | n_1 l_1 n_2 l_2; LM \rangle \\
= & \int d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 \left(\sum_{m_1' m_2'} C^{LM}_{l_1' m_1' l_2' m_2'} Y^*_{l_1' m_1'}(\hat{n}_1) Y^*_{l_2' m_2'}(\hat{n}_2) \right) \phi_{n_1' l_1'}(r_1) \phi_{n_2' l_2'}(r_2) \\
& \times V(\boldsymbol{r}_1 - \boldsymbol{r}_2) \left(\sum_{m_1 m_2} C^{LM}_{l_1 m_1 l_2 m_2} Y_{l_1 m_1}(\hat{n}_1) Y_{l_2 m_2}(\hat{n}_2) \right) \phi_{n_1 l' 1}(r_1) \phi_{n_2 l_2}(r_2) \\
= & \sum_{k=0}^{\infty} \Bigg[\sum_{m_1' m_2'} \sum_{m_1 m_2} \sum_{m_k=-k}^{k} \frac{4\pi(-1)^k}{\sqrt{2k+1}} C^{00}_{k m_k, k-m_k} C^{LM}_{l_1' m_1' l_2' m_2'} C^{LM}_{l_1 m_1 l_2 m_2} \\
& \times \left(\int d^2\Omega_1 Y^*_{l_1' m_1'}(\hat{n}_1) Y_{k m_k}(\hat{n}_1) Y_{l_1 m_1}(\hat{n}_1) \right) \left(\int d^2\Omega_2 Y^*_{l_2' m_2'}(\hat{n}_2) Y_{k-m_k}(\hat{n}_2) Y_{l_2 m_2}(\hat{n}_2) \right) \Bigg] \\
& \times \left[\int dr_1 r_1^2 dr_2 r_2^2 \phi_{n_1' l_1'}(r_1) \phi_{n_2' l_2'}(r_2) v_k(r_1, r_2) \phi_{n_1 l' 1}(r_1) \phi_{n_2 l_2}(r_2) \right] \\
= & \sum_k f_k R^k
\end{aligned} \tag{13.122}$$

in terms of slater integrals R^k,

$$\begin{aligned}
R^k &= \int_0^\infty \int_0^\infty u_{n_1' l_1'}(r_1) u_{n_2' l_2'}(r_2) v_k(r_1, r_2) u_{n_1 l_1}(r_1) u_{n_2 l_2}(r_2) dr_1 dr_2 \\
&= \frac{2k+1}{2} \int_{-1}^{1} \int_0^\infty \int_0^\infty V(|\boldsymbol{r}_1 - \boldsymbol{r}_2|) P_k(\cos\theta_{12}) u_{n_1' l_1'}(r_1) u_{n_2' l_2'}(r_2) v_k(r_1, r_2) u_{n_1 l_1}(r_1) u_{n_2 l_2}(r_2) dr_1 dr_2 d\cos\theta_{12}
\end{aligned}$$

The angular integral part can be simplified by using tensor decomposition,

$$\begin{aligned}
f_k &= \langle l_1' l_2'; LM | P_k(\cos\theta_{12}) | l_1 l_2; LM \rangle \\
&= \frac{4\pi(-1)^k \sqrt{2L+1}}{\sqrt{2k+1}} \langle l_1' || Y_k || l_1 \rangle \langle l_2' || Y_k || l_2 \rangle \begin{Bmatrix} l_1' & l_1 & k \\ l_2' & l_2 & k \\ L & L & 0 \end{Bmatrix} \\
&= \frac{4\pi(-1)^{l_1 + l_2' + L}}{2k+1} \langle l_1' || Y_k || l_1 \rangle \langle l_2' || Y_k || l_2 \rangle \begin{Bmatrix} l_1' & l_1 & k \\ l_2 & l_2' & L \end{Bmatrix}
\end{aligned} \tag{13.123}$$

Unlike the Moshinsky transformation which is only valid for H.O. basis, slater integral expression is valid for any basis. But, if we use H.O. basis wave function, we can simplify the slater integrals into a sum of Talmi integrals. It is because the Laguerre polynomial can be expanded in powers of argument, and thus we can express

$$\frac{u_{nl}(r)}{r} = \sum_m C_{nl,m} r^m e^{-\nu r^2}. \tag{13.124}$$

This implies that we may express the product of two s.p. waves

$$\frac{u_{n_1 l_1}(r_1)}{r_1} \frac{u_{n_2 l_2}(r_2)}{r_2} = \sum_{s_1 s_2} C_{n_1 l_1, s_1} C_{n_2 l_2, s_2} r_1^{s_1} r_2^{s_2} e^{-\nu(r_1^2 + r_2^2)} \tag{13.125}$$

and we may separate integrals over relative coordinate and C.M. coordinates. (In other words, both Slater integral and Moshinski transformation braket formula should give the same expression in terms of Talmi-integrals. Advantage of Moshinsky braket is to directly connect TBME with Talmi integrals without intermediate step of Slater integrals.)

13.12 TBME of interaction

Then, TBME between antisymmetric two-particle wave functions becomes

$$\begin{aligned} & \langle\rho_a\rho_b|V|\rho_c\rho_d\rangle^{JT}_{nas}, \quad \rho_i=(n_il_ij_i) \\ = & \frac{1}{\sqrt{(1+\delta_{ab})}}\frac{1}{\sqrt{(1+\delta_{cd})}} \\ & \times\Big[{}_p\langle k_1k_2JT|V|k_3k_4JT\rangle_p-(-1)^{j_3+j_4-J+1-T}{}_p\langle k_1k_2JT|V|k_4k_3JT\rangle_p\Big] \end{aligned} \tag{13.126}$$

Note that

$$\begin{aligned} & |[(n_1l_1\frac{1}{2})j_1(n_2l_2\frac{1}{2})j_2]JT\rangle_p \\ = & \sum_{LS}\sqrt{(2j_1+1)(2j_2+1)(2L+1)(2S+1)}\left\{\begin{array}{ccc} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ L & S & J \end{array}\right\} \\ & \times|[(n_1l_1n_2l_2)LS]JT\rangle_p \end{aligned} \tag{13.127}$$

we can rewrite the last ket as

$$|[(n_1l_1n_2l_2)LS]JT\rangle_p=\sum_{nlN\Lambda}\langle(nlN\Lambda)L|(n_1l_1n_2l_2)L\rangle\times|[(nlN\Lambda)LS]JT\rangle_p \tag{13.128}$$

In a similar way, if the order of particle changes from 12 to 21, we gets (isospin is considered separately)

$$\begin{aligned} & |[(n_2l_2\frac{1}{2})j_2(n_1l_1\frac{1}{2})j_1]JT\rangle_p \\ = & \sum_{LS}\sqrt{(2j_1+1)(2j_2+1)(2L+1)(2S+1)}\left\{\begin{array}{ccc} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ L & S & J \end{array}\right\} \\ & \times(-1)^{l_1+l_2+L+1+S+j_1+j_2+J}|[(n_2l_2n_1l_1)LS]JT\rangle_p \\ = & \sum_{LS}\sqrt{(2j_1+1)(2j_2+1)(2L+1)(2S+1)}\left\{\begin{array}{ccc} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ L & S & J \end{array}\right\} \\ & \times(-1)^{l_1+l_2+L+1+S+j_1+j_2+J}\sum_{nlN\Lambda}(-1)^{\Lambda-L}\langle(nlN\Lambda)L|(n_1l_1n_2l_2)L\rangle|[(nlN\Lambda)LS]JT\rangle \end{aligned} \tag{13.129}$$

Thus, for the TBME, we can use

$$\begin{aligned} & |[(n_2l_2\frac{1}{2})j_2(n_1l_1\frac{1}{2})j_1]JT\rangle_p-(-1)^{j_1+j_2-J+1-T}|[(n_2l_2\frac{1}{2})j_2(n_1l_1\frac{1}{2})j_1]JT\rangle_p \\ = & \sum_{LS}\sqrt{(2j_1+1)(2j_2+1)(2L+1)(2S+1)}\left\{\begin{array}{ccc} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ L & S & J \end{array}\right\} \\ & \times\sum_{nlN\Lambda}\left(1-(-1)^{j_1+j_2-J+1-T}(-1)^{l_1+l_2+L+1+S+j_1+j_2+J}(-1)^{\Lambda-L}\right) \\ & \times\langle(nlN\Lambda)L|(n_1l_1n_2l_2)L\rangle\times|[(nl,N\Lambda)LS]JT\rangle_p \\ = & \sum_{LS}\sqrt{(2j_1+1)(2j_2+1)(2L+1)(2S+1)}\left\{\begin{array}{ccc} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ L & S & J \end{array}\right\} \\ & \times\sum_{nlN\Lambda}\left(1-(-1)^{l+S+T}\right)\langle(nlN\Lambda)L|(n_1l_1n_2l_2)L\rangle\times|[(nl,N\Lambda)LS]JT\rangle_p \end{aligned} \tag{13.130}$$

also we can rewrite the last ket as

$$\begin{aligned}|[(nl,N\Lambda)LS]JT\rangle_p &= \sum_j (-1)^{l+S+L+j}\sqrt{(2L+1)(2j+1)}\left\{\begin{array}{ccc}\Lambda & l & L\\ S & J & j\end{array}\right\}|[(nl,S)j,N\Lambda]JT\rangle_p \\ &= \sum_j (-1)^{\Lambda+S+j}\sqrt{(2L+1)(2j+1)}\left\{\begin{array}{ccc}\Lambda & l & L\\ S & J & j\end{array}\right\}|[(nl,S)j,N\Lambda]JT\rangle_p\end{aligned}$$

Now we can separate the relative part and center of mass part of the ket.

Thus, we eventually have matrix elements,

$$\langle[(nlS)j,N\Lambda]JT|V(r)|[(n'l'S')j,N'\Lambda']JT\rangle \tag{13.131}$$

Because $V(r)$ only depends on the relative distance, it will be

$$\begin{aligned}\langle[(nlS)j,N\Lambda]JT|V(\boldsymbol{r})|[(n'l'S')j',N'\Lambda']JT\rangle &= \delta_{NN'}\delta_{\Lambda,\Lambda'}\delta_{jj'}\sum_{m_1m_2}C^{JM}_{jm_1,\Lambda m_2}C^{JM}_{jm_1,\Lambda m_2}\langle(nlS)jm_1|V(\boldsymbol{r})|(n'l'S')jm_1\rangle \\ &= \delta_{NN'}\delta_{\Lambda,\Lambda'}\delta_{jj'}\delta_{SS'}\langle(nlS)j|V(\boldsymbol{r})|(n'l'S)j\rangle \end{aligned}\tag{13.132}$$

where we assumed the potential does not change two nucleon spin and $\langle(nlS)jm_1|V(r)|(n'l'S)jm_1\rangle$ actually does not depends on m_1(Because V(r) is a rank-0 operator) and the completeness relation of C.G. coefficients.

In summary: Note that potential operator can be rank 0,1,2 for orbital or spin.

$$\begin{aligned}&\langle\rho_a\rho_b|V|\rho_c\rho_d\rangle^{JT}_{nas} \\ =\ & 2\left[\frac{(2j_a+1)(2j_b+1)(2j_c+1)(2j_d+1)}{(1+\delta_{ab})(1+\delta_{cd})}\right]^{\frac12} \\ &\times\sum_{\Lambda\Lambda'S}(-1)^{\Lambda-\Lambda'}(2\Lambda+1)(2\Lambda'+1)(2S+1)\left\{\begin{array}{ccc}l_a & \frac12 & j_a\\ l_b & \frac12 & j_b\\ \Lambda & S & J\end{array}\right\}\left\{\begin{array}{ccc}l_c & \frac12 & j_c\\ l_d & \frac12 & j_d\\ \Lambda' & S & J\end{array}\right\} \\ &\times\sum_{nl,n'l',NL}\langle nlNL|n_al_an_bl_b\rangle_\Lambda\delta^{odd}_{l+S+T}\langle n'l'NL|n_cl_cn_dl_d\rangle_{\Lambda'}\delta^{odd}_{l'+S+T} \\ &\times\sum_j(2j+1)\left\{\begin{array}{ccc}L & l & \Lambda\\ S & J & j\end{array}\right\}\left\{\begin{array}{ccc}L & l' & \Lambda'\\ S & J & j\end{array}\right\} \\ &\times\sum_\nu\langle nlS;j|U^T_\nu(r)W_\nu|n'l'S;j\rangle.\end{aligned}\tag{13.133}$$

Isospin projection gives $\langle T|P_{T'}|T\rangle=\delta_{TT'}$. (We used the fact that S does not change for considered operators.) [7] Though we expressed potential $V(\boldsymbol{r})=\sum_\nu U_\nu P_\nu$, it is can be written in more general form as (for spin and parity conserving interactions)

$$\langle nlS;j|V(\boldsymbol{r})|n'l'S;j\rangle=\int d^3\boldsymbol{R}\mathcal{R}_{nl}(R)\left[Y_l(\hat{R})\otimes\chi_S\right]^\dagger_j V(\boldsymbol{r})\mathcal{R}_{n'l'}(R)\left[Y_{l'}(\hat{R})\otimes\chi_S\right]_j \tag{13.137}$$

[7] The equation may be calculated in steps first step

$$\begin{aligned}\langle\rho_a\rho_b|V|\rho_c\rho_d\rangle^{JT}_{nas} &= 2\left[\frac{(2j_a+1)(2j_b+1)(2j_c+1)(2j_d+1)}{(1+\delta_{ab})(1+\delta_{cd})}\right]^{\frac12} \\ &\times\sum_{\Lambda\Lambda'S}(-1)^{\Lambda-\Lambda'}(2\Lambda+1)(2\Lambda'+1)(2S+1)\left\{\begin{array}{ccc}l_a & \frac12 & j_a\\ l_b & \frac12 & j_b\\ \Lambda & S & J\end{array}\right\}\left\{\begin{array}{ccc}l_c & \frac12 & j_c\\ l_d & \frac12 & j_d\\ \Lambda' & S & J\end{array}\right\} \\ &\times\langle\rho_a\rho_b;\Lambda|V|\rho_c\rho_d;\Lambda'\rangle^{SJT}_p\end{aligned}\tag{13.134}$$

and second

$$\begin{aligned}\langle\rho_a\rho_b;\Lambda|V|\rho_c\rho_d;\Lambda'\rangle^{SJT}_p &= \sum_{nl,n'l',NL}\langle nlNL|n_al_an_bl_b\rangle_\Lambda\delta^{odd}_{l+S+T}\langle n'l'NL|n_cl_cn_dl_d\rangle_{\Lambda'}\delta^{odd}_{l'+S+T} \\ &\times\langle nlNL,\Lambda S|V|n'l'NL,\Lambda'S\rangle^{JT}\end{aligned}\tag{13.135}$$

13.13 Example of TBME

We can compute the last matrix elements according to the spin and orbital structures.

$$\langle nlS;j|U^T_{S'}(r)W_{S'}|n'l'S;j\rangle^T = \langle nl|U^T_S(r)|n'l\rangle\delta_{SS'}\delta_{ll'} \tag{13.138}$$

For spin-orbit interaction,

$$\langle nls;j|U^T_{LS}(r)W_{LS}|n'l's;j\rangle^T \quad = \quad \delta_{S1}\delta_{ll'}\frac{1}{2}(j(j+1)-l(l+1)-s(s+1))\langle nl|U^T_{LS}(r)|n'l\rangle \tag{13.139}$$

$$\begin{aligned} & \langle nlS;j|U^T_{TN}(r)W_{TN}|n'l'S;j\rangle^T \\ = \quad & \delta_{S1}\Big[\delta_{l,j}\delta_{l',j}(2)+\delta_{l',j-1}\delta_{l,j-1}(-2\frac{j-1}{2j+1}) \\ & +\delta_{l',j\pm1}\delta_{l,j\mp1}(6\frac{\sqrt{j(j+1)}}{2j+1})+\delta_{l,j+1}\delta_{l',j+1}(-2\frac{j+2}{2j+1})\Big]\langle nl|U^T_{TN}(r)|n'l'\rangle \end{aligned}$$

For a special case of delta potential, exact integral is possible.
From the original expression

$$\begin{aligned} \langle nlS;j|V_0\delta^{(3)}(\boldsymbol{r})|n'l'S;j\rangle \quad &= \quad \int d^3R\mathcal{R}_{nl}(R)[Y_l\otimes\chi_S]^\dagger_{jm}V_0\frac{\delta(r)}{r^2}\delta(\cos\theta)\delta(\phi)\mathcal{R}_{n'l'}(R)[Y_{l'}\otimes\chi_S]_{jm} \\ &= \quad \left(\int dRR^2\mathcal{R}_{nl}(R)\mathcal{R}_{n'l'}(R)\frac{V_0}{(\sqrt{2}b)^3}\frac{\delta(R)}{R^2}\right)(C^{jm}_{00,Sm})^2\delta_{l0}\delta_{l'0}\frac{1}{4\pi} \\ &= \quad V_0\delta_{l0}\delta_{l'0}\delta_{jS}\frac{1}{4\pi}\frac{1}{(\sqrt{2}b)^3}\mathcal{R}_{nl}(0)\mathcal{R}_{n'l}(0) \\ &= \quad V_0\delta_{l0}\delta_{l'0}\delta_{jS}\frac{1}{4\pi}\frac{\sqrt{(2n+1)!(2n'+1)!}}{2^{n+n'}n!n'!}\sqrt{\frac{2}{\pi}}\frac{1}{b^3} \end{aligned} \tag{13.140}$$

One can obtain the same expression from Brody-Moshinsky coefficients (angular factor $1/(4\pi)$ have to be supplied)

$$\begin{aligned} \langle nl|V_0\frac{\delta(r)}{r^2}|n'l'\rangle \quad &= \quad V_0\delta_{l0}\delta_{l'0}B(n0n'0;0)I_{p=0} \\ &= \quad V_0\delta_{l0}\delta_{l'0}\frac{\sqrt{(2n+1)!(2n'+1)!}}{2^{n+n'}n!n'!}\sqrt{\frac{2}{\pi}}\frac{1}{b^3} \end{aligned} \tag{13.141}$$

By using dimension-less R, such as $|\boldsymbol{r}_1-\boldsymbol{r}_2|=\sqrt{2}bR$,

$$\begin{aligned} H^{(A=2)}_{rel} \quad &= \quad \frac{1}{2mA}(\boldsymbol{p}_1-\boldsymbol{p}_2)^2+\frac{1}{2A}m\omega^2(\boldsymbol{r}_1-\boldsymbol{r}_2)^2 \\ &= \quad \frac{\omega}{A}\left(\frac{b^2}{2}(\boldsymbol{p}_1-\boldsymbol{p}_2)^2+\frac{1}{2b^2}(\boldsymbol{r}_1-\boldsymbol{r}_2)^2\right) \\ &= \quad \frac{\omega}{A}\left(-\nabla^2_R+R^2\right), \end{aligned} \tag{13.142}$$

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and third

$$\begin{aligned} \langle nlNL,\Lambda S|V|n'l'NL,\Lambda'S\rangle^{JT} \quad &= \quad \sum_j(2j+1)\left\{\begin{array}{ccc} L & l & \Lambda \\ S & J & j\end{array}\right\}\left\{\begin{array}{ccc} L & l' & \Lambda' \\ S & J & j\end{array}\right\} \\ & \quad \times\sum_\nu\langle nlS;j|U^T_\nu(r)W_\nu|n'l'S;j\rangle. \end{aligned} \tag{13.136}$$

$$\langle nl|(-\nabla_R^2 + R^2)|n'l'\rangle = 2\delta_{nn'}\delta_{ll'}(2n + l + \frac{3}{2}) = 2(2n + l + \frac{3}{2})\delta_{nn'}\delta_{ll'} \quad (13.143)$$

$\langle nl|p^2|n'l'\rangle = \langle nl| - \nabla_R^2|n'l'\rangle$ are known.

If one use units of $\hbar\omega$(or use $\hbar\omega = 1$ MeV), the matrix elements becomes

$$\begin{aligned} \langle nl|H_{rel}^{(A=2)}|n'l'\rangle &= \frac{2\omega}{A}\left(\frac{1}{2}\langle nl|(-\nabla_R^2 + R^2)|n'l'\rangle\right), \\ \langle nl|T_{rel}^{(A=2)}|n'l'\rangle &= \frac{\omega}{A}\langle nl| - \nabla_R^2|n'l'\rangle \end{aligned} \quad (13.144)$$

Or $1/A = 1/2$ should be included in the matrix elements?

Chapter 14

RMF

14.1 Nuclear Matter

Note that in many cases, the notation does not distinguish the operator and its expectation values. So, be careful.

- Nuclear wave function in Infinite Nuclear Matter is a plane wave without explicit calculation because of homogeneous isotropic condition. This implies the nuclear density simply becomes the same as free gas case,

$$\begin{aligned} \rho &= \frac{A}{V} = \sum_{k\lambda} \psi^*_{\boldsymbol{k},\lambda}(\boldsymbol{r})\psi_{\boldsymbol{k},\lambda}(\boldsymbol{r}) = \frac{\gamma}{(2\pi)^3}\int d^3k\; n(\boldsymbol{k}) \\ &\to \frac{\gamma}{6\pi^2}k_F^3 \quad \text{for } n(\boldsymbol{k}) = \theta(k_F - |\boldsymbol{k}|) \end{aligned} \tag{14.1}$$

  note that this relation holds even when there is a interaction among nucleons. However, the interaction can change the relation between energy and momentum and thus change the relation between Fermi momentum and Fermi energy.

  Because there will be other definition of density, let us denote this nucleon number density as ρ_B(Baryon density).

- The main quantity we need to compute is a energy density $\epsilon = \frac{E}{V}$ (or equivalently, $\frac{E}{A} = \frac{\epsilon}{\rho}$.) as a functional of density ρ which in turn related with particle wave function. We may compute the energy density by computing $\langle\Phi|H|\Phi\rangle$ which is related with energy-momentum tensor $T^{\mu\nu}$,($H = T^{00}$). Energy momentum tensor is defined as

$$T^{\mu\nu} = \sum_i \frac{\partial\mathcal{L}}{\partial(\partial_\mu\Phi_i)}\partial^\nu\Phi_i - g^{\mu\nu}\mathcal{L}. \tag{14.2}$$

  We may compute also the pressure of the system by computing T^{ii}. [1] We expect the homogeneous isotropic system have the relation with energy density and pressure

$$T^{\mu\nu} = (\epsilon + P)u^\mu u^\nu - Pg^{\mu\nu} \tag{14.3}$$

  with u^μ to be a velocity of the system, $u^\mu = (\gamma, \gamma\vec{v})$.

[1] The energy momentum tensor, $\langle T^{00}\rangle$ and $\langle T^{0i}\rangle$ corresponds to the energy and momentum density of the system. $\langle T^{ij}\rangle$ corresponds to stress tensor(pressure) of the system.

- Energy density in a mean-field picture is something like

$$\epsilon[\rho] = \left(\frac{\gamma}{(2\pi)^3} \int d^3k \frac{\boldsymbol{k}^2}{2M} n(\boldsymbol{k}) \right) + U[\rho] \tag{14.4}$$

where, the first term is an integration of free particle energy over particle density, the second term is a correction to single particle energy from mean field effects.

Equivalently, we can write

$$\frac{E}{A} = \frac{\epsilon}{\rho} = \frac{3k_F^2}{10M} + \frac{U[\rho]}{\rho} \tag{14.5}$$

- Thermodynamic consistency: We may compute the pressure in two different way. The first is by computing energy-momentum tensor of the system.

$$P = \frac{1}{3} \sum_i \langle T^{ii} \rangle \tag{14.6}$$

The second is to use thermodynamic relations,

$$P = -\frac{\partial E}{\partial V} = \rho_B \frac{\partial \epsilon}{\partial \rho_B} - \epsilon = \rho_B^2 \frac{\partial}{\partial \rho_B} \left(\frac{\epsilon}{\rho_B} \right) \tag{14.7}$$

Thermodynamic consistency requires both P are the same.

- Any theory of nuclear matter have to satisfy Saturation property of nuclear matter:

$$\frac{E}{A} \simeq -16MeV \quad \rho_0 \simeq 0.16 fm^{-3}, \quad k_F \simeq 1.36 fm^{-1} \simeq 260MeV \tag{14.8}$$

- Around normal symmetric nuclear matter (normal nuclear matter density and $N = Z$), we may expand the energy density in terms of small density changes and iso-spin dependences. Let us denote the variation as $\rho_B - \rho_0$ and β,

$$\begin{aligned} \rho_B &= \rho_p + \rho_n, \quad \rho_3 = \rho_p - \rho_n, \\ \beta &= \frac{\rho_n - \rho_p}{\rho_B} = -\frac{\rho_3}{\rho_B}, \quad \rho_{p,n} = \frac{1}{2}(\rho_B \pm \rho_3) \end{aligned} \tag{14.9}$$

Because the saturation density is defined as a minimum energy per particle, E/A [2], the first derivative of $\frac{E}{A}$ over density or β becomes zero at saturation density. Then the second derivative of $\frac{E}{A}$ over density is called *incompressibility* and the second derivative over β is called *symmetry energy.*

- Define binding energy per particle,

$$E_B(\rho_B, \beta) = \frac{E}{A} - M = \frac{\epsilon}{\rho_B} - M. \tag{14.10}$$

Then, expansion in density,

$$E_B(\rho_0 + \delta\rho, \beta = 0) = a_4 + \frac{L}{3} \left(\frac{\rho_B - \rho_0}{\rho_0} \right) + \frac{K}{18} \left(\frac{\rho_B - \rho_0}{\rho_0} \right)^2 + \cdots \tag{14.11}$$

where, slope L is

$$L = 3\rho_0 \frac{\partial E_B}{\partial \rho_B}|_{\rho_B = \rho_0} = \frac{3}{\rho_0} P(\rho_0). \tag{14.12}$$

[2]Nuclear matter is assumed to have lowest energy per particle at saturation density and also iso-spin symmetric case.

and incompressibility or compress modulus K is

$$K = 9\frac{\partial P}{\partial \rho_B}|_{\rho_B=\rho_0} = 9\rho_B^2 \frac{\partial^2(\epsilon/\rho_B)}{\partial \rho_B^2}|_{\rho_B=\rho_0}. \tag{14.13}$$

Thus, the minimum condition of saturation density is equivalent to the zero pressure at saturation density, $P(\rho_0) = 0$.

- Also, the expansion around symmetric matter,

$$\begin{aligned} E_B(\rho_B, \beta) &= E_B|_{\beta=0} + \frac{\partial E_B}{\partial \beta}|_{\beta=0}\beta + \frac{1}{2}\frac{\partial^2 E_B}{\partial \beta^2}|_{\beta=0}\beta^2 + \cdots \\ &= E_B(\rho_B) + E_{sym}\beta^2 + \mathcal{O}(\beta^4) + \cdots \end{aligned} \tag{14.14}$$

In may approximation, the most symmetric nuclear matter($\beta = 0$) and asymmetric nuclear matter $\beta = 1$ are related only up to symmetry energy term.

14.2 QHD-I

The main feature of RMF is that the nucleon's are considered as a non-interacting quasi-particles which satisfies equation of motion under repulsive vector potential and attractive scalar mean-field potential,

$$[\gamma_\mu(i\partial^\mu + V^\mu[\rho]) - (M + S[\rho])]\,\Psi_i = 0 \tag{14.15}$$

Depending on the exact formulation, the form of vector potential and scalar potential changes. In QHD-I, the vector potential is generated by vector mesons and scalar potential is generated by scalar mesons, which in turn is related with the nuclear density. In Point-coupling models, they are non-linear functions of nuclear density. Regardless formulation, the basic concept is that the system will be described by the product of single particle solutions of Dirac equations.

Thus, in mean-field model, the many-body problem is equivalent to solve one-body Dirac equation.

- QHD-I Lagrangian: with $\sigma, \omega_\mu, \rho_\mu$ mesons and photon A_μ,

$$\begin{aligned} \mathcal{L} &= \bar{\Psi}(i\gamma_\mu\partial^\mu - M)\Psi + \frac{1}{2}(\partial_\mu\sigma\partial^\mu\sigma - m_\sigma^2\sigma^2) - U(\sigma) \\ &\quad -\frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\omega^2\omega_\mu\omega^\mu - \frac{1}{4}\boldsymbol{R}_{\mu\nu}\boldsymbol{R}^{\mu\nu} + \frac{1}{2}m_\rho^2\boldsymbol{\rho}_\mu\boldsymbol{\rho}^\mu - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} \\ &\quad -g_\sigma\bar{\Psi}\sigma\Psi - g_\omega\bar{\Psi}\gamma_\mu\omega^\mu\Psi - g_\rho\bar{\Psi}\gamma_\mu\boldsymbol{\tau}\boldsymbol{\rho}^\mu\Psi - e\frac{1+\tau_3}{2}\bar{\Psi}\gamma_\mu A^\mu\Psi, \end{aligned} \tag{14.16}$$

with

$$\begin{aligned} U(\sigma) &= \frac{1}{3}g_2\sigma^3 + \frac{1}{4}g_3\sigma^4, \\ \Omega^{\mu\nu} &= \partial^\mu\omega^\nu - \partial^\nu\omega^\mu, \\ \boldsymbol{R}^{\mu\nu} &= \partial^\mu\boldsymbol{\rho}^\nu - \partial^\nu\boldsymbol{\rho}^\mu, \\ F^{\mu\nu} &= \partial^\mu A^\nu - \partial^\nu A^\mu. \end{aligned} \tag{14.17}$$

- equation of motion of QHD-I: From Euler-Lagrange equation of motion,

$$\partial_\mu\left(\frac{\partial\mathcal{L}}{\partial\partial_\mu q}\right) - \frac{\partial\mathcal{L}}{\partial q} = 0, \tag{14.18}$$

gives

$$\left[\gamma_\mu(i\partial^\mu - g_\omega\omega^\mu - g_\rho\vec{\tau}\cdot\vec{\rho}^\mu - e\frac{1+\tau_3}{2}A^\mu) - M - g_\sigma\sigma\right]\Psi_i = 0, \tag{14.19}$$

and meson equations[3]

$$\begin{aligned}\left[\partial^2 + m_\sigma^2\right]\sigma &= -g_\sigma\bar{\psi}\psi - g_2\sigma^2 - g_3\sigma^3,\\ \partial^\nu\Omega_{\mu\nu} + m_\omega^2\omega_\mu &= g_\omega\bar{\psi}\gamma_\mu\psi,\\ \partial^\nu\vec{R}_{\mu\nu} + m_\rho^2\vec{\rho}_\mu &= g_\rho\bar{\psi}\gamma_\mu\vec{\tau}\psi,\end{aligned} \tag{14.21}$$

Note that the photon energy will be eventually computed as a Coulomb energy between nucleons, thus, we don't need equation for photon. Also, in nuclear matter, we ignore Coulomb interaction.

- We may define various nuclear density and currents,

$$\begin{aligned}\hat{\rho}_s &= \bar{\psi}\psi,\\ \hat{j}_\mu &= \bar{\psi}\gamma_\mu\psi = (\hat{\rho}_B, \vec{j}), \quad \ldots\end{aligned} \tag{14.22}$$

It is important to distinguish the scalar density ρ_S and Baryon density ρ_B. Note that in usual convention of Dirac spinors, we have relation,

$$\bar{u}(\boldsymbol{k})u(\boldsymbol{k}) = \frac{M}{\sqrt{k^2+M^2}}u^\dagger(\boldsymbol{k})u(\boldsymbol{k}). \tag{14.23}$$

- **RMF ground state wave function:** The ground state of the nuclear system is approximated as a Slater determinant of single particle states (In other words, Hartree-Fock states). However, because the meson fields are classical fields in RMF, all nuclear contributions to the energy expectation value becomes the one-body operators and thus only diagonal terms contributes. (Hartree level).
- **RMF meson wave function:** In Relativistic Mean Field Theory (RMF), we replace the quantum fields as classical fields (their expectation values). So that the field operators become a numeric functions. It may be justified by the argument that in nuclear matter the density of mesons are so large that can be treated as classical density. However, nucleons are still treated as a quantum mechanical object.
- **Why no pion? :** Because Pions are pseudo scalar, the coupling term of pions and nucleons change parity of nucleons. Then, the equations of motion for nucleon becomes coupled among different parities. Also, if we only consider Hartree level, they do not contribute to the energy expectation values.

14.3 QHD-I for nuclear matter

In case of nuclear matter, the problem becomes simple because of the static homogeneous isotropic property of the system. In this case, the nucleon wave function simply becomes plane waves.

[3]Useful relation,

$$\frac{\partial}{\partial(\partial_\mu A_\nu)}\left(-\frac{1}{4}F^{\alpha\beta}F_{\alpha\beta}\right) = -F^{\mu\nu} \tag{14.20}$$

- static, homogeneous, isotropic: time derivative is replaced by static energy. Also, in the rest frame of matter, nuclear currents vanishes, $\langle \jmath_\mu \rangle \to (\rho_B, 0)$ and so the spatial component of meson fields too. there is no spatial dependence of currents and density. Thus, all densities and meson mean fields becomes a constant. Also, we will only consider iso-spin eigen states. Thus, only third component of isospin survives.
- To simplify the problem, let us **ignore non-linear potential** $U(\sigma)$ from now on.
- From the equation of motion for meson, we get

$$\langle \sigma \rangle = -\frac{g_\sigma}{m_\sigma^2}\rho_S, \quad \langle \omega_0 \rangle = \frac{g_\omega}{m_\omega^2}\rho_B, \quad \langle \rho_0^z \rangle = \frac{g_\rho}{m_\rho^2}\langle \bar{\psi}\gamma_0\tau^z\psi \rangle = \frac{g_\rho}{m_\rho^2}(\rho_p - \rho_n). \quad (14.24)$$

- The energy momentum tensor:

14.4 Dirac equation for nuclear matter

Let us consider Dirac equation for nuclear matter.

- We know that the nucleon wave function is a plane wave. Thus, let us put $\psi_k(\boldsymbol{r}, t) = e^{-ik\cdot x}u(\boldsymbol{k})$, with $k^\mu = (E, \boldsymbol{k})$.

$$\hat{\psi}(\boldsymbol{x}) = \frac{1}{\sqrt{V}}\sum_{\boldsymbol{k}\lambda}\left[u_\lambda(\boldsymbol{k})\hat{a}_{\boldsymbol{k}\lambda}e^{i\boldsymbol{k}\cdot\boldsymbol{x}} + v_\lambda(-\boldsymbol{k})\hat{b}^\dagger_{\boldsymbol{k}\lambda}e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}\right]. \quad (14.25)$$

$$\begin{aligned} & \left[\gamma_\mu(i\partial^\mu - g_\omega\omega^\mu - g_\rho\vec{\tau}\cdot\vec{\rho}^\mu) - (M + g_\sigma\sigma)\right]\Psi_k = 0, \\ \to \quad & \left[\gamma_0 E - \vec{\gamma}\cdot\boldsymbol{k} + \gamma_0(-g_\omega\omega_0 - g_\rho\tau^3\rho_0^3) - (M + g_\sigma\sigma)\right]u(\boldsymbol{k}) = 0, \\ \to \quad & \left[\vec{\alpha}\cdot\boldsymbol{k} + \beta(M + g_\sigma\sigma)\right]u(\boldsymbol{k}) = (E - g_\omega\omega_0 - g_\rho\tau^3\rho_0^3)u(\boldsymbol{k}). \end{aligned} \quad (14.26)$$

- If we define 'effective mass', M^*, we have the relation between energy eigen values E and momentum $\boldsymbol{k}$,

$$\begin{aligned} M^* &\equiv M + g_\sigma\sigma, \\ E_k &= \pm\sqrt{\boldsymbol{k}^2 + M^{*2}} + g_\omega\omega_0 + \tau_3 g_\rho\rho_0^3, \\ &= \pm E^* + g_\omega\omega_0 + \tau_3 g_\rho\rho_0^3, \quad E^* \equiv \sqrt{\boldsymbol{k}^2 + M^{*2}} \end{aligned} \quad (14.27)$$

  where, $\tau_3 = +1$ for proton and -1 for neutron.
- Because the only isospin dependence appears from rho meson contribution, we may compute the ρ_p (or ρ_n) separately and then change sign of g_ρ for the other. Also, the symmetry energy in QHD-I is originate from this rho meson.
- For the case of finite nuclei, let us introduce Scalar potential $S(r)$ and Vector potential $V(r)$, and rewrite the equation as

$$\left[-i\vec{\alpha}\cdot\nabla + \beta(M + S(r))\right]\psi(\boldsymbol{r}) = (E - V(r))\psi(\boldsymbol{r}). \quad (14.28)$$

- This equation can be written as

$$(\gamma_\mu k^{*\mu} - M^*)u(\boldsymbol{k}) = 0 \quad (14.29)$$

  by define

$$k^{*\mu} \equiv k^\mu - g_\omega V^\mu - g_\rho\tau^3\rho^{3\mu} = (E^*, \vec{k}^*) \quad (14.30)$$

- This is the same as free Dirac equation ans thus spinors $u(\boldsymbol{k})$ are the same except replacing $M \to M^*, E \to E^*$. It implies the relation,

$$\bar{u}(\boldsymbol{k})u(\boldsymbol{k}) = \frac{M^*}{\sqrt{k^2 + M^{*2}}} u^\dagger(\boldsymbol{k})u(\boldsymbol{k}). \tag{14.31}$$

Usual convention of Dirac spinor is

$$\begin{aligned} u_i^\dagger(\boldsymbol{k})u_j(\boldsymbol{k}) &= 2E_k\delta_{ij}, \quad \bar{u}_i(\boldsymbol{k})u_j(\boldsymbol{k}) = 2M\delta_{ij}, \\ u_s(\boldsymbol{k}) &= \sqrt{E+m}\begin{pmatrix} \chi_s \\ \frac{\boldsymbol{\sigma}\cdot\boldsymbol{k}}{E+m}\chi_s \end{pmatrix} \end{aligned} \tag{14.32}$$

Or we may use, (in this note)

$$\begin{aligned} u_i^\dagger(\boldsymbol{k})u_j(\boldsymbol{k}) &= \delta_{ij}, \quad \bar{u}_i(\boldsymbol{k})u_j(\boldsymbol{k}) = \frac{M}{E}\delta_{ij}, \\ u_s(\boldsymbol{k}) &= \sqrt{\frac{E+m}{2E}}\begin{pmatrix} \chi_s \\ \frac{\boldsymbol{\sigma}\cdot\boldsymbol{k}}{E+m}\chi_s \end{pmatrix} \end{aligned} \tag{14.33}$$

- Density : From the definition of Baryon density, we can write the Baryon density operator. However, this involves

$$\hat{\rho}_B = \hat{\psi}^\dagger(\boldsymbol{x})\hat{\psi}(\boldsymbol{x}) \to \frac{1}{V}\sum_{\boldsymbol{k}\lambda}\left(u_{k\lambda}^\dagger u_{k\lambda}\hat{a}_{k\lambda}^\dagger\hat{a}_{k\lambda} + v_{-k\lambda}^\dagger v_{-k,\lambda}\hat{b}_{k\lambda}\hat{b}_{k\lambda}^\dagger\right) \tag{14.34}$$

And the last term for anti-particle gives infinity from $\sum_{k\lambda} 1$, if we replace it to $-b_{k\lambda}^\dagger b_{k\lambda}$. To avoid this, we may assume that the all anti-particle states are occupied (filled Dirac sea). This is equivalent to subtract vaccum contribution, thus,

$$\hat{\rho}_B \to :\hat{\psi}^\dagger(\boldsymbol{x})\hat{\psi}(\boldsymbol{x}) := \frac{1}{V}\sum_{\boldsymbol{k}\lambda}\left(\hat{a}_{k\lambda}^\dagger\hat{a}_{k\lambda} - \hat{b}_{k\lambda}^\dagger\hat{b}_{k\lambda}\right) \tag{14.35}$$

Also correspondingly, the energy calculation also involves subtracting zero-point energy.

14.5 Energy and Pressure of QHD-I

- For the case $\beta \neq 0$, let us define ρ_p and ρ_n.

$$\rho_p = \bar{\psi}\gamma_0\frac{1+\tau_3}{2}\psi, \quad \rho_n = \bar{\psi}\gamma_0\frac{1-\tau_3}{2}\psi, \tag{14.36}$$

Then, the density and fermi momentum can be related as

$$\rho_{p,n} = \frac{2}{(2\pi)^3}\int^{k_F^{p,n}} d^3k = \frac{2}{6\pi^2}(k_F^{p,n})^3. \tag{14.37}$$

- Some relation for Energy-momentum tensor

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial(\partial_\mu \bar{\psi})}\partial^\nu \bar{\psi} &= 0, \\
\frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)}\partial^\nu \psi &= \bar{\psi} i\gamma^\mu \partial^\nu \psi, \\
\frac{\partial \mathcal{L}}{\partial(\partial_\mu \sigma)}\partial^\nu \sigma &= \partial^\mu \sigma \partial^\nu \sigma, \\
\frac{\partial \mathcal{L}}{\partial(\partial_\mu \omega_\lambda)}\partial^\nu \omega_\lambda &= -\Omega^{\mu\lambda}\partial^\nu \omega_\lambda, \\
\frac{\partial \mathcal{L}}{\partial(\partial_\mu \rho^i_\lambda)}\partial^\nu \rho^i_\lambda &= -R^{\mu\lambda,i}\partial^\nu \rho^i_\lambda,
\end{aligned} \tag{14.38}$$

Thus, energy-momentum tensor becomes

$$\begin{aligned}
T^{\mu\nu} &= \bar{\psi} i\gamma^\mu \partial^\nu \psi + \partial^\mu \sigma \partial^\nu \sigma - \Omega^{\mu\lambda}\partial^\nu \omega_\lambda - R^{\mu\lambda,i}\partial^\nu \rho^i_\lambda - F^{\mu\lambda}\partial^\nu A_\lambda \\
&\quad -g^{\mu\nu}\Big[+ \frac{1}{2}(\partial_\mu \sigma \partial^\mu \sigma - m_\sigma^2 \sigma^2) - U(\sigma) \\
&\quad -\frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\omega^2 \omega_\mu \omega^\mu - \frac{1}{4}\boldsymbol{R}_{\mu\nu}\boldsymbol{R}^{\mu\nu} + \frac{1}{2}m_\rho^2 \boldsymbol{\rho}_\mu \boldsymbol{\rho}^\mu - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} \\
&\quad \bar{\Psi}\left(i\gamma_\mu \partial^\mu - g_\omega \gamma_\mu \omega^\mu - g_\rho \gamma_\mu \boldsymbol{\tau}\boldsymbol{\rho}^\mu - e\frac{1+\tau_3}{2}\gamma_\mu A^\mu - M - g_\sigma \sigma \right)\Psi \Big]
\end{aligned} \tag{14.39}$$

Then, when we compute the expectation value, we may use equation of motion of nucleon for the last line.

- Let us consider expectation values[4]

$$\rho_B = \langle \sum_{k\lambda} a^\dagger_{k\lambda} a_{k\lambda} \rangle = \frac{\gamma}{(2\pi)^3}\int d^3k n(\boldsymbol{k}) = \frac{\gamma}{6\pi^2}k_F^3, \tag{14.41}$$

$$\begin{aligned}
\rho_S &= \langle \sum_{k\lambda} \frac{M^*}{E^*_k} a^\dagger_{k\lambda} a_{k\lambda} \rangle = \frac{\gamma}{(2\pi)^3}\int_0^{k_F} d^3k \frac{M^*}{\sqrt{k^2 + M^{*2}}} \\
&= \frac{\gamma}{4\pi^2}M^* \left[k_F \sqrt{k_F^2 + M^{*2}} - M^{*2} \ln \frac{k_F + \sqrt{k_F^2 + M^{*2}}}{M^*} \right].
\end{aligned} \tag{14.42}$$

$$\begin{aligned}
\langle \sum_{k\lambda} E^*_k a^\dagger_{k\lambda} a_{k\lambda} \rangle &= \frac{\gamma}{(2\pi)^3}\int d^3k E^*_k n(\boldsymbol{k}) \\
&= \underbrace{\frac{\gamma}{(2\pi)^3}4\pi}_{\equiv \alpha}\int_0^{k_F} dk k^2 \sqrt{k^2 + M^{*2}} = \alpha \int dk \frac{k^2(k^2 + M^{*2})}{\sqrt{k^2 + M^{*2}}} \\
&= \alpha \int dk k^3 \frac{k}{E^*} + M^* \rho_S = M^* \rho_S + \alpha k_F^3 \sqrt{k_F^2 + M^{*2}} - 3\alpha \int_0^{k_F} dk k^2 E^*_k, \\
&\to \frac{3}{4}\rho_B E^*(k_F) + \frac{1}{4}M^* \rho_S(k_F)
\end{aligned} \tag{14.43}$$

[4]From the Dirac spinor

$$\bar{u}(\boldsymbol{k})\vec{\gamma}\cdot\boldsymbol{k}u(\boldsymbol{k}) = \frac{E^* + M^*}{2E^*}\left(\chi\ \chi^\dagger \frac{\boldsymbol{\sigma}\cdot\boldsymbol{k}}{E^* + M^*} \right)\begin{pmatrix} 0 & \boldsymbol{\sigma}\cdot\boldsymbol{k} \\ \boldsymbol{\sigma}\cdot\boldsymbol{k} & 0 \end{pmatrix}\begin{pmatrix} \chi \\ \frac{\boldsymbol{\sigma}\cdot\boldsymbol{k}}{E^* + M^*}\chi \end{pmatrix} = \frac{\boldsymbol{k}^2}{E^*} \tag{14.40}$$

$$\sum_i \langle \bar{\psi} i\gamma^i \partial^i \psi \rangle = \sum_{k\lambda} \frac{\boldsymbol{k}^2}{E_k^*} \langle a_{k\lambda}^\dagger a_{k\lambda} - b_k^\dagger b_k \rangle = \frac{\gamma}{(2\pi)^3} \int d^3k \frac{\boldsymbol{k}^2}{E_k^*} n(\boldsymbol{k})$$
$$= \frac{3}{4}\rho_B E^*(k_F) - \frac{3}{4} M^* \rho_S(k_F) \tag{14.44}$$

- Note that if we consider proton and neutron separately, for $i = (n, p)$,

$$\rho_i = \frac{2}{(2\pi)^3} \int d^3k n_i(\boldsymbol{k}) = \frac{2}{6\pi^2} (k_F^{(i)})^3,$$
$$\rho_B = \rho_p + \rho_n \tag{14.45}$$

and

$$\rho_S^{(i)} = \frac{2}{4\pi^2} M^* \left[k_F^{(i)} \sqrt{k_F^{(i)2} + M^{*2}} - M^{*2} \ln \frac{k_F^{(i)} + \sqrt{k_F^{(i)2} + M^{*2}}}{M^*} \right],$$
$$\rho_S = \rho_S^{(p)} + \rho_S^{(n)} \tag{14.46}$$

- Self-consistent equation: from the relation of ρ_S and M^*,

$$M^* = M + g_\sigma \sigma = M - \frac{g_\sigma^2}{m_\sigma^2} \rho_S \tag{14.47}$$

The right hand side ρ_S is also a function of M^*. Thus, this equation is a self-consistency equation. The solution of above equation is $M^*(k_F)$, effective mass as a function of k_F or density ρ_B. Once it is obtained, we can get energy density and pressure as a function of density or k_F.

- energy of nuclear matter: all derivatives on meson fields vanish. Also we neglect Coulomb interaction. Thus,

$$\langle T^{00} \rangle = \langle \bar{\psi} \gamma^0 i \partial_0 \psi \rangle + \frac{1}{2} m_\sigma^2 \sigma^2 + U(\sigma) - \frac{1}{2} m_\omega^2 \omega_0^2 - \frac{1}{2} m_\rho^2 (\rho_0^z)^2 \tag{14.48}$$

From now let us ignore non-linear term $U(\sigma)$.

Using the energy of a nucleon and meson equation,

$$E_k = +E_k^* + g_\omega \omega_0 + \tau_3 g_\rho \rho_0^z,$$
$$\langle \sigma \rangle = -\frac{g_\sigma}{m_\sigma^2} \rho_S, \quad \langle \omega_0 \rangle = \frac{g_\omega}{m_\omega^2} \rho_B, \quad \langle \rho_0^z \rangle = \frac{g_\rho}{m_\rho^2} \langle \bar{\psi} \gamma_0 \tau^z \psi \rangle = \frac{g_\rho}{m_\rho^2} (\rho_p - \rho_n). \tag{14.49}$$

$$\langle T^{00} \rangle = \langle \sum_{k\lambda} E_k^* a_{k\lambda}^\dagger a_{k\lambda} \rangle + g_\omega \omega_0 (\rho_p + \rho_n) + g_\rho \rho_0^z (\rho_p - \rho_n) + \frac{1}{2} m_\sigma^2 \sigma^2 - \frac{1}{2} m_\omega^2 \omega_0^2 - \frac{1}{2} m_\rho^2 (\rho_0^z)^2$$
$$\to \langle \sum_{k\lambda} E_k^* a_{k\lambda}^\dagger a_{k\lambda} \rangle - \frac{1}{2} g_\sigma \sigma \rho_S + \frac{1}{2} g_\omega \omega_0 \rho_B + \frac{1}{2} g_\rho \rho_0^z (\rho_p - \rho_n)$$
$$\epsilon = \frac{3}{4}\rho_B E^*(k_F) + \frac{1}{4} M^* \rho_S(k_F) - \frac{1}{2} g_\sigma \sigma \rho_S + \frac{1}{2} g_\omega \omega_0 \rho_B + \frac{1}{2} g_\rho \rho_0^z (\rho_p - \rho_n) \tag{14.50}$$

- Pressure of nuclear matter

$$\begin{aligned} P &= \frac{1}{3}\sum_i \langle T^{ii}\rangle = \frac{1}{3}\sum_i \left(\langle \bar{\psi} i\gamma^i \partial^i \psi\rangle - \frac{1}{2}m_\sigma^2\sigma^2 + \frac{1}{2}m_\omega^2\omega_0^2 + \frac{1}{2}m_\rho^2\rho_z^2\right) \\ &= \frac{1}{3}\sum_i \langle \bar{\psi} i\gamma^i \partial^i \psi\rangle + \frac{1}{2}g_\sigma\sigma\rho_S + \frac{1}{2}g_\omega\omega_0\rho_B + \frac{1}{2}g_\rho\rho_0^z(\rho_p - \rho_n) \\ &= \frac{1}{4}\rho_B E^*(k_F) - \frac{1}{4}M^*\rho_S(k_F) + \frac{1}{2}g_\sigma\sigma\rho_S + \frac{1}{2}g_\omega\omega_0\rho_B + \frac{1}{2}g_\rho\rho_0^z(\rho_p - \rho_n) \end{aligned} \quad (14.51)$$

- or in $\sigma - \omega$ model

$$\begin{aligned} \epsilon(\rho_B;\phi_0) &= \frac{g_v^2}{2m_v^2}\rho_B^2 + \frac{m_s^2}{2g_s^2}(M - M^*)^2 + \frac{\gamma}{(2\pi)^3}\int_0^{k_F} d^3k(\boldsymbol{k}^2 + M^{*2})^{\frac{1}{2}}, \\ p(\rho_B;\phi_0) &= \frac{g_v^2}{2m_v^2}\rho_B^2 - \frac{m_s^2}{2g_s^2}(M - M^*)^2 + \frac{\gamma}{3(2\pi)^3}\int_0^{k_F} d^3k\frac{\boldsymbol{k}^2}{(\boldsymbol{k}^2 + M^{*2})^{\frac{1}{2}}} \end{aligned} \quad (14.52)$$

  while $M^* = M - g_s\phi_0$. If we require, the energy to be minimized at a certain ϕ_0 value, V is volume, B is baryon number,

$$\left(\frac{\partial E}{\partial \phi_0}\right)_{V,B} = 0 \quad (14.53)$$

  gives condition,

$$\begin{aligned} \phi_0 &= \frac{g_s}{m_s^2}\rho_s, \\ \rho_s &= \frac{\gamma}{(2\pi)^3}\int_0^{k_F} d^3k\frac{M^*}{(\boldsymbol{k}^2 + M^{*2})^{\frac{1}{2}}} \end{aligned} \quad (14.54)$$

- Fixing parameters: In case of $\sigma - \omega$ model, only unknown parameters are g_σ and g_ω and they can be fixed by requiring the saturation property of energy density. This fixes

$$C_\sigma^2 = g_\sigma^2\frac{M^2}{m_\sigma^2} = 267.1, \quad C_\omega^2 = g_\omega^2\frac{M^2}{m_\omega^2} = 195.9, \quad (14.55)$$

  with $M = 939$ MeV. This gives $k_{F0} = 1.42fm^{-1}$ in $\sigma - \omega$ model. it needs some improvement.

- Compressibility: Let us consider symmetric matter only. ($\rho_p = \rho_n = \frac{1}{2}\rho_B$ and $k_F = k_F^{(p)} = k_F^{(n)}$.)

$$\begin{aligned} E_B &= \frac{\epsilon}{\rho_B} - M \\ &= \frac{3}{4}E^*(k_F) + \frac{1}{4}M^*\frac{\rho_S}{\rho_B} - \frac{1}{2}g_\sigma\sigma\frac{\rho_S}{\rho_B} + \frac{1}{2}g_\omega\omega_0 - M \\ &= \frac{3}{4}E^*(k_F) + \frac{1}{4}M^*\frac{\rho_S}{\rho_B} + \frac{g_\sigma^2}{2m_\sigma^2}\frac{\rho_S^2}{\rho_B} + \frac{g_\omega^2}{2m_\omega^2}\rho_B - M \end{aligned} \quad (14.56)$$

  we would need[5]

$$\begin{aligned} &\frac{\partial}{\partial\rho_B} = (\frac{\partial k_F}{\partial\rho_B})\frac{\partial}{\partial k_F}, \quad \frac{\partial k_F}{\partial\rho_B} = \frac{2\pi^2}{\gamma k_F^2}, \\ &\frac{\partial E_F^*}{\partial\rho_B} = \frac{2\pi^2}{\gamma k_F}\frac{1}{E_F^*}, \\ &\frac{\partial\rho_S}{\partial\rho} = \frac{M^*}{E_F^*} \quad \text{(correct?)} \end{aligned} \quad (14.57)$$

[5] **Problem?** Question is how we should compute $\frac{\partial\rho_S}{\partial\rho_B}$ or $\frac{\partial M^*}{\partial\rho_B}$. Because implicitly, $M^*[\rho_B]$ is also a function of ρ_B, it is not clear whether the partial derivative is actually meant to be full derivative or not. As far as I can understand, it should be full derivative. **Let us at the moment ignore derivative on M^*.**

Then,

$$L = 3\rho_0 \frac{\partial E_B}{\partial \rho_B}|_{\rho_B=\rho_0} = \frac{3}{\rho_0} P(\rho_0) \tag{14.58}$$

The condition $L = 0$ determines ρ_0 value. And the second derivative

$$K = 9\frac{\partial P}{\partial \rho_B}|_{\rho_B=\rho_0} = 9\rho_B^2 \frac{\partial^2(\epsilon/\rho_B)}{\partial \rho_B^2}|_{\rho_B=\rho_0} \tag{14.59}$$

gives

$$K = 9\rho_0 \left[\frac{k_F^2}{3E_F^*\rho_B} + \frac{g_\omega^2}{m_\omega^2} - \frac{g_\sigma^2}{m_\sigma^2}\frac{M^{*2}}{E_F^{*2}}\right]_{\rho_B=\rho_0}, \quad \text{(correct?)}. \tag{14.60}$$

- Symmetry energy: By using

$$\epsilon = \sum_{i=p,n}\left[\frac{3}{4}\rho_i E_{F_i}^* + \frac{1}{4}M^*\rho_{S_i}\right] - \frac{1}{2}g_\sigma\sigma\rho_S + \frac{1}{2}g_\omega\omega_0\rho_B + \frac{1}{2}g_\rho\rho_0^z(\rho_p - \rho_n) \tag{14.61}$$

Then derivative over β becomes,

$$\frac{\partial}{\partial\beta} = -\rho_B\frac{\partial}{\partial\rho_3}, \quad \frac{\partial\rho_S}{\partial\rho} = \frac{M^*}{E_F^*}, \quad \frac{\partial k_{Fi}}{\partial\rho_i} = \frac{\pi^2}{k_{Fi}^2} \tag{14.62}$$

- **Unfinished...**

Chapter 15

HFB

15.1 Bogoliubov transformation

Let us assume that the ground state of the full Hamiltonian with paring interaction is given as a quasi-particle vacuum state $|\Phi\rangle$ such as $\alpha_k|\Phi\rangle = 0$. This assumption is motivated from the BCS theory.

The quasi-particle operators are defined such as[1]

$$\begin{aligned}
&\{\alpha_k, \alpha_{k'}^\dagger\} = \delta_{kk'}, \quad \{\alpha_k, \alpha_{k'}\} = \{\alpha_k^\dagger, \alpha_{k'}^\dagger\} = 0, \\
&\alpha_k = \sum_n (U_{nk}^* c_n + V_{nk}^* c_n^\dagger), \quad \alpha_k^\dagger = \sum_n (V_{nk} c_n + U_{nk} c_n^\dagger).
\end{aligned} \tag{15.1}$$

Here, note that U and V are matrices. We may write the relation as matrix form

$$\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} = W^\dagger \begin{pmatrix} c \\ c^\dagger \end{pmatrix} \tag{15.2}$$

And it's inverse

$$\begin{pmatrix} c \\ c^\dagger \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} = W \begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} \tag{15.3}$$

and the same commutation relations implies W to be unitary ($WW^\dagger = W^\dagger W = I$) and relations

$$U^\dagger U + V^\dagger V = I, \quad U^T V + V^T U = 0, \quad UU^\dagger + V^* V^T = I, \quad UV^\dagger + V^* U^T = 0. \tag{15.4}$$

We can define normal ρ and paring κ one-body density matrices as

$$\begin{aligned}
\rho_{nn'} &= \langle\Phi|c_{n'}^\dagger c_n|\Phi\rangle = \langle\Phi|(V\alpha + U^*\alpha^\dagger)_{n'}(U\alpha + V^*\alpha^\dagger)_n|\Phi\rangle \\
&= \langle\Phi|\sum_{k,k'} V_{n'k'} V_{nk}^* \alpha_{k'} \alpha_k^\dagger|\Phi\rangle = (V^* V^T)_{nn'} = (1 - UU^\dagger)_{nn'}, \\
\kappa_{nn'} &= \langle\Phi|c_{n'} c_n|\Phi\rangle = \langle\Phi|(U\alpha + V^*\alpha^\dagger)_{n'}(U\alpha + V^*\alpha^\dagger)_n|\Phi\rangle \\
&= \langle\Phi|\sum_{k,k'} U_{n'k'} V_{nk}^* \alpha_{k'} \alpha_n^\dagger|\Phi\rangle = (V^* U^T)_{nn'} = -(UV^\dagger)_{nn'}.
\end{aligned} \tag{15.5}$$

(Now there are relations $\kappa^T = -\kappa$, $\rho^2 - \rho = -\kappa\kappa^\dagger$, $\rho\kappa = \kappa\rho^*$.) Here note again that V and U are matrices in state indices n and state index includes r, k_i, σ_i, q_i , position or momentum/energy, spin and isospin.

[1] In case of H.F. theory, we can identify $U \to 0$, $V \to 1$. In case of BCS theory, $U_{nk} \to u_k \delta_{nk}$, $V_{nk} \to v_k \delta_{nk}$.

By using

$$\begin{aligned}
\langle\Phi|c^\dagger_{n_1}c^\dagger_{n_2}c_{n_4}c_{n_3}|\Phi\rangle &= \langle\Phi|(V\alpha+U^*\alpha^\dagger)_{n_1}(V\alpha+U^*\alpha^\dagger)_{n_2}(U\alpha+V^*\alpha^\dagger)_{n_4}(U\alpha+V^*\alpha^\dagger)_{n_3}|\Phi\rangle \\
&= \sum_{k_1,k_2,k_3,k_4} V_{n_1k_1}V^*_{n_3k_3}V_{n_2k_2}V^*_{n_4k_4}\langle\Phi|\alpha_{k_1}\alpha_{k_2}\alpha^\dagger_{k_4}\alpha^\dagger_{k_3}|\Phi\rangle \\
&\quad + \sum_{k_1,k_2,k_3,k_4} V_{n_1k_1}V^*_{n_3k_3}U^*_{n_2k_2}U_{n_4k_4}\langle\Phi|\alpha_{k_1}\alpha^\dagger_{k_2}\alpha_{k_4}\alpha^\dagger_{k_3}|\Phi\rangle \\
&= \sum_{k_1,k_2,k_3,k_4} V_{n_1k_1}V^*_{n_3k_3}V_{n_2k_2}V^*_{n_4k_4}\langle\Phi|\Phi\rangle\left(-\delta_{k_1k_4}\delta_{k_3k_2}+\delta_{k_1k_3}\delta_{k_4k_2}\right) \\
&\quad + \sum_{k_1,k_2,k_3,k_4} V_{n_1k_1}V^*_{n_3k_3}U^*_{n_2k_2}U_{n_4k_4}\langle\Phi|\Phi\rangle\delta_{k_1k_2}\delta_{k_3k_4} \\
&= \langle\Phi|\Phi\rangle\left(-(V^*V^T)_{n_1n_4}(V^*V^T)_{n_2n_3}+(V^*V^T)_{n_3n_1}(V^*V^T)_{n_4n_2}+(VU^\dagger)_{n_1n_2}(V^*U^T)_{n_3n_4}\right) \\
&= \langle\Phi|\Phi\rangle(-\rho_{n_4n_1}\rho_{n_2n_3}+\rho_{n_3n_1}\rho_{n_4n_2}+\kappa^*_{n_1n_2}\kappa_{n_3n_4}) \qquad (15.6)
\end{aligned}$$

Thus, we can write the energy expectation value as (need to use antisymmetry of $\bar{v}$)

$$H=\sum_{n_1n_2}e_{n_1n_2}c^\dagger_{n_1}c_{n_2}+\frac{1}{4}\sum_{n_1n_2n_3n_4}\bar{v}_{n_1n_2n_3n_4}c^\dagger_{n_1}c^\dagger_{n_2}c_{n_4}c_{n_3}, \qquad (15.7)$$

$$E[\rho,\kappa] = \frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle}=\mathrm{Tr}[(e+\frac{1}{2}\Gamma)\rho]-\frac{1}{2}\mathrm{Tr}[\Delta\kappa^*], \qquad (15.8)$$

where

$$\begin{aligned}
\Gamma_{n_1n_3} &= \sum_{n_2n_4}\bar{v}_{n_1n_2n_3n_4}\rho_{n_4n_2}, \\
\Delta &= \frac{1}{2}\sum_{n_3n_4}\bar{v}_{n_1n_2n_3n_4}\kappa_{n_3n_4}. \qquad (15.9)
\end{aligned}$$

We may do this easily if we do the Unitary transformation from the Hamiltonian.

$$\begin{aligned}
H &= H^0+:\frac{1}{2}\begin{pmatrix} c^\dagger & c\end{pmatrix}\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^*\end{pmatrix}\begin{pmatrix} c \\ c^\dagger\end{pmatrix}:+\frac{1}{4}\sum_{l_1l_2l_3l_4}\bar{v}_{l_1l_2l_3l_4}:c^\dagger_{l_1}c^\dagger_{l_2}c_{l_4}c_{l_3}:, \\
H^0 &= \langle\Phi|H|\Phi\rangle=\mathrm{Tr}[(e+\frac{1}{2}\Gamma)\rho]-\frac{1}{2}\mathrm{Tr}[\Delta\kappa^*], \\
h &= e+\Gamma, \qquad (15.10)
\end{aligned}$$

For the HFB approximation, we neglect the last term and only keeps the quadratic terms. Note that the ground state $|\Phi\rangle$ is not known yet and the normal ordered operator of c or $c^\dagger$ does not vanish in general, $\langle\Phi|:O(c,c^\dagger):|\Phi\rangle$. Finding a ground state is equivalent to find a basis transformation such that the second term becomes diagonalized. Then in that basis, we can define the ground state such that $\beta_k|\Phi\rangle=0$. In other words, we want to find transformation W such that

$$W^\dagger\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^*\end{pmatrix}W=\begin{pmatrix} E & 0 \\ 0 & E\end{pmatrix}. \qquad (15.11)$$

This is equivalent to HFB equation.

If we consider the constraints on the total number of particles and the normalization of each single particle states, we may use

$$H\to H-\lambda\sum_k c^\dagger_kc_k+\sum_k E_kc^\dagger_kc_k \qquad (15.12)$$

With Bogoliubov transformation(replace vacuum and operators), we will have

$$H = (H^0 - \lambda \mathrm{Tr}\rho + \mathrm{Tr}[E\rho]) + : \frac{1}{2} \begin{pmatrix} \beta^\dagger & \beta \end{pmatrix} W^\dagger \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} W \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} : + \dots \quad (15.13)$$

15.1.1 Useful mathematical theorems for product wave functions

These theorems are explained in the book by P. Ring.

- Bloch-Messiah Theorem: A unitary matrix W of the following special form can be decomposed into three matrices,

$$W = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix} \begin{pmatrix} \bar{U} & \bar{V} \\ \bar{V} & \bar{U} \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix} \quad (15.14)$$

  ,where the real matrices $\bar{U}$ and $\bar{V}$ are diagonal and of "quasi-canonical" form.

- Thouless' Theorem: Staring with a general product wave function $|\Phi_0\rangle$ which is the vacuum to quasi-particle operator β, any general product wave function $|\Phi_1\rangle$ which is not orthogonal to $|\Phi_0\rangle$ may be expressed in the form

$$|\Phi_1\rangle = \mathcal{N} \exp\left(\sum_{k<k'} Z_{kk'} \beta_k^\dagger \beta_{k'}^\dagger \right) |\Phi_0\rangle, \quad (15.15)$$

  where $\mathcal{N} = \langle \Phi_0 | \Phi_0 \rangle$ is a normalization constant and Z a skew symmetric matrix, $Z^T = -Z$.

15.2 HFB equation

Because the number of particles are not conserved for $|\Phi\rangle$, we have to use chemical potential(Fermi energy) to fix the average number of particle. Also the various constraints on U and V have to be included at the same time. Thus, we may introduce two Lagrange multipliers λ and E and find a minimization condition. Then, the variation of energy

$$\delta(E[\rho, \kappa] - \lambda \langle \hat{N} \rangle) = 0. \quad (15.16)$$

leads to the HFB euqations, (**Requires verification!! At the moment, it is not confirmed yet.**)

$$\begin{pmatrix} e + \Gamma - \lambda & \Delta \\ -\Delta^* & -(e+\Gamma)^* + \lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix} \quad (15.17)$$

The index n can be single particle quantum number of basis states or also can be the position, spin, isospin $(\boldsymbol{r}, \sigma, q)$.

In fact, it is often assumed that V and U are diagonal, and use paring density $\tilde{\rho}$ instead of pairing tensor κ,

$$\tilde{\rho}(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') = -2\sigma' \kappa(\boldsymbol{r}, \sigma, \boldsymbol{r}', -\sigma') \quad (15.18)$$

Note that the energy density functional for paring is written as

$$-\frac{1}{2}\mathrm{Tr}[\Delta\kappa^*] = -\frac{1}{2} \sum_{n_1 n_2} \frac{1}{2} \sum_{n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} \kappa_{n_3 n_4} \kappa^*_{n_2 n_1} \quad (15.19)$$

Chapter 16

Coupled cluster theory

Reference: Thomas Papenbrock's lecture at RISP.

Reference state is defined as

$$|\Phi\rangle = \prod_{i=1,A} a_i^\dagger |0\rangle. \tag{16.1}$$

Coupled cluster ansatz: full A-body wave function $|\Psi\rangle$ can be obtained by applying $e^{\hat{T}}$ operator on the H.F. ground state $|\Phi_0\rangle$(slater determinant for A-body occupied states).[1]

$$|\Psi\rangle = e^{\hat{T}}|\Phi_0\rangle = \left(\sum_{n=1}^{A} \frac{1}{n!}\hat{T}^n\right)|\Phi_0\rangle \tag{16.2}$$

Cluster Operator $\hat{T}$ is considered for one-body and two-body correlations (즉, T가 correlation을 만들어내는 역할을 한다.)

$$\begin{aligned}
\hat{T} &= \hat{T}_1 + \hat{T}_2 + \cdots, \\
\hat{T}_1 &= \sum_{ia} t_i^a \hat{a}_a^\dagger \hat{a}_i, \\
\hat{T}_2 &= \frac{1}{4}\sum_{ijab} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i, \\
\hat{T}_A &= \frac{1}{(A!)^2}\sum t_{i_1\ldots i_A}^{a_1\ldots a_A} a_{a_1}^\dagger \ldots a_{a_A}^\dagger a_{i_A}\ldots a_{i_1}.
\end{aligned} \tag{16.3}$$

여기서, i, j, a, b 는 모든 가능한 occupied and unoccupied states 이다. 가능한 single particle state의 수를 N이라고 하면, T_1에는 N^2개, T_2에는 N^4개의 unknown parameter 가 있는 셈이다. (더 정확히는 CCSD라면 A^2N^4이라고 한다. 확인 필요.) 여기서, 만약 가능한 모든 excitation을 고려한다면 (즉, T_A 까지 포함한다면), unoccupied single particle level의 수를 N_u라고 할 때 unknown 파라미터의 수는 $\sum_{n=0}^{A} {}_{N_u}C_{nA}C_{A-n} = {}_{A+N_u}C_A = {}_NC_A$로 Full configuration interaction의 coefficient의 수와 같다.

In practice, one have to truncate the operators in T. CCSD (coupled cluster singles doubles) approximation use

$$T \equiv \sum_{ia} t_i^a \hat{a}_a^\dagger \hat{a}_i + \frac{1}{4}\sum_{ijab} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i. \tag{16.4}$$

[1] This looks similar to the VMC wave function which acts correlation operators. Because operator is in the exponential, it creates series of excitations.

여기서, 주의할 것은 T operator가 exponential 위에 있다는 것이다. 따라서, e^T는 1p1h, 2p2h states 뿐 아니라, ApAh 까지를 모두 만들수 있다. 앞으로 1p1h state 는 $|\Phi_i^a\rangle$, 2p2h state는 $|\Phi_{ij}^{ab}\rangle$ 로 타나내도록 하자. (T operator는 particle creation and hole annihilation operator 들로 구성되어 있다. particle annihilation, hole creation operator는 나타나지 않음.)

Suppose $|\Psi\rangle$ is a ground state of Hamiltonian $\hat{H}$.

$$\begin{aligned} &\hat{H}|\Psi\rangle = E|\Psi\rangle, \quad \hat{H}e^{\hat{T}}|\Phi_0\rangle = Ee^{\hat{T}}|\Phi_0\rangle, \\ &\left(\bar{H} \equiv e^{-\hat{T}}\hat{H}e^{\hat{T}}\right)|\Phi_0\rangle = E|\Phi_0\rangle \end{aligned} \tag{16.5}$$

여기서 $\bar{H}$ 는 similarity-transformed Hamiltonian from $\hat{H}$. **즉, $\bar{H}$ 는 reference state $|\Phi_0\rangle$가 정확한 ground state eigenvalue를 주도록 만든다. 이러한 similarity transform T 를 찾을 수 있다면 $\langle\Phi_0|\bar{H}|\Phi_0\rangle = E$ 를 계산하면 ground state energy를 계산할 수 있다.** (For Hermitian $\bar{H}_N$, e^T have to be unitary and thus, T must be anti-Hermitian, $T = -T^\dagger$. However, in coupled cluster theory, $\bar{H}$ is non-hermitian.)

$$\langle\Phi_0|\bar{H}|\Phi_0\rangle = \langle\Phi_0|\bar{H}_N|\Phi_0\rangle + E_0 = E \tag{16.6}$$

이므로, $\langle\Phi_0|\bar{H}_N|\Phi_0\rangle = E_c$.

Coupled cluster theory employs non-Hermitian Hamiltonian $\bar{H}_N$.

Note that $\bar{H}_N$ has the same eigenvalues as H_N for arbitrary T.

$$\begin{aligned} H_N|\lambda\rangle &= \lambda|\lambda\rangle, \\ (e^{-T}H_Ne^T)e^{-T}|\lambda\rangle &= \lambda e^{-T}|\lambda\rangle \end{aligned} \tag{16.7}$$

(즉, $H|\lambda\rangle = \lambda|\lambda\rangle$ 일 때, $\bar{H}|e^{-T}\lambda\rangle = \lambda|e^{-T}\lambda\rangle$는 같은 eigenvalue를 가진다.) $\bar{H}_N$ 의 eigen-value를 E_α 라고 할 때, non-hermitian operator는 left eigen state와 right eigen state를 가지므로,

$$\bar{H}_N = \sum_\alpha |R_\alpha\rangle E_\alpha \langle L_\alpha|, \quad \langle L_\alpha|R_\beta\rangle = \delta_\alpha^\beta \tag{16.8}$$

로 나타낼 수 있다. Then,

$$\begin{aligned} \langle\Phi_0|\bar{H}_N|\Phi_0\rangle &= E_c, \\ \langle\Phi_i^a|\bar{H}_N|\Phi_0\rangle &= 0, \\ \langle\Phi_{ij}^{ab}|\bar{H}_N|\Phi_0\rangle &= 0, \cdots \end{aligned} \tag{16.9}$$

가 얻어진다. CCSD apprpximation에서 $\bar{H}$를 얻는 것은 위의 coupled equation의 해를 찾는 것과 같다. E_c 는 correlation energy. 어떤 operator 에 대해 eigen-state라는 것은 model space 안에서 operator에 의해 다른 state로 가지 않는다는 것. In general,

$$\bar{H}_N|\Phi_0\rangle = E_c|\Phi_0\rangle + \sum|\Phi_i^a\rangle + \sum|\Phi_{ij}^{ab}\rangle + \cdots \tag{16.10}$$

가 되는데, 위 조건을 만족시킨다는 것은 1p-1h과 2p-2h까지 고려한 모델스페이스에서는 $\bar{H}_N|\Phi_0\rangle = E_c|\Phi_0\rangle$ 로 근사시킬수 있다는 뜻. (We note that in the CCSD approximation the reference state is not an exact eigenstates. Rather, it is decoupled from simple states but $\bar{H}_N$ still connects this state to 3p-3h, and 4p-4h states etc.) (But, full wave $e^T|\Phi_0\rangle$ contains all possible excitations. Thus, it is not simply limited to 2p-2h excitations.)

We see that the coupled-cluster method in its CCSD approximation yields a similarity-transformed Hamiltonian that is of a two-body structure with respect to a non-trivial vacuum. Thus, the coupled-cluster method "transforms" an A-body problem (in CCSD) into a two-body problem, albeit with respect to a nontrivial vacuum.

따라서, 밑의 두 식을 이용하여 parameter들을 결정하면, 이를 이용하여 correlation energy E_c 를 구할 수 있다.

$$\begin{aligned}\bar{H}_N &= e^{-T} H_N e^T \\ &= H_N + [H_N, T] + \frac{1}{2!}[[H_N, T], T] + \frac{1}{3!}[[[H_N, T], T], T] + \dots \end{aligned} \tag{16.11}$$

여기서, 주의할 것은 cluster operator는 particle creation and hole annihilation operator(but no particle annihilation or hole creation)로 이루어져 있다는 것이다. 따라서, all terms that enter T commute each other. 이것은 위 expansion에서 non-zero가 나오는 경우는 각각의 T가 H_N과 connect되어야만 한다.(But no T with another T). 따라서, above expansion terminates at finite terms. Thus one can express $\bar{H}_N$ exactly with finite terms. [2] 예를 들어, $[[[H_N, T_1], T_1], T_1]$ contribute to CCSD equations from 1-body part of Hamiltonian, But $[[[H_N, T_2], T_2], T_2]$ are three-body rank or higher and does not contribute in CCSD equation. 또는, 2-body interaction까지 생각할 때 H_N은 최대 $a_p^\dagger a_q^\dagger a_s a_r$의 4개 operator를 가지는데, 하나의 T와의 commutation으로 최소한 하나의 operator를 connect할 수 있으므로, 4개의 T로 전부 connect할 수 있고, 그 이상의 term은 contribute 하지 않는다. 즉, 전개했을때 Hamiltonian 과 T의 operator간에 전부 contract 하고도 모든 항에 남는 normal ordered operator가 생기므로, CCSD equation에 contribute 하지 않는다.

Connected Cluster theorem can be used to simplify the expansion,

$$\bar{H} = \hat{H}_N + \left(\hat{H}_N \hat{T}\right)_c + \frac{1}{2}\left(\hat{H}_N \hat{T}^2\right)_c + \dots + \frac{1}{n!}\left(\hat{H}_N \hat{T}^n\right)_c + \dots \tag{16.12}$$

(commutaor 의 expansion은 결국, H_N과 T^n의 connected diagram 이 된다는 것이다. 즉, 일단 H_N과 T^n이 fully connect되면, 그보다 더 높은 order에서는 connected diagram을 만들수 없고, 따라서, series가 멈춘다. 위에서 설명한 것과 같은 이유.)

Then, we can write

$$\bar{H}_N = \sum_{pq} \bar{H}_q^p a_q^\dagger a_p + \frac{1}{4}\sum_{pqrs} \bar{H}_{rs}^{pq} a_p^\dagger a_q^\dagger a_s a_r + \dots \tag{16.13}$$

with

$$\begin{aligned}\bar{H}_q^p &= \langle p|\bar{H}_N|q\rangle, \\ \bar{H}_{rs}^{pq} &= \langle pq|\bar{H}_N|rs\rangle. \end{aligned} \tag{16.14}$$

In CCSD, $\bar{H}_i^a = 0$ and $\bar{H}_{ij}^{ab} = 0$. (But, $\bar{H}_a^i$, $\bar{H}_{ab}^{ij}$ etc can be non-zero.)

For example, matrix element for $\bar{H}_{ab}^{ij} = \langle ij|\bar{H}_N|ab\rangle$ 를 직접 Hamiltonian으로 계산해 보면(즉 $e^{-T}H_N e^T$를 넣어서), $\bar{H}_{ab}^{ij} a_i^\dagger a_j^\dagger a_b a_a$ 형태를 최종적으로 얻어야하므로 no contraction with any cluster operator T is possible. (cluster operator는 annihilate holes and create particles) 따라서, we simply have $\bar{H}_{ab}^{ij} = \langle ij|V|ab\rangle$.

16.0.1 HF state is "good" reference?

If HF basis is used(each $|p\rangle = \sum_x c_{px}|\phi_x\rangle$ of simple basis $|\phi_x\rangle$), the f_q^p becomes diagonal, so does 1-body part of $\hat{H}_N$. If potential is weak, we would expect small off-diagonal terms in the Hamiltonian. Thus, full solution will be close to initial diagonal one, i.e. HF state. Also, if there is a clear gap in the single particle spectrum, it will justify the truncation of model space.

CCSD의 경우, for a good reference, we might reasonably expect that the inclusion of 1p-1h and 2p-2h excitations could result in an accurate approximation. (Usually 90% of correlation can be accounted by CCSD. And inclusion of triples yields usually 99% of correlation energy.)

[2](It is because $\bar{H}_N$ is non-Hermitian Hamiltonian. For Hermitian $\bar{H}_N$ (which implies anti-hermitian T), the expansion does not terminate and one have to use some truncation approximation.)

16.1 bi-variational point of view

Suppose a problem of minimizing energy functional

$$E(T,L) = \langle\Phi|Le^{-T}He^{T}|\Phi\rangle = \langle\Phi|L\bar{H}|\Phi\rangle \tag{16.15}$$

where $L = l_0 + L_1 + L_2 + \cdots + L_A$ is a de-excitation operator,

$$\begin{aligned} L_1 &= \sum_{ia} l_a^i a_i^\dagger a_a \\ L_2 &= \frac{1}{4}\sum_{ijab} l_{ab}^{ij} a_i^\dagger a_j^\dagger a_b a_a, \end{aligned} \tag{16.16}$$

(For example $L_1|\Phi_{1h}^{1p}\rangle \to 0, |\Phi\rangle$. We may view the minimization of $E(T,L)$ as an independent variation over bra state $\langle\Phi|Le^{-T}$ and ket state $e^T|\Phi\rangle$. Also, $\langle\Phi|Le^{-T}e^T|\Phi\rangle = \langle\Phi|\Phi\rangle = 1$ if $l_0 = 1$.) Then, variation w.r.t. L gives equations

$$\begin{aligned} \langle\Phi_i^a|\bar{H}|\Phi\rangle &= 0 \\ \langle\Phi_{ij}^{ab}|\bar{H}|\Phi\rangle &= 0 \end{aligned} \tag{16.17}$$

these equation gives solution of t_i^a, t_{ij}^{ab}. Variation w.r.t. T gives

$$\begin{aligned} \langle\Phi|L[\bar{H}, a_a^\dagger a_i]|\Phi\rangle &= 0, \\ \langle\Phi|L[\bar{H}, a_a^\dagger a_b^\dagger a_j a_i]|\Phi\rangle &= 0 \end{aligned} \tag{16.18}$$

which gives equations for l_a^i, l_{ab}^{ij}. If we are only interested in ground state energy, we don't need l's.

Above equation implies that if we truncate the series of T, reference $|\Phi\rangle$ becomes an eigen-state of $\bar{H}$ within this model space. (i.e. $\langle\Phi|L_n\bar{H}|\Phi\rangle = 0$) then, energy functional becomes

$$E = \langle\Phi|\bar{H}|\Phi\rangle \tag{16.19}$$

which implies $He^T|\Phi\rangle = Ee^T|\Phi\rangle$ in the model space. (In other words, exact ground state energy for H.)

16.2 Correlation energy

We will find CC equations which determines operators T_1,T_2 and so on. Here, let us assume amplitudes are known and just show how to compute correlation energy in CCSD approximation,$\hat{T} \simeq \hat{T}_1 + \hat{T}_2$.

The correlation energy is

$$\begin{aligned} E_{CC} &= \langle\Phi_0|\bar{H}_N|\Phi_0\rangle \\ &= \langle\Phi_0|H_N + [H_N,T] + \frac{1}{2!}[[H_N,T],T] + \frac{1}{3!}[[[H_N,T],T],T] + \ldots|\Phi_0\rangle \end{aligned} \tag{16.20}$$

- The first term is zero by construction,

$$\langle\Phi_0|\hat{H}_N|\Phi_0\rangle = 0. \tag{16.21}$$

- The second term can be split

$$\langle\Phi_0|[H_N,T]|\Phi\rangle = \langle\Phi_0|([F_N,T_1] + [F_N,T_2] + [V_N,T_1] + [V_N,T_2])|\Phi_0\rangle \tag{16.22}$$

– the first term

$$\begin{aligned}
[F_N, T_1] &= \sum_{pqia} \left(f_q^p N(a_p^\dagger a_q) t_i^a N(a_a^\dagger a_i) - t_i^a N(a_a^\dagger a_i) f_q^p N(a_p^\dagger a_q) \right) \\
&= \sum_{pqia} f_q^p t_i^a \left(N(a_p^\dagger a_q) N(a_a^\dagger a_i) - N(a_a^\dagger a_i) N(a_p^\dagger a_q) \right) \\
&= \sum_{pqia} f_q^p t_i^a \left(\delta_{qa} N(a_p^\dagger a_i) + \delta_{pi} N(a_q a_a^\dagger) + \delta_{qa}\delta_{pi} \right) \\
&= \sum_{pai} f_a^p t_i^a N[a_p^\dagger a_i] + \sum_{qai} f_q^i t_i^a N[a_q a_a^\dagger] + \sum_{ai} f_a^i t_i^a \qquad (16.23)
\end{aligned}$$

Thus, finally

$$\langle \Phi_0 | [F_N, T_1] | \Phi_0 \rangle = \sum_{ai} f_a^i t_i^a \qquad (16.24)$$

– the second term (after some lengthy calculation)

$$\begin{aligned}
[F_N, T_2] &= \frac{1}{4} \sum_{pq,ij,ab} f_q^p t_{ij}^{ab} \Big(N[a_p^\dagger a_q] N[a_a^\dagger a_b^\dagger a_j a_i] - N[a_a^\dagger a_b^\dagger a_j a_i] N[a_p^\dagger a_q] \Big) \\
&= \frac{1}{4} \sum_{pq,ij,ab} f_q^p t_{ij}^{ab} \Big(-\delta_{pj} N[a_q a_a^\dagger a_b^\dagger a_i] + \delta_{pi} N[a_q a_a^\dagger a_b^\dagger a_j] + \delta_{qa} N[a_p^\dagger a_b^\dagger a_j a_i] - \delta_{qb} N[a_p^\dagger a_a^\dagger a_j a_i] \\
&\quad -\delta_{pj}\delta_{qa} N[a_b^\dagger a_i] + \delta_{pi}\delta_{qa} N[a_b^\dagger a_j] + \delta_{pj}\delta_{qb} N[a_a^\dagger a_i] - \delta_{pi}\delta_{qb} N[a_a^\dagger a_j] \Big) \\
&= \frac{1}{2} \sum_{q,ij,ab} f_q^i t_{ij}^{ab} N[a_q a_a^\dagger a_b^\dagger a_j] + \frac{1}{2} \sum_{p,ij,ab} f_a^p t_{ij}^{ab} N[a_p^\dagger a_b^\dagger a_j a_i] + \sum_{ijab} f_a^i t_{ij}^{ab} N[a_b^\dagger a_j] \qquad (16.25)
\end{aligned}$$

Thus,

$$\langle \Phi_0 | [F_N, T_2] | \Phi_0 \rangle = 0. \qquad (16.26)$$

– other terms

$$\langle \Phi_0 | [V_N, T_1] | \Phi_0 \rangle = 0. \qquad (16.27)$$

$$\langle \Phi_0 | [V_N, T_2] | \Phi_0 \rangle = \frac{1}{4} \sum_{ijab} \langle ij | \hat{v} | ab \rangle t_{ij}^{ab} \qquad (16.28)$$

- Correlation energy from non-linear terms with amplitudes squared

$$\langle \Phi_0 | \frac{1}{2} (V_N T_1^2) | \Phi_0 \rangle = \frac{1}{2} \sum_{ijab} \langle ij | \hat{v} | ab \rangle t_i^a t_j^b \qquad (16.29)$$

- Collecting all terms

$$\Delta E = \sum_{ai} \langle i | \hat{f} | a \rangle t_i^a + \frac{1}{2} \sum_{ijab} \langle ij | \hat{v} | ab \rangle t_i^a t_j^b + \frac{1}{4} \sum_{ijab} \langle ij | \hat{v} | ab \rangle t_{ij}^{ab} \qquad (16.30)$$

16.3 diagrams

With

$$\hat{H}_N = \sum_{pq} \langle p | \hat{f} | q \rangle N[c_p^\dagger c_q] + \frac{1}{4} \sum_{pqrs} \langle pq | v | rs \rangle N[c_p^\dagger c_q^\dagger c_s c_r] \qquad (16.31)$$

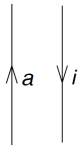
From the linked cluster theorem, all terms in $\bar{H}_N$ comes from

$$\frac{1}{n!}\left(\hat{H}_N\hat{T}^n\right)_c. \tag{16.32}$$

Because it is connected, one can express those terms as a connected diagrams. One have to draw all possible ways to connect operators.

16.3.1 Convention and rules

Lines



- Denote hole lines (i,j,k..) are pointing down.
- Denote particle lines (a,b,c..) are pointing up.
- incoming line to a point means annihilation operator
- outgoing line from a point means creation operator
- In other words, $a_i^\dagger$ is a outgoing-down arrow. a_i is incoming-down arrow. $a_a^\dagger$ is a outgoing-up arrow. a_a is incoming-up arrow.
- line connecting two vertex is a contraction. (connected up line means $\overbrace{a_a a_a^\dagger} = 1$. connected down line means $\overbrace{a_i^\dagger a_i} = 1$)

Operators

Let us use notation f_q^p, v_{rs}^{pq}.(즉, 위에 있는 index가 left bra, 아래 index가 ket을 나타낸다.)

- F_N One-body operator

$$\sum_{ab} f_{ab}\{a_a^\dagger a_b\} \quad + \quad \sum_{ij} f_{ij}\{a_i^\dagger a_j\} \quad + \quad \sum_{ia} f_{ia}\{a_i^\dagger a_a\} \quad + \quad \sum_{ia} f_{ai}\{a_a^\dagger a_i\}$$

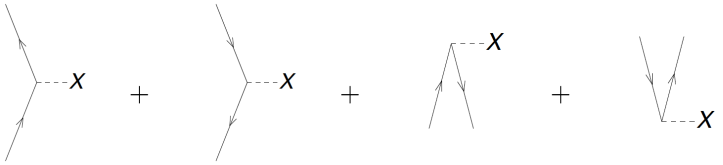


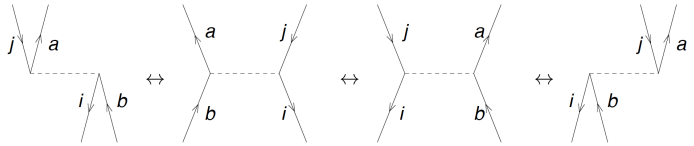
Figure 16.1: F_N terms. One identify $f_{pq} \leftrightarrow f_q^p$.

- V_N Two-body operator

$$\frac{1}{4}\sum_{pqrs}\langle pq|v|rs\rangle\{a_p^\dagger a_q^\dagger a_s a_r\} \tag{16.33}$$

We can expand it in terms of particles and holes (each p, q, r, s can be either particle or hole) and each one corresponds to one diagram.

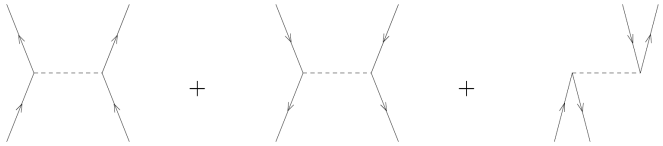
- $\langle ai|v|jb\rangle a_a^\dagger a_i^\dagger a_b a_j$ structure. Following figures have the same operator structures and thus topologically equivalent. (Position of line is not important but number of lines of incoming and outgoing, and particle and hole to the operator have to be the same. In this case, one for each incoming/outgoing particle/holes.)



$$\langle ai|v|jb\rangle = -\langle ai|v|bj\rangle = -\langle ia|v|jb\rangle = \langle ia|v|bj\rangle$$

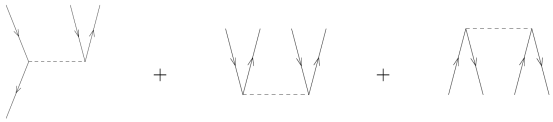
In fact, one have to consider factor and sign. But these will be counted at the last moment. (For example, if one computes $\langle \Phi_{jb}^{ai}|V_N|\Phi_0\rangle$ the external index have to contract in 4 possible ways. Also, one have to take into account the original operator is normal ordered.)

- $\langle ab|v|cd\rangle a_a^\dagger a_b^\dagger a_d a_c + \langle ij|v|kl\rangle a_i^\dagger a_j^\dagger a_l a_k + \langle ia|v|bj\rangle a_i^\dagger a_a^\dagger a_j a_b$



- $\langle ai|b|bc\rangle a_a^\dagger a_i^\dagger a_c a_b + \langle ij|v|ka\rangle a_i^\dagger a_j^\dagger a_a a_k + \langle ab|v|ci\rangle a_a^\dagger a_b^\dagger a_i a_c$

- $\langle ia|v|jk\rangle a_i^\dagger a_a^\dagger a_k a_i + \langle ab|v|ij\rangle a_a^\dagger a_b^\dagger a_j a_i + \langle ij|v|ab\rangle a_i^\dagger a_j^\dagger a_b a_a$



CC amplitudes

- T-amplitudes : Single and Double amplitudes

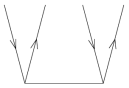
Rules

Rules to construct diagrams of $\bar{H}_N$ matrix elements

- Write down all topologically different diagrams corresponding to the desired matrix element. Topologically different diagrams differ in the number and type of lines (particle or hole) that

$$\hat{T}_1 = \sum_{ia} t_i^a \{a_a^\dagger a_i\} =$$

$$\hat{T}_2 = \frac{1}{4}\sum_{ijab} t_{ij}^{ab} \{a_a^\dagger a_b^\dagger a_j a_i\} =$$



connect the Fock matrix F or the interaction V to the cluster amplitudes T, but not whether these connections are left or right (as those are related by antisymmetry). (Only one diagram for given in-out particle-hole lines and F,V,T_1,T_2.)

- Write down the matrix elements that enter the diagram, and sum over all internal lines.
- The overall sign is (-1) to the power of [(number of hole lines) – (number of loops)].
- Symmetry factor: For each pair of equivalent lines (i.e. lines that connect the same two operators.) multiply with a factor 1/2. For n identical vertices, multiply the algebraic expression by the symmery factor 1/n! to account properly for the number of ways the diagram can be constructed.
- Antisymmetrize the outgoing and incoming lines as necessary. One can use anti-symmetrization operators,

$$\begin{aligned} \hat{P}(ab) &= 1 - \hat{P}_{ab}, \\ \hat{P}(ij|ab) &= (1 - \hat{P}_{ij})(1 - \hat{P}_{ab}) \end{aligned} \tag{16.34}$$

The sign comes obviously from the arrangement of creation and annilhilation operators, while the symmetry factor stems from all the different ways, one can contract the cluster operator with the normal-ordered Hamiltonian.

Example: CCSD correlation energy with two-body interaction

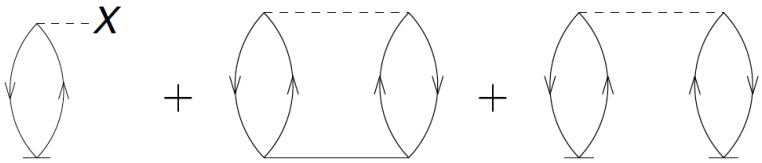


Figure 16.2: Correlation energy in CCSD

For example, CCSD correlation energy

$$\Delta E = \sum_{ai} \langle i|\hat{f}|a\rangle t_i^a + \frac{1}{4}\sum_{ijab} \langle ij|\hat{v}|ab\rangle t_{ij}^{ab} + \frac{1}{2}\sum_{ijab} \langle ij|\hat{v}|ab\rangle t_i^a t_j^b \tag{16.35}$$

can be expressed as a diagrams with no external line, and one f or v of Hamiltonian with suitable number of singles or doubles. How about the signs and factors?

- The first diagram comes from

$$\langle\Phi_0|\left(\hat{F}_N\hat{T}_1\right)_c|\Phi_0\rangle = \sum_{pq}\sum_{ai} f_p^q t_i^a \{\overbrace{a_q^\dagger \overbrace{a_p\}\{a_a^\dagger}^{}}^{} a_i\}.$$

  This diagram has one hole line and one loop. Thus, sign is positive. No equivalent lines or vertices. Thus no symmetry factor.

- Second diagram comes from

$$\langle\Phi_0|\left(\hat{V}_N\hat{T}_2\right)_c|\Phi_0\rangle = \frac{1}{4}\sum_{pqrs}\frac{1}{4}\sum_{abij}\langle pq|v|rs\rangle t_{ij}^{ab}\left(\{a_p^\dagger a_q^\dagger a_s a_r\}\{a_a^\dagger a_b^\dagger a_j a_i\}\right)_c$$

  Because there are 4-ways to contract operators, the factor $\frac{1}{4}$ remains.

  According to the diagram rule, sign is positive (for two hole lines and two loops). Two particle lines are equivalent because they connect the same operators($\hat{V}$ and $\hat{T}_2$). (Same for hole lines). Thus symmetry factor is $(\frac{1}{2})^2$.

- Third diagram is from

$$\langle\Phi_0|\frac{1}{2}\hat{V}_N\hat{T}_1^2|\Phi_0\rangle = \frac{1}{2}\frac{1}{4}\sum_{pqrs}\sum_{ai}\sum_{bj}\langle pq|v|rs\rangle t_i^a t_j^b\left(\{a_p^\dagger a_q^\dagger a_s a_r\}\{a_a^\dagger a_i\}\{a_b^\dagger a_j\}\right)_c$$

  Because there are four ways to contract operators, factor $\frac{1}{2}$ remains.

  According to the diagram rule, sign is positive (for two hole lines and two loops). Because two $\hat{T}_1$ are in the same form, symmetry factor is 1/2!. (이 경우 particle line들은 다른 operator와 amplitude를 연결하고 있으므로 equivalent가 아니다.)

16.4 CCD approximation

Simplification can be done with only 2p-2h correlations, $\hat{T} \simeq T_2$,

$$|\Psi_0\rangle \simeq |\Psi_{CCD}\rangle = \exp(\hat{T}_2)|\Phi_0\rangle \tag{16.36}$$

In this case, the ground state energy is

$$\begin{aligned} E_{CCD} &= \langle\Phi_0|e^{-\hat{T}_2}\hat{H}_N e^{\hat{T}_2}|\Phi_0\rangle = \langle\Phi_0|\hat{H}_N(1+\hat{T}_2)|\Phi_0\rangle \\ &= E_{ref} + \frac{1}{4}\sum_{abij}\langle ij|\hat{v}|ab\rangle t_{ij}^{ab} \end{aligned} \tag{16.37}$$

Note that CCD approximation corresponds to

$$\bar{H}_N|\Phi_0\rangle \simeq E_{CCD}|\Phi_0\rangle + \cdots \tag{16.38}$$

where additional terms are higher than 2p-2h excitations. Thus CCD is a similarity transformation plus a truncation, which decouples the ground state only from 2p-2h states.

CCD equations/diagrams

CCD equations for amplitudes

$$\langle\Phi_{ij}^{ab}|e^{-T_2}H_N e^{T_2}|\Phi_0\rangle = 0 \tag{16.39}$$

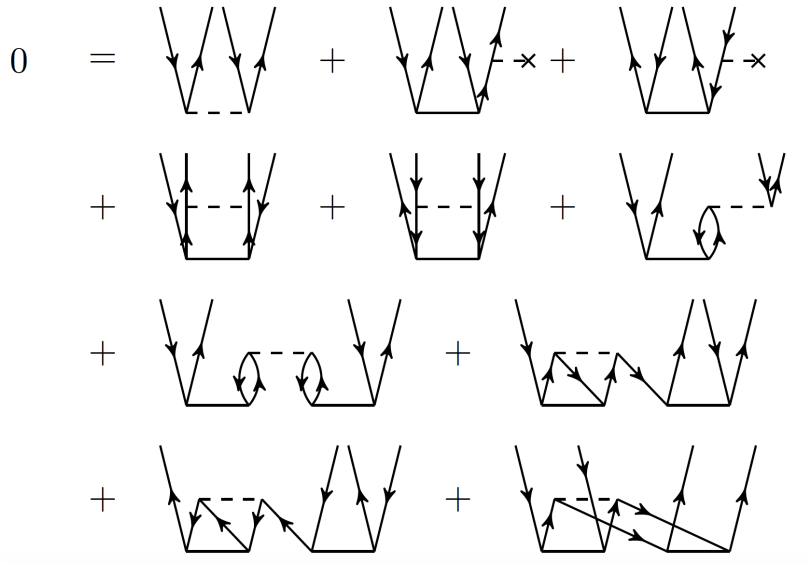


Figure 16.3: CCD equation

for all $i > j$ and all $a > b$.

It can be expressed as diagrams as

These comes from ($\hat{T}_2^3$ and higher orders are zero.)

$$0 = \langle \Phi_{ij}^{ab} | H_N | \Phi_0 \rangle + \langle \Phi_{ij}^{ab} | H_N T_2 | \Phi_0 \rangle + \frac{1}{2} \langle \Phi_{ij}^{ab} | H_N T_2^2 | \Phi_0 \rangle. \tag{16.40}$$

The first diagram is from the first term, 2nd-5th diagrams are from the second term, and other diagrams are from the third term.

Let us explicitly calculate CCD equations and diagrams.

- one can use symmetry of amplitudes and potential,

$$t_{ij}^{ab} = -t_{ji}^{ab} = -t_{ij}^{ba} = t_{ji}^{ba} \tag{16.41}$$

$$\langle ab|v|ij\rangle = -\langle ab|v|ji\rangle = -\langle ba|v|ij\rangle = \langle ba|v|ji\rangle \tag{16.42}$$

- the first term is obvious

$$\langle \Phi_{ij}^{ab} | H_N | \Phi_0 \rangle = \frac{1}{4} \sum_{pqrs} \langle \Phi_0 | \{a_i^\dagger a_j^\dagger a_b a_a\} \{a_p^\dagger a_q^\dagger a_s a_r\} | \Phi_0 \rangle_c = \langle ab|v|ij\rangle. \tag{16.43}$$

- The second term have two contributions,

$$\begin{aligned} \langle \Phi_{ij}^{ab} | F_N T_2 | \Phi_0 \rangle &= \frac{1}{4} \sum_{pq} \sum_{cdkl} f_q^p t_{kl}^{cd} \langle \Phi_{ij}^{ab} | \{a_p^\dagger a_q\} \{a_c^\dagger a_d^\dagger a_l a_k\} | \Phi_0 \rangle_c \\ &= \frac{1}{4} \sum_{pq} \sum_{cdkl} f_q^p t_{kl}^{cd} \langle \Phi_0 | \{a_i^\dagger a_j^\dagger a_b a_a\} \{a_p^\dagger a_q\} \{a_c^\dagger a_d^\dagger a_l a_k\} | \Phi_0 \rangle_c \end{aligned} \tag{16.44}$$

  If the amplitude operator contracts with particles, we have the second diagram. If the amplitude operator contracts with holes, we have the third diagram. Thus,

$$\langle \Phi_{ij}^{ab} | F_N T_2 | \Phi_0 \rangle \to P(ab) \sum_c f_c^b t_{ij}^{ac} - P(ij) \sum_k f_j^k t_{ik}^{ab}, \tag{16.45}$$

where $P(ab)$ and $P(ij)$ is to make the results to be antisymmetric with external index. In terms of diagram rules, the second term has negative sign because of 3-hole lines.

The other contribution is

$$\langle\Phi_{ij}^{ab}|V_N T_2|\Phi_0\rangle = \frac{1}{4}\frac{1}{4}\sum_{pqrs}\sum_{cdkl}\langle pq|v|rs\rangle t_{kl}^{cd}\langle\Phi_{ij}^{ab}|\{a_p^\dagger a_q^\dagger a_s a_r\}\{a_c^\dagger a_d^\dagger a_l a_k\}|\Phi_0\rangle_c \tag{16.46}$$

If external ab contracts with potential and external ij contracts with t_2 amplitude , we get the 4th diagram. If external ab contracts with amplitude and external ij contracts with potential, we get 5th diagram. If external ij contracts with both potential and amplitude, we get 6th diagram. Thus,

$$\langle\Phi_{ij}^{ab}|V_N T_2|\Phi_0\rangle \to +\frac{1}{2}\sum_{cd}\langle ab|\hat{v}|cd\rangle t_{ij}^{cd} + \frac{1}{2}\sum_{kl}\langle kl|\hat{v}|ij\rangle t_{kl}^{ab} + \hat{P}(ij|ab)\sum_{kc}\langle kb|\hat{v}|cj\rangle t_{ik}^{ac} \tag{16.47}$$

signs are all positive (two hole lines, four hole lines, 3-hole lines and 1-loop). One can count the symmetry factor is 1/2 for 4-th (two equivalent particle lines), and 5-th (two equivalent hole lines) diagrams. No equivalent lines for 6-th. The last contribution have to be anti-symmetrized.

- Some diagrams can be topologically equivalent even though they looks very different. One can exchange two incoming/outgoing lines in left and right side of operator. If one can get a loop by exchanging lines, it is better to use diagram with loop.

- Let us split the third term.

$$\frac{1}{2}\langle\Phi_{ij}^{ab}|F_N T_2^2|\Phi_0\rangle + \frac{1}{2}\langle\Phi_{ij}^{ab}|V_N T_2^2|\Phi_0\rangle \tag{16.48}$$

The first contribution is zero because no contraction is possible. Then,

$$\begin{aligned}\frac{1}{2}\langle\Phi_{ij}^{ab}|V_N T_2^2|\Phi_0\rangle &= \frac{1}{2}\frac{1}{4}\frac{1}{4}\frac{1}{4}\sum_{pqrs}\sum_{cdkl}\sum_{efmn}\langle pq|v|rs\rangle t_{kl}^{cd}t_{mn}^{ef} \\ &\times\langle\Phi_0|\{a_i^\dagger a_j^\dagger a_b a_a\}\{a_p^\dagger a_q^\dagger a_s a_r\}\{a_c^\dagger a_d^\dagger a_l a_k\}\{a_e^\dagger a_f^\dagger a_n a_m\}|\Phi_0\rangle\end{aligned} \tag{16.49}$$

Because there are 4-particle operators but external has only 2-particles, 2-particles must contract with potential. (Same for holes.) Thus, potential cannot contract with external lines.

If external ai and bj contracts to different amplitudes, we get the 7-th diagram. If external i and abj contracts to different amplitudes, we get 8-th diagram. If external a and bij contacts to different amplitudes, we get 9-th diagram. If external ab and ij contracts to different amplitudes, we get 10-th diagram.

Thus,

$$\begin{aligned}\frac{1}{2}\langle\Phi_{ij}^{ab}|V_N T_2^2|\Phi_0\rangle \to\ & +\frac{1}{2}\hat{P}(ij|ab)\sum_{klcd}\langle kl|\hat{v}|cd\rangle t_{ik}^{ac}t_{jl}^{bd} \\ & +\frac{1}{2}\hat{P}(ij)\sum_{klcd}\langle kl|\hat{v}|cd\rangle t_{ik}^{cd}t_{lj}^{ab} + \frac{1}{2}\hat{P}(ab)\sum_{klcd}\langle kl|\hat{v}|cd\rangle t_{kl}^{ac}t_{ij}^{db} \\ & +\frac{1}{4}\sum_{klcd}\langle kl|\hat{v}|cd\rangle t_{ij}^{cd}t_{kl}^{ab}\end{aligned} \tag{16.50}$$

For 7-th diagram, sign is positive and symmetry factor is 1/2 (from two symmetric T_2 amplitudes). For 8-th diagram, sign is positive(4 hole lines and no-loop) and symmetry factor is 1/2(two T_2 are not symmetric. There is one equivalent pair of particle line.). For 9-th diagram, sign is positive(4 hole lines and no-loop) and symmetry factor is 1/2(two T_2 are not symmetric. There is one equivalent pair of hole line.). For 10-th diagram, sign is positive and symmetry factor is 1/4 (two T_2 are not symmetric. There are two pairs of equivalent lines.)

In summary, (all 10 terms),

$$\begin{aligned} 0 &= \langle ab|\hat{v}|ij\rangle + P(ab)\sum_c f_c^b t_{ij}^{ac} - P(ij)\sum_k f_j^k t_{ik}^{ab} \\ &+\frac{1}{2}\sum_{cd}\langle ab|\hat{v}|cd\rangle t_{ij}^{cd} + \frac{1}{2}\sum_{kl}\langle kl|\hat{v}|ij\rangle t_{kl}^{ab} \\ &+\hat{P}(ij|ab)\sum_{kc}\langle kb|\hat{v}|cj\rangle t_{ik}^{ac} \\ &+\frac{1}{2}\hat{P}(ij|ab)\sum_{klcd}\langle kl|\hat{v}|cd\rangle t_{ik}^{ac} t_{jl}^{bd} \\ &+\frac{1}{2}\hat{P}(ij)\sum_{klcd}\langle kl|\hat{v}|cd\rangle t_{ik}^{cd} t_{lj}^{ab} + \frac{1}{2}\hat{P}(ab)\sum_{klcd}\langle kl|\hat{v}|cd\rangle t_{kl}^{ac} t_{ij}^{db} \\ &+\frac{1}{4}\sum_{klcd}\langle kl|\hat{v}|cd\rangle t_{ij}^{cd} t_{kl}^{ab} \end{aligned} \tag{16.51}$$

(In HF basis, f is diagonal and the second and third terms cancels out.)

How to solve CCD equation

Above non-linear equations can be solved by iterative methods. For example, one may start from guess of amplitudes

$$(t_{ij}^{ab})^{(0)} = \frac{\langle ab|v|ij\rangle}{(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b)} \tag{16.52}$$

and then iterate to update t_{ij}^{ab}. (Here $\epsilon_i = f_i^i$ for Fock operator.)

Actual implementation of CCD equation, requires some additional technique. One can linearize the equation for amplitudes by introducing 'intermediates'. (The exact form is only for CCD approximation. In case of CCSD, one needs different definitions)

- Diagram 7

$$+\frac{1}{2}\hat{P}(ij|ab)\sum_{klcd}\langle kl|\hat{v}|cd\rangle t_{ik}^{ac} t_{jl}^{bd} \to \frac{1}{2}\hat{P}(ij|ab)\sum_{ld}\chi_{id}^{al} t_{lj}^{db} \tag{16.53}$$

  with (intermediate for 'phph' type)

$$\chi_{id}^{al} = \sum_{kc}\langle kl|\hat{v}|cd\rangle t_{ik}^{ac} \tag{16.54}$$

- Diagram 8

$$+\frac{1}{2}\hat{P}(ij)\sum_{klcd}\langle kl|\hat{v}|cd\rangle t_{ik}^{cd} t_{lj}^{ab} \to -P(ij)\sum_{l}\chi_i^l t_{lj}^{ab} \tag{16.55}$$

  with (intermediate for 'hh' type)

$$\chi_i^l = -\frac{1}{2}\sum_{kcd}\langle kl|v|cd\rangle t_{ik}^{cd} \tag{16.56}$$

- Diagram 9

$$+\frac{1}{2}\hat{P}(ab)\sum_{klcd}\langle kl|\hat{v}|cd\rangle t_{kl}^{ac} t_{ij}^{db} \to P(ab)\sum_{d}\chi_d^a t_{ij}^{db} \tag{16.57}$$

with (intermediate for 'pp' type)

$$\chi_d^a = \frac{1}{2}\sum_{kcl}\langle kl|v|cd\rangle t_{kl}^{ac} \tag{16.58}$$

- Diagram 10 or the last term of equation can be expressed as

$$+\frac{1}{4}\sum_{klcd}\langle kl|\hat{v}|cd\rangle t_{ij}^{cd}t_{kl}^{ab} \rightarrow \frac{1}{2}\sum_{kl}\chi_{ij}^{kl}t_{kl}^{ab} \tag{16.59}$$

with (intermediate for 'hhhh' type)

$$\chi_{ij}^{kl} = \frac{1}{2}\sum_{cd}\langle kl|v|cd\rangle t_{ij}^{cd} \tag{16.60}$$

Then, after using intermediates, we get CCD equation as

$$\begin{aligned}
0 &= \langle ab|\hat{v}|ij\rangle + P(ab)\sum_c f_c^b t_{ij}^{ac} - P(ij)\sum_k f_j^k t_{ik}^{ab} \\
&+\frac{1}{2}\sum_{cd}\langle ab|\hat{v}|cd\rangle t_{ij}^{cd} + \frac{1}{2}\sum_{kl}\langle kl|\hat{v}|ij\rangle t_{kl}^{ab} \\
&+\hat{P}(ij|ab)\sum_{kc}\langle kb|\hat{v}|cj\rangle t_{ik}^{ac} \\
&+\frac{1}{2}\hat{P}(ij|ab)\sum_{ld}\chi_{id}^{al}t_{lj}^{db} \\
&-\hat{P}(ij)\sum_l \chi_i^l t_{lj}^{ab} + \hat{P}(ab)\sum_d \chi_d^a t_{ij}^{db} \\
&+\frac{1}{2}\sum_{kl}\chi_{ij}^{kl}t_{kl}^{ab}
\end{aligned} \tag{16.61}$$

This equation is solved in iterative way as

$$(t_{ij}^{ab})_{new} = (t_{ij}^{ab(n)})_{old} + \frac{\bar{H}_{ij}^{ab}}{f_i^i + f_j^j - f_a^a - f_b^b} \tag{16.62}$$

In reality, it is better to use mixed update with fraction x,

$$(t_{ij}^{ab}) \leftarrow x(t_{ij}^{ab})_{new} + (1-x)(t_{ij}^{ab(n)})_{old} \tag{16.63}$$

16.5 CCSD equations

Let us look at the full CCSD equation(without three-body interaction) Following expressions are obtained by symPy program.

- $\langle\Phi_0|\bar{H}_N|\Phi_0\rangle = 0$ gives CCSD correlation energy expression.
- $\langle\Phi_i^a|\bar{H}_N|\Phi_0\rangle = 0$.

$$\begin{aligned}
0 &= f_i^a + t_{ik}^{ac}\left(f_c^k + v_{dc}^{lk}t_l^d\right) + t_i^c\left(f_c^a + t_k^d v_{dc}^{ka}\right) \\
&-t_k^a f_i^k + t_k^a t_l^c v_{ic}^{lk} + \frac{t_k^a t_{il}^{cd}v_{cd}^{lk}}{2} - t_k^a t_i^c f_c^k \\
&+t_k^c v_{ic}^{ak} \\
&-\frac{t_i^c t_{kl}^{ad}v_{cd}^{kl}}{2} + \frac{t_{ik}^{cd}v_{cd}^{ak}}{2} - \frac{t_{kl}^{ac}v_{ic}^{kl}}{2} - t_l^a t_k^c t_i^d v_{cd}^{kl}
\end{aligned} \tag{16.64}$$

- $\langle \Phi_{ij}^{ab} | \bar{H}_N | \Phi_0 \rangle = 0$.

$$
\begin{aligned}
0 \;=\;& f_c^k t_i^c t_{jk}^{ab} P(ij) + f_c^k t_k^a t_{ij}^{bc} P(ab) + f_i^k t_{jk}^{ab} P(ij) \\
& - f_c^a t_{ij}^{bc} P(ab) + t_k^c t_i^d t_{jl}^{ab} v_{cd}^{kl} P(ij) + t_k^c t_l^a t_{ij}^{bd} v_{cd}^{kl} P(ab) \\
& - t_k^c t_{ij}^{ad} v_{cd}^{bk} P(ab) + t_k^c t_{il}^{ab} v_{jc}^{kl} P(ij) + t_i^c t_j^d t_k^a t_l^b v_{cd}^{kl} + t_i^c t_j^d t_k^a v_{cd}^{bk} P(ab) \\
& + \frac{t_i^c t_j^d t_{kl}^{ab} v_{cd}^{kl}}{2} + t_i^c t_j^d v_{cd}^{ab} - t_i^c t_k^a t_l^b v_{jc}^{kl} P(ij) \\
& - t_i^c t_k^a t_{jl}^{bd} v_{cd}^{kl} P(ab) P(ij) - t_i^c t_k^a v_{jc}^{bk} P(ab) P(ij) - t_i^c t_{jk}^{ad} v_{cd}^{bk} P(ab) P(ij) \\
& - \frac{t_i^c t_{kl}^{ab} v_{jc}^{kl} P(ij)}{2} - t_i^c v_{jc}^{ab} P(ij) \\
& + \frac{t_k^a t_l^b t_{ij}^{cd} v_{cd}^{kl}}{2} + t_k^a t_l^b v_{ij}^{kl} + \frac{t_k^a t_{ij}^{cd} v_{cd}^{bk} P(ab)}{2} + t_k^a t_{il}^{bc} v_{jc}^{kl} P(ab) P(ij) + t_k^a v_{ij}^{bk} P(ab) \\
& + \frac{t_{ij}^{cd} t_{kl}^{ab} v_{cd}^{kl}}{4} + \frac{t_{ij}^{cd} v_{cd}^{ab}}{2} + \frac{t_{jk}^{cd} t_{il}^{ab} v_{cd}^{kl} P(ij)}{2} + t_{ik}^{ac} v_{jc}^{bk} P(ab) P(ij) \\
& - \frac{t_{ij}^{ac} t_{kl}^{bd} v_{cd}^{kl} P(ab)}{2} - t_{jk}^{ac} t_{il}^{bd} v_{cd}^{kl} P(ab) + \frac{t_{kl}^{ab} v_{ij}^{kl}}{2} + v_{ij}^{ab}
\end{aligned}
\tag{16.65}
$$

- With **intermediates**, the sum of intermediates and amplitude is similar to

$$C_{ij} = \sum_k A_{ik} B_{kj} \tag{16.66}$$

matrix multiplication with mapping $kl \to K$, $ij \to I$, $cd \to C$. One can use BLAS for matrix multiplication.

Intermediates are defined as

$$\langle b|\chi|c\rangle = \langle b|f|c\rangle - \frac{1}{2}\sum_{kld} \langle bd|t|kl\rangle\langle kl|v|cd\rangle \tag{16.67}$$

$$\langle k|\chi|j\rangle = \langle k|f|j\rangle + \frac{1}{2}\sum_{cdl} \langle kl|v|cd\rangle\langle cd|t|jl\rangle \tag{16.68}$$

$$\langle k|\chi|c\rangle = \langle k|f|c\rangle + \frac{1}{2}\sum_{ld} \langle kl|v|cd\rangle\langle d|t|l\rangle \tag{16.69}$$

$$\langle kl|\chi|ij\rangle = \langle kl|v|ij\rangle + \frac{1}{2}\sum_{cd} \langle kl|v|cd\rangle\langle cd|t|ij\rangle \tag{16.70}$$

$$\langle kb|\chi|cj\rangle = \langle kb|v|cj\rangle + \frac{1}{2}\sum_{dl} \langle kl|v|cd\rangle\langle db|t|lj\rangle \tag{16.71}$$

$$\langle ab|\chi|cd\rangle = \langle ab|v|cd\rangle \tag{16.72}$$

Then, CCSD equation becomes

$$0 = \tag{16.73}$$

$$0 = \tag{16.74}$$

16.6 Minnesota potential

$$V(r) = \frac{1}{2}\left(V_R + \frac{1}{2}(1+P_{12}^{\sigma})V_T + \frac{1}{2}(1-P_{12}^{\sigma})V_S\right)(1-P_{12}^{\sigma}P_{12}^{\tau}) \tag{16.75}$$

where

$$V_\alpha(r) = V_\alpha \exp(-\alpha r^2) \tag{16.76}$$

with coefficients,

$$\begin{aligned} V_R &= 200 \text{ MeV}, \alpha_R = 1.487 \text{ fm}^{-2}, \\ V_T &= 178 \text{ MeV}, \alpha_T = 0.639 \text{ fm}^{-2}, \\ V_S &= 91.85 \text{ MeV}, \alpha_S = 0.465 \text{ fm}^{-2}. \end{aligned} \tag{16.77}$$

The matrix element in momentum,

$$(\boldsymbol{k}_p\boldsymbol{k}_q|V_\alpha|\boldsymbol{k}_r\boldsymbol{k}_s) = \frac{V_\alpha}{L^3}\left(\frac{\pi}{\alpha}\right)^{3/2}\exp(\frac{-q^2}{4\alpha})\delta_{\boldsymbol{k}_p+\boldsymbol{k}_q,\boldsymbol{k}_r+\boldsymbol{k}_s}, \quad \boldsymbol{q} = \frac{1}{2}(\boldsymbol{k}_p - \boldsymbol{k}_q - \boldsymbol{k}_r + \boldsymbol{k}_s) \tag{16.78}$$

For neutron matter, only $\alpha = R, S$ contributes. Including spin,

$$(k_p s_p, k_q s_q|V_\alpha|k_r s_r, k_s s_s) = (\boldsymbol{k}_p\boldsymbol{k}_q|V_\alpha|\boldsymbol{k}_r\boldsymbol{k}_s)\frac{1}{2}\left(\delta_{s_p}^{s_r}\delta_{s_q}^{s_s} - \delta_{s_p}^{s_s}\delta_{s_q}^{s_r}\right), \tag{16.79}$$

Note that the matrix elements are not anti-symmetrized. One have to use

$$\langle k_p s_p, k_q s_q|V_\alpha|k_r s_r, k_s s_s\rangle_{AS} = (k_p s_p, k_q s_q|V_\alpha|k_r s_r, k_s s_s) - (k_p s_p, k_q s_q|V_\alpha|k_s s_s, k_r s_r) \tag{16.80}$$

- To store $\langle pq|v|rs\rangle$ or $\langle ab|t|ij\rangle$, it is useful to use 1-dimensional arrays, instead of 4-dimensional arrays. such that

$$index(p,q,r,s) = p \times N_{sp}^3 + q \times N_{sp}^2 + r \times N_{sp} + s \tag{16.81}$$

- But, in this index space, $v(index)$, $t(index)$ may have many zeroes.
- For neutron matter, one have to use channel structure. Thus, interaction is written as $v_{\sigma_1\sigma_2}^{\sigma_s igma_3}(\boldsymbol{p},\boldsymbol{k})$ instead of $v_{\sigma_1\sigma_2}^{\sigma_s igma_3}(\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4)$. In a similar way, amplitude is $t_{\sigma_1\sigma_2}^{\sigma_s igma_3}(\boldsymbol{Q};\boldsymbol{p},\boldsymbol{k})$. Notice $\boldsymbol{Q}$ in amplitude.
- Because of momentum conservation, it has block structure for each total momentum. For neutron matter, CCD correlation energy becomes for total momentum P_{ij} and relative momentum k_{ij}

$$E_c = \frac{1}{4}\sum_{P_{ij}}\sum_{k_{ij}s_is_j}\sum_{k_{ab}s_as_b} t(P_{ij})_{k_{ij}s_is_j}^{k_{ab}s_as_b} V(P_{ij})_{k_{ij}s_is_j}^{k_{ab}s_as_b} \tag{16.82}$$

Neutron matter code is structured as

- For a given density and UV cutoff, set up the lattice, i.e. determine the single-particle basis.
- Determine the channels allowed by the (Minnesota) interaction, i.e. sets of two-body states that are connected by the interaction.
- Exploit this channel structure when computing the diagrams.

- Solve the coupled-cluster equations.

$$
\begin{aligned}
0 \;=\;& +f_i^a - f_c^k t_i^c t_k^a + f_c^k t_{ik}^{ac} - f_i^k t_k^a + f_c^a t_i^c \\
& -t_k^c t_i^d t_l^a v_{cd}^{kl} - t_k^c t_i^d v_{cd}^{ak} \\
& +t_k^c t_l^a v_{ic}^{kl} + t_k^c t_{il}^{ad} v_{cd}^{kl} \\
& +t_k^c v_{ic}^{ak} \\
& -\frac{t_i^c t_{kl}^{ad} v_{cd}^{kl}}{2} + \frac{t_l^a t_{ik}^{cd} v_{cd}^{kl}}{2} + \frac{t_{ik}^{cd} v_{cd}^{ak}}{2} - \frac{t_{kl}^{ac} v_{ic}^{kl}}{2}
\end{aligned}
\tag{16.83}
$$

$$
\begin{aligned}
0 \;=\;& f_c^k t_i^c t_{jk}^{ab} P(ij) + f_c^k t_k^a t_{ij}^{bc} P(ab) \\
& +f_i^k t_{jk}^{ab} P(ij) - f_c^a t_{ij}^{bc} P(ab) \\
& +t_k^c t_i^d t_{jl}^{ab} v_{cd}^{kl} P(ij) + t_k^c t_l^a t_{ij}^{bd} v_{cd}^{kl} P(ab) \\
& -t_k^c t_{ij}^{ad} v_{cd}^{bk} P(ab) + t_k^c t_{il}^{ab} v_{jc}^{kl} P(ij) + t_i^c t_j^d t_k^a t_l^b v_{cd}^{kl} + t_i^c t_j^d t_k^a v_{cd}^{bk} P(ab) \\
& +\frac{t_i^c t_j^d t_{kl}^{ab} v_{cd}^{kl}}{2} + t_i^c t_j^d v_{cd}^{ab} \\
& -t_i^c t_k^a t_l^b v_{jc}^{kl} P(ij) - t_i^c t_k^a t_{jl}^{bd} v_{cd}^{kl} P(ab) P(ij) \\
& -t_i^c t_k^a v_{jc}^{bk} P(ab) P(ij) - t_i^c t_{jk}^{ad} v_{cd}^{bk} P(ab) P(ij) \\
& -\frac{t_i^c t_{kl}^{ab} v_{jc}^{kl} P(ij)}{2} - t_i^c v_{jc}^{ab} P(ij) \\
& +\frac{t_k^a t_l^b t_{ij}^{cd} v_{cd}^{kl}}{2} + t_k^a t_l^b v_{ij}^{kl} \\
& +\frac{t_k^a t_{ij}^{cd} v_{cd}^{bk} P(ab)}{2} + t_k^a t_{il}^{bc} v_{jc}^{kl} P(ab) P(ij) \\
& +t_k^a v_{ij}^{bk} P(ab) \\
& +\frac{t_{ij}^{cd} t_{kl}^{ab} v_{cd}^{kl}}{4} + \frac{t_{ij}^{cd} v_{cd}^{ab}}{2} \\
& +\frac{t_{jk}^{cd} t_{il}^{ab} v_{cd}^{kl} P(ij)}{2} + t_{ik}^{ac} v_{jc}^{bk} P(ab) P(ij) \\
& -\frac{t_{ij}^{ac} t_{kl}^{bd} v_{cd}^{kl} P(ab)}{2} - t_{jk}^{ac} t_{il}^{bd} v_{cd}^{kl} P(ab) \\
& +\frac{t_{kl}^{ab} v_{ij}^{kl}}{2} + v_{ij}^{ab}
\end{aligned}
\tag{16.84}
$$

Chapter 17

EDFT

17.1 Note: 2016.08.30. Summary of PCPK1 paper?

- Lagrangian

$$\begin{aligned}
\mathcal{L} &= \mathcal{L}^{free} + \mathcal{L}^{4f} + \mathcal{L}^{hot} + \mathcal{L}^{der} + \mathcal{L}^{em} \\
\mathcal{L}^{free} &= \bar{\psi}(i\gamma_\mu \partial^\mu - m)\psi, \\
\mathcal{L}^{4f} &= -\frac{1}{2}\alpha_S(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) \\
&\quad -\frac{1}{2}\alpha_{TS}(\bar{\psi}\vec{\tau}\psi)(\bar{\psi}\vec{\tau}\psi) - \frac{1}{2}\alpha_{TV}(\bar{\psi}\vec{\tau}\gamma_\mu\psi)(\bar{\psi}\vec{\tau}\gamma^\mu\psi), \\
\mathcal{L}^{hot} &= -\frac{1}{3}\beta_S(\bar{\psi}\psi)^3 - \frac{1}{4}\gamma_S(\bar{\psi}\psi)^4 - \frac{1}{4}\gamma_V[(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi)]^2, \\
\mathcal{L}^{der} &= -\frac{1}{2}\delta_S\partial_\nu(\bar{\psi}\psi)\partial^\nu(\bar{\psi}\psi) - \frac{1}{2}\delta_V\partial_\nu(\bar{\psi}\gamma_\mu\psi)\partial^\nu(\bar{\psi}\gamma^\mu\psi) \\
&\quad -\frac{1}{2}\delta_{TS}\partial_\nu(\bar{\psi}\vec{\tau}\psi)\partial^\nu(\bar{\psi}\vec{\tau}\psi) - \frac{1}{2}\delta_{TV}\partial_\nu(\bar{\psi}\vec{\tau}\gamma_\mu\psi)\partial^\nu(\bar{\psi}\vec{\tau}\gamma^\mu\psi), \\
\mathcal{L}^{em} &= -\frac{1}{4}F^{\mu\nu}F^{\mu\nu} - e\frac{1-\tau_3}{2}\bar{\psi}\gamma^\mu\psi A_\mu.
\end{aligned} \tag{17.1}$$

- RMF: replace operator by their expectation values

$$\bar{\psi}(\hat{O}\Gamma)_i\psi \to \langle\Phi|\bar{\psi}(\hat{O}\Gamma)_i\psi|\Phi\rangle = \sum_k v_k^2\bar{\psi}_k(\hat{O}\Gamma)_i\psi_k \tag{17.2}$$

  where, sum is over positive energy states with occupation probability v_k^2 and ψ_k is a single particle wave function for state k.

- EDF:

$$E_{tot} = \mathcal{E}_{EDF}[\boldsymbol{\tau}, \rho_S, j_i^\mu, A_\mu] + E_{pair}[\kappa, \kappa^*] + E_{c.m.}^{mic} \tag{17.3}$$

  with

$$\mathcal{E}_{EDF}[\boldsymbol{\tau}, \rho_S, j_i^\mu, A_\mu] = \int d^3r\mathcal{E}(\boldsymbol{r}), \quad \mathcal{E}(\boldsymbol{r}) = \mathcal{E}^{kin}(\boldsymbol{r}) + \mathcal{E}^{int}(\boldsymbol{r}) + \mathcal{E}^{em}(\boldsymbol{r}). \tag{17.4}$$

$$
\begin{aligned}
\mathcal{E}^{kin}(\boldsymbol{r}) &= \sum_k v_k^2 \psi_k^\dagger(\boldsymbol{r})(\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta m)\psi_k, \\
\mathcal{E}^{int}(\boldsymbol{r}) &= \frac{\alpha_S}{2}\rho_S^2 + \frac{\beta_S}{3}\rho_S^3 + \frac{\gamma_S}{4}\rho_S^4 + \frac{\delta_S}{2}\rho_S\Delta\rho_S \\
&\quad + \frac{\alpha_V}{2} j_\mu j^\mu + \frac{\gamma_V}{4}(j_\mu j^\mu)^2 + \frac{\delta_V}{2} j_\mu \Delta j^\mu + \frac{\alpha_{TV}}{2}(\vec{j}_{TV})^\mu\cdot(\vec{j}_{TV})_\mu + \frac{\delta_{TV}}{2}(\vec{j}_{TV})^\mu\cdot\Delta(\vec{j}_{TV})_\mu, \\
\mathcal{E}^{em}(\boldsymbol{r}) &= \frac{1}{4}F_{\mu\nu}F^{\mu\nu} - F^{0\mu}\partial_0 A_\mu + eA_\mu j_p^\mu. \qquad (17.5)
\end{aligned}
$$

- Local densities and currents

$$
\begin{aligned}
\rho_S(\boldsymbol{r}) &= \sum_k v_k^2 \bar{\psi}_k(\boldsymbol{r})\psi_k(\boldsymbol{r}), \\
j_V^\mu(\boldsymbol{r}) &= \sum_k v_k^2 \bar{\psi}_k(\boldsymbol{r})\gamma^\mu\psi_k(\boldsymbol{r}), \\
\vec{j}_{TV}^\mu(\boldsymbol{r}) &= \sum_k v_k^2 \bar{\psi}_k(\boldsymbol{r})\vec{\tau}\gamma^\mu\psi_k(\boldsymbol{r}) \qquad (17.6)
\end{aligned}
$$

- Pairing: Density independent δ force in the pairing channel is adopted

$$
E_{pair}[\kappa,\kappa^*] = -\sum_{\tau=n,p}\frac{V_\tau}{4}\int d^3r \kappa_\tau^*(\boldsymbol{r})\kappa_\tau(\boldsymbol{r}), \qquad (17.7)
$$

$$
\kappa(\boldsymbol{r}) = -2\sum_{k>0} f_k u_k v_k |psi_k(\boldsymbol{r})|^2. \qquad (17.8)
$$

  with cutoff weighting factor

$$
f_k = \frac{1}{1+\exp[(\epsilon_k-\epsilon_F-\Delta E_\tau)/\mu_\tau]}, \qquad (17.9)
$$

- center of mass correction

$$
E_{c.m.}^{mic} = -\frac{1}{2mA}\langle \hat{\boldsymbol{P}}_{c.m.}^2\rangle, \quad \hat{\boldsymbol{P}}_{c.m.} = \sum_i^A \hat{p}_i \qquad (17.10)
$$

- From above expression, if we know
  - coefficients of Lagrangian (α's , β's and so on)
  - single particle states k and occupation probability v_k and u_k
  - single particle wave function $\psi_k(\boldsymbol{r})$. Note that this would be a four component wave function.
  - single particle energy ϵ_k
  - EM field $A_\mu(\boldsymbol{r})$
  - chemical potential ϵ_F
  - V_τ, ΔE_τ, μ_τ.

  we can compute energy density and its total energy. Now the problem is how to determine them.

Some of parameters can be determined once other quantities are determined.

- k is determined by the shell model assumption. Number of single particle shells.
- the chemical potential ϵ_F can be fixed by the condition, $\langle\Phi|\hat{N}_\tau|\Phi\rangle = N_\tau$, particle number of neutrons and protons.
- ΔE_τ and $\mu_\tau = \Delta E_\tau/10$ can be determined by choice $2\sum_{k>0} f_k = N_\tau + 1.65N_\tau^{2/3}$.
- V_τ can be adjusted by fiting the average single-particle pairing gap to the data,

$$\langle\Delta\rangle \equiv \frac{\sum_k f_k u_k v_k \Delta_k}{f_k u_k v_k} \tag{17.11}$$

  where Δ_k is known from $u_k, v_k, \psi_k(?)$.
- single particle level, energy and wave function is determined by solving

$$[\gamma_\mu(i\partial^\mu - V^\mu) - (m+S)]\psi_k = 0. \tag{17.12}$$

  with

$$S(\boldsymbol{r}) = \Sigma_S, \quad V^\mu(\boldsymbol{r}) = \Sigma^\mu + \vec{\tau}\cdot\vec{\Sigma}^\mu_{TV}, \tag{17.13}$$

  When solving these equation one assumes that the $S(\boldsymbol{r})$ and $V^\mu(\boldsymbol{r})$ is already known.
- In practice, single particle equation have to be solved self-consistently with single particle wave functions ψ_k, v_k

$$\begin{aligned}
\Sigma_S &= \alpha_S\rho_S + \beta_S\rho_S^2 + \gamma_S\rho_S^3 + \delta_S\Delta\rho_S, \\
\Sigma^\mu &= \alpha_V j_V^\mu + \gamma_V (j_V^\mu)^3 + \delta_V \Delta j_V^\mu + eA^\mu, \\
\vec{\Sigma}^\mu_{TV} &= \alpha_{TV}\vec{j}^\mu_{TV} + \delta_{TV}\Delta\vec{j}^\mu_{TV}.
\end{aligned} \tag{17.14}$$

  Also, assumming time-reversal invariance, only j_i^0, $V^0(\boldsymbol{r})$ are non-zero. Also, only third component of iso-vector τ_3 survives. Coulomb field A_0 is determined by the Poisson's equation.

  In BCS approximation, $v_k = \frac{1}{2}\left(1 - \frac{\epsilon_k - \epsilon_F}{\sqrt{(\epsilon_k-\epsilon_F)^2+\Delta_k^2}}\right)$.

Chapter 18

IM-SRG

18.1 Similarity Renormalization Group

For unitary operator $\hat{U}_\alpha$, where α is a flow parameter, $\hat{U}_\alpha^\dagger \hat{U}_\alpha = 1$, unitary transformation of Hamiltonian,

$$\begin{aligned}
\hat{H}_\alpha &\equiv \hat{U}_\alpha^\dagger \hat{H}_0 \hat{U}_\alpha, \\
\frac{d\hat{H}_\alpha}{d\alpha} &= \frac{d}{d\alpha}(\hat{U}_\alpha^\dagger \hat{H}_0 \hat{U}_\alpha) = \frac{d\hat{U}_\alpha^\dagger}{d\alpha}\hat{H}_0\hat{U}_\alpha + \hat{U}_\alpha^\dagger \hat{H}_0 \frac{d\hat{U}_\alpha}{d\alpha}, \\
&= \left(-\hat{U}_\alpha^\dagger \frac{d\hat{U}_\alpha}{d\alpha}\hat{U}_\alpha^\dagger\right)\hat{H}_0\hat{U}_\alpha + \hat{U}_\alpha^\dagger \hat{H}_0 \hat{U}_\alpha \hat{U}_\alpha^\dagger \frac{d\hat{U}_\alpha}{d\alpha}, \quad \text{(from Unitarity)} \\
&= -\hat{U}_\alpha^\dagger \frac{d\hat{U}_\alpha}{d\alpha}\hat{H}_\alpha + \hat{H}_\alpha \hat{U}_\alpha^\dagger \frac{d\hat{U}_\alpha}{d\alpha} \\
&\equiv [\hat{\eta}_\alpha, \hat{H}_\alpha] \qquad (18.1)
\end{aligned}$$

Thus, flow equation with generator $\hat{\eta}_\alpha$,

$$\frac{d\hat{H}_\alpha}{d\alpha} = [\hat{\eta}_\alpha, \hat{H}_\alpha], \quad \hat{\eta}_\alpha = -\hat{U}_\alpha^\dagger \frac{d\hat{U}_\alpha}{d\alpha}. \qquad (18.2)$$

where, generator is anti-hermitian, $\hat{\eta}_\alpha^\dagger = -\hat{\eta}_\alpha$. The choice of generator is to determine the nature of transformation.

- one may choose $\hat{\eta}_\alpha = [\hat{G}_\alpha, \hat{H}_\alpha]$ with hermitian operator $\hat{G}_\alpha$,

  $$\hat{G}_\alpha = \hat{H}_\alpha^{diag} = \sum_i \langle i|\hat{H}_\alpha|i\rangle |i\rangle\langle i|. \qquad (18.3)$$

  This choice makes the generator $\hat{\eta}_\alpha$ vanishes as soon as $\hat{H}_\alpha$ becomes diagonal.

- The other choice of intrinsic kinetic energy, $\hat{G}_\alpha = \hat{T}_{int}$, leads to

  $$\hat{\eta}_\alpha = (2\mu)^2 [\hat{T}_{int}, \hat{H}_\alpha] \qquad (18.4)$$

  with reduced mass $\mu = m_N/2$.

Disadvantage of the SRG is the generation of irreucible higher-oerder forces(induced higher body forces). One have to choose a resonable tradeoff between pre-diagonalization and higher-order contributions. Once SRG is done for Hamiltoninan, the same SRG have to be applied to operators.

Chapter 19

Numerical practice

One have to so tests

- Validation test : can code reproduce known results?
- unit test : each part of the code acts correctly?
- integration test: how each components work together?

Optimization ideas for MBPT code

- Use symmetry: introduce channel structure so that only non-zero block of potential is calculated.
- Store some intermediates in memory. (reduce redundant calls.)
- reduce number of evaluation of functions.
- use parallelism. (openMp and MPI)