Nuclear Many-Body Theory in "occupation number representation" (2nd quant.)

So far, we have discussed the nuclear many-body problem in coordinate space, including spin and isospin degrees of freedom; using the shorthand notations

$$x \equiv (\vec{r}, s_z, t_z) \qquad (1a)$$

$$\int dx \equiv \int d^3r \sum_{s_z=-\frac{1}{2}}^{+\frac{1}{2}} \sum_{t_z=-\frac{1}{2}}^{+\frac{1}{2}} . \qquad (1b)$$

The many-particle Schrödinger eq. has the structure

$$\left[H(1,\dots,A) - i\hbar \frac{\partial}{\partial t} \right] \psi(1,\dots,A;t) = 0 \qquad (2a)$$

with

$$H = \sum_{i=1}^{A} -\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} \sum_{i,j=1}^{A} v_{ij}^{(2)}(x_i,x_j) + \frac{1}{6} \sum_{i,j,k=1}^{A} v_{ijk}^{(3)}(x_i,x_j,x_k) \qquad (2b)$$

According to Pauli's spin-statistic theorem, the many-body WF $\psi(1,\dots,A;t)$ has to be antisymmetric under the interchange of any particle coordinate $x_i \leftrightarrow x_j$. We have seen that Slater-determinants composed of single-particle basis states $\varphi_i(x) \equiv \langle x|i\rangle$ have this property; suppose we order the s.p. states according to their energy:

$$E_1 < E_2 < E_3 \dots < E_N < E_{N+1} \dots \qquad (3a)$$

According to the Pauli principle, no quantum state $|i\rangle$

can be occupied by more than one particle, i.e. the particle numbers allowed are

$$n_i = 0 \text{ or } 1 \tag{3b}$$

To avoid confusion, we clarify that the kets $|i\rangle$ are a shorthand notation for <u>all</u> quantum numbers. <u>For example</u>, in the <u>Fermi gas model</u> for nucleons we have

$$|i\rangle \equiv |\varphi_i\rangle = \underset{\text{space}}{|\vec{k}\rangle} \otimes \underset{\text{spin}}{|s=\tfrac{1}{2}, s_z = \pm\tfrac{1}{2}\rangle} \otimes \underset{\text{isospin}}{|t=\tfrac{1}{2}, t_z = \pm\tfrac{1}{2}\rangle} \tag{4a}$$

with the s.p. wavefctns

$$\langle x|i\rangle = \langle x|\varphi_i\rangle = \underbrace{L^{-3/2} e^{i\vec{k}\cdot\vec{r}}}_{\text{space}} \underset{\text{spin}}{\chi_{s_z}^{s=\frac{1}{2}}} \underset{\text{isospin}}{\zeta_{t_z}^{t=\frac{1}{2}}} \tag{4b}$$

with the familiar representation $\chi_{\uparrow}^{\frac{1}{2}} = \begin{pmatrix}1\\0\end{pmatrix}$, $\chi_{\downarrow}^{\frac{1}{2}} = \begin{pmatrix}0\\1\end{pmatrix}$, etc.

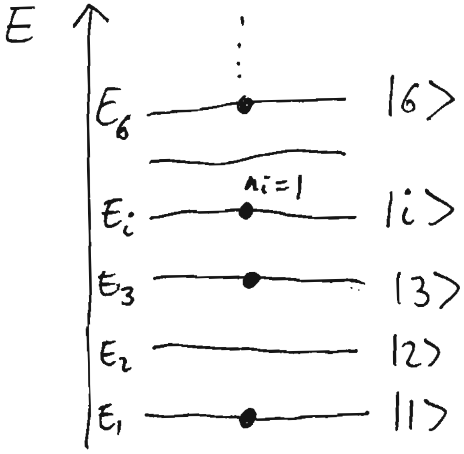
Another <u>example</u>: <u>spherical shell model</u>

$$|i\rangle \equiv |\varphi_i\rangle = |n, \ell, s=\tfrac{1}{2}, j, m_j\rangle \otimes |t=\tfrac{1}{2}, t_z\rangle \tag{5a}$$

with s.p. wavefctns

$$\left\{\begin{aligned} \langle x|i\rangle &= \varphi_{n\ell\frac{1}{2}jm_j,\frac{1}{2}t_z}(\vec{r}, s_z, t_z) = R_{n\ell}(r) \sum_{m_\ell, m_s} \langle \ell m_\ell, \tfrac{1}{2} m_s | j m_j\rangle \\ &\quad \cdot Y_{\ell m_\ell}(\theta,\varphi)\, \chi_{m_s}^{\frac{1}{2}} \otimes \zeta_{t_z}^{\frac{1}{2}} \end{aligned}\right. \tag{5b}$$

<u>etc.</u> As discussed earlier (section 2.2.1), the <u>Slater determinant</u> has the structure (suppose, levels 1, 3, 4 and 6 are filled with one nucleon, all others are unfilled):



$$\Phi^{(1,2,3,4)}_{n_1=1,\,n_2=0,\,n_3=1,\,n_4=1,\,n_5=0,\,n_6=1,\,n_{>6}=0} = \frac{1}{\sqrt{4!}}\begin{vmatrix} \varphi_1(1) & \varphi_1(2) & \varphi_1(3) & \varphi_1(4) \\ \varphi_3(1) & \varphi_3(2) & \varphi_3(3) & \varphi_3(4) \\ \varphi_4(1) & \varphi_4(2) & \varphi_4(3) & \varphi_4(4) \\ \varphi_6(1) & \varphi_6(2) & \varphi_6(3) & \varphi_6(4) \end{vmatrix} \quad (6)$$

Clearly, this complicated structure of the many-body WF is simply a reflection of the fact that the particles are identical and we can't really say which particle is in what quantum state! The mathematical structure of the Slater determinant takes care of the Pauli principle

$$\text{if} \quad |i\rangle \equiv |j\rangle \;\Rightarrow\; \phi(1,\dots,A) \equiv 0 \qquad (7a)$$

and the antisym. of the WF: $P_{ij}\,\phi(1,\dots,i,\dots,j\dots) \stackrel{\text{def}}{=}$

$$\phi(1,\dots,j,\dots,i,\dots) = -\phi(1,\dots,i,\dots,j,\dots). \qquad (7b)$$

One can prove that the most general soln. of the many-body Schrödinger eq. is an infinite linear superposition of Slater determinants:

$$\boxed{\psi(1,\dots,A;t) = \underbrace{\sum_{n_1,n_2,\dots,n_\infty=0}^{1}}_{\substack{\text{occupation numbers}\\ (0\text{ or }1)}} \underbrace{f(n_1,n_2,\dots,n_\infty;t)}_{\text{configuration amplitude}}\;\underbrace{\Phi^{(1,\dots,A)}_{n_1 n_2 \dots n_\infty}}_{\substack{\text{Slater determinant}\\ \text{(configuration)}}}} \qquad (8)$$

Occupation number representation

Ref: Fetter and Walecka, Quantum Theory of Many-Particle systems, chapter 1

One gets the feeling that there has to be a better way than using antisym. products of s.p. wavefunctions (Slater determinants). Our discussion above seems to indicate that all one really needs to know is which s.p. states $|i\rangle$ are occupied or not. Furthermore, we need to satisfy the Pauli restrictions. This suggests that we introduce creation and annihilation operators

$$\hat{c}_i^+ \text{ and } \hat{c}_i$$

for the quantum states $|i\rangle$. The state vector $|\phi\rangle$ corresponding to the Slater determinant in eq. (6) has the structure

$$\underset{\substack{\text{many-particle}\\ \text{state vector}}}{|\phi\rangle} = \underbrace{\hat{c}_1^+ \hat{c}_3^+ \hat{c}_4^+ \hat{c}_6^+}_{\substack{\text{creation}\\ \text{operators}}} \underset{\text{vacuum}}{|0\rangle} \tag{9}$$

This appears to make sense! But how do we take care of the Pauli restrictions? Recall the commutation relations, according to Dirac, for the 1-D harmonic oscillator (spin-zero $\Rightarrow$ bosons):

$$[A, B] = AB - BA \quad \text{commutator}$$

$$[\hat{a}, \hat{a}^+] = \hat{a}\hat{a}^+ - \hat{a}^+\hat{a} = 1 .$$

In 1928, Jordan and Wigner showed that the Pauli principle for fermions can be incorporated by requiring anti-commutation relations for the $\hat{c}_i, \hat{c}_i^+$:

define anti-commutator $\boxed{\{A, B\} = AB + BA}$ (10a)

with the requirements

$$\boxed{\{\hat{c}_i, \hat{c}_j\} = 0, \quad \{\hat{c}_i^+, \hat{c}_j^+\} = 0, \quad \{\hat{c}_i, \hat{c}_j^+\} = \delta_{ij}} \qquad (10b)$$

Let's clarify the shorthand notation with an example (nuclear Fermi gas with quantum states $|i\rangle = |\vec{k}, s_z, t_z\rangle$, see eq. (4a)):

$$\{\hat{c}_i, \hat{c}_j^+\} = \delta_{ij} \Longleftrightarrow \left\{\hat{c}_{\vec{k}, s_z, t_z}, \hat{c}^+_{\vec{k}' s_z' t_z'}\right\} = \delta_{\vec{k}, \vec{k}'}\, \delta_{s_z s_z'}\, \delta_{t_z, t_z'}.$$

Similar expressions for nuclear shell model basis states given in eq. (5a). (11)

Consequences of anti-commutation relations (10b)

① Pauli principle is contained, because for $j = i$

$$0 = \{\hat{c}_i^+, \hat{c}_i^+\} = \hat{c}_i^+ \hat{c}_i^+ + \hat{c}_i^+ \hat{c}_i^+ = 2\, \hat{c}_i^+ \hat{c}_i^+ \Rightarrow \boxed{\hat{c}_i^+ \hat{c}_i^+ |0\rangle = 0}$$

$\Downarrow$ no 2 fermions in same quantum state!

② The number of fermions n_i in a given quantum state $|i\rangle$ is either zero or one (note: unrestricted for bosons!).

Proof: We define the fermion number operator in state $|i\rangle$ as

$$\boxed{\hat{n}_i = \hat{c}_i^+ \hat{c}_i} \qquad (12)$$

and construct eigenstates $\hat{n}_i |n_i\rangle = n_i |n_i\rangle$.

$$\hat{n}_i = \hat{c}_i^+ \hat{c}_i \overset{(10b)}{=\!=} 1 - \hat{c}_i \hat{c}_i^+$$ take square of this eq.

$$\boxed{\hat{n}_i^2} = (\hat{c}_i^+ \hat{c}_i)^2 = (1 - \hat{c}_i \hat{c}_i^+)^2 = 1 - 2\hat{c}_i \hat{c}_i^+ + \hat{c}_i (\hat{c}_i^+ \hat{c}_i) \hat{c}_i^+$$

$$\overset{(10b)}{=\!=} 1 - 2\hat{c}_i \hat{c}_i^+ + \hat{c}_i (1 - \hat{c}_i \hat{c}_i^+) \hat{c}_i^+ = 1 - 2\hat{c}_i \hat{c}_i^+ + \hat{c}_i \hat{c}_i^+ - \underbrace{\hat{c}_i^2}_{0} \underbrace{(\hat{c}_i^+)^2}_{0} =$$

$$= 1 - \hat{c}_i \hat{c}_i^+ \underset{(10b)}{=} \hat{c}_i^+ \hat{c}_i = \boxed{\hat{n}_i} \quad \Rightarrow \quad \hat{n}_i^2 = \hat{n}_i \quad \text{or} \quad \hat{n}_i^2 - \hat{n}_i = 0$$

$$\boxed{\hat{n}_i (\hat{n}_i - 1) = 0}$$ Apply this op. eq. to the $\hat{n}_i$ eigenstates:

$$\hat{n}_i (\hat{n}_i - 1) |n_i\rangle = 0 \Rightarrow \underbrace{n_i (n_i - 1)}_{\text{eigenvalues}} |n_i\rangle = 0 \Rightarrow \boxed{n_i = 0 \text{ or } 1}$$

q.e.d.

From the anticomm. relations (10b) and the properties of the fermion number operators one can prove:

③ ~~def~~ $\boxed{\hat{c}_i |0\rangle = 0} \Rightarrow \hat{c}_i^+ \hat{c}_i |0\rangle = 0 \Rightarrow \hat{n}_i |0\rangle = 0$

i.e. $|0\rangle$ is the fermion vacuum state.

④ Define the state $\boxed{|n_i = 1\rangle = \hat{c}_i^+ |0\rangle}$

$\Rightarrow \hat{c}_i |n_i = 1\rangle = |0\rangle$ and

$\hat{c}_i^+ |n_i = 1\rangle = (c_i^+)^2 |0\rangle = 0$.

⑤ Because $[n_i, n_j] = 0$ for arbitrary states $|i\rangle, |j\rangle$ we can ~~..~~ construct simultaneous eigenstates of all number operators

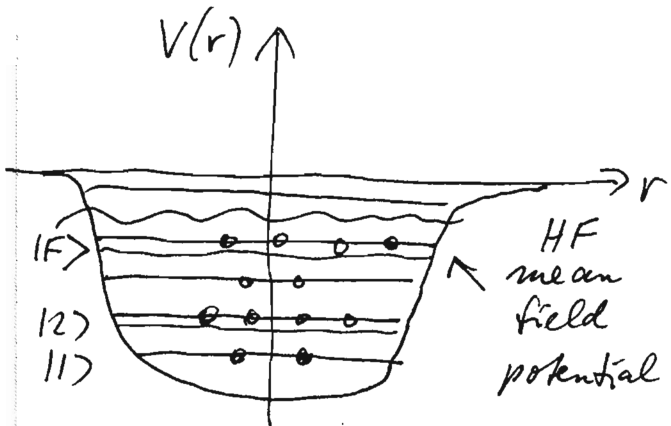
$$\boxed{|n_1, n_2, \ldots, n_\infty\rangle \overset{\text{def}}{=} |n_1\rangle |n_2\rangle \ldots |n_\infty\rangle} \qquad (13)$$

with the property $\boxed{\hat{n}_j |n_1, n_2, \ldots, n_j, \ldots, n_\infty\rangle = n_j |n_1, n_2, \ldots\rangle}$

$\boxed{\text{Slater determinant (coord. space)} \longleftrightarrow \text{state vector} \left(\begin{matrix}\text{occup.}\\ \text{\# space}\end{matrix}\right)}$

The Slater determinants given in eqns (6) and (8) correspond to the following state vectors $|\phi\rangle$ in occupation number space

$$\left.\begin{aligned} |\phi\rangle &= |n_1, n_2, \dots, n_\infty\rangle = |n_1\rangle|n_2\rangle \dots |n_\infty\rangle = \\ &= \left(\hat{c}_1^+\right)^{n_1} \left(\hat{c}_2^+\right)^{n_2} \dots \left(\hat{c}_\infty^+\right)^{n_\infty} |0\rangle = \\ &= \prod_{k=1}^{\infty} \left(\hat{c}_k^+\right)^{n_k} |0\rangle \quad \left\{ \begin{array}{l} \text{with } n_k = 0 \text{ or } 1 \\ \text{and } \sum_{k=1}^{\infty} n_k = A \end{array} \right. \end{aligned}\right\} \quad (14)$$



We will see that in the Hartree-Fock theory, nucleons occupy the lowest single-particle energies in their ground state:

$$\boxed{\underset{\text{HF-ground state}}{\left|\phi_0^{HF}\right\rangle} = \hat{c}_1^+ \hat{c}_2^+ \dots \underset{\substack{\uparrow \\ \text{Fermi level}}}{\hat{c}_F^+} |0\rangle} \quad (15)$$

The single-particle "orbitals" $\varphi_i(x)$ are self-consistently generated from the HF differential equations.

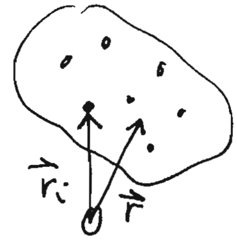
One-body operators in occupation # space

In coordinate space, one-body operators are defined by (see section 2.2.1):

$$\boxed{A = \sum_{i=1}^{N} A(x_i)} \quad \text{coord. space} \qquad (16)$$

Examples: kinetic energy $T = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_i^2 \right)$

linear momentum $\vec{P} = \sum_{k=1}^{N} \left(-i\hbar \nabla_k \right)$



$\left.\begin{array}{l}\text{particle density}\\ \text{(N point particles)}\end{array}\right\}$ $\rho(\vec{r}) = \sum_{i=1}^{N} \delta(\vec{r} - \vec{r}_i)$

QM Many-Body Theory Books (e.g. Fetter & Walecka) show that the corresponding expression in occupation # space is given by

$$\boxed{\hat{A} = \sum_{k,l=1}^{\infty} \langle k | A | l \rangle \, \hat{c}_k^{+} \hat{c}_l} \qquad (17)$$

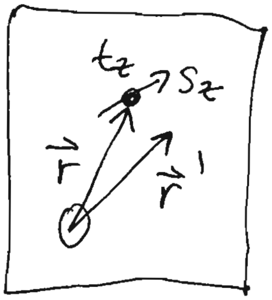
with the s.p. matrix element $\boxed{\langle k | A | l \rangle = \int dx \, \varphi_k^{+}(x) \, A(x) \, \varphi_l(x)}$

and $A(x)$ is determined from $A = \sum_{i=1}^{N} A(x_i)$.

Note: a) $\hat{A}$ contains an infinite sum over all ~~of~~ single-particle quantum states

b) there is no sum over particles in occup. # repr. This info is contained in the state vector $|\Phi_0\rangle$.

Example 1: ground state density $\langle \rho \rangle_{g.s.}$



density operator in occup. # representation:

$$\hat{\rho} = \sum_{k,l=1}^{\infty} \langle k | \underset{\substack{\uparrow \\ \text{s.p. density op.}}}{\rho} | l \rangle \, \hat{c}_k^+ \hat{c}_l \qquad \underline{(18)}$$

Consider s.p. element

$$\langle k | \rho | l \rangle = \int dx' \, \varphi_k^*(x') \, \rho(x') \, \varphi_l(x') \qquad \boxed{x' = (\vec{r}\,', s_z', t_z')}$$

$$\rightarrow \left. \int d^3r' \sum_{s_z'} \sum_{t_z'} \varphi_k^*(\vec{r}\,', s_z', t_z') \, \underbrace{\delta(\vec{r}\,' - \vec{r}) \, \delta_{s_z' s_z} \, \delta_{t_z' t_z}}_{\text{s.p. density operator}} \cdot \varphi_l(\vec{r}\,', s_z', t_z') \right\}$$

Because of δ-function and Kronecker delta's, integral and sums collapse:

$$\langle k | \rho | l \rangle \rightarrow \varphi_k^*(\vec{r}, s_z, t_z) \, \varphi_l(\vec{r}, s_z, t_z) \qquad \underline{(19)}$$

The ground state density is defined as the expectation value

$$\left. \begin{aligned} \langle \rho \rangle_{g.s.} &= \langle \phi_{g.s.} | \hat{\rho} | \phi_{g.s.} \rangle \overset{(18)}{=} \\ &\sum_{k,l=1}^{\infty} \langle k | \rho | l \rangle \underbrace{\langle \phi_{g.s.} | \hat{c}_k^+ \hat{c}_l | \phi_{g.s.} \rangle}_{\overset{\text{def}}{=} \rho_{lk}} \end{aligned} \right\} \qquad \underline{(20)}$$

The density parameters ρ_{lk} depend on the nature of the ground state. In <u>Hartree-Fock theory</u>, one assumes a simple <u>single Slater determinant given by (15)</u>.

Many-body theory shows that in this case

$$\boxed{\rho_{\ell k}^{HF} = \langle \phi_{g.s.}^{HF} | \hat{c}_k^{+} \hat{c}_\ell | \phi_{g.s.}^{HF} \rangle = \delta_{k\ell}\ \theta(\varepsilon_F - \varepsilon_k)} \qquad (21)$$

Inserting (21) into (20):

$$\langle \rho \rangle_{g.s.}^{HF} = \sum_{k,\ell=1}^{\infty} \langle k|\rho|\ell\rangle \delta_{k\ell}\ \theta(\varepsilon_F - \varepsilon_k) =$$

$$= \sum_{k=1}^{\infty} \langle k|\rho|k\rangle \theta(\varepsilon_F - \varepsilon_k) = \sum_{k=1}^{F} \langle k|\rho|k\rangle .$$

Inserting the expr. (19) for $\langle k|\rho|\ell\rangle$, we obtain:

$$\boxed{\langle \rho \rangle_{g.s.}^{HF} = \sum_{k=1}^{F} \underbrace{\varphi_k^{*}(\vec{r}, s_z, t_z)\, \varphi_k(\vec{r}, s_z, t_z)}_{=\rho_k(\vec{r}, s_z, t_z)}} \qquad (22)$$

In words: the g.s. density is the sum of the probability densities $|\varphi_k|^2 = \rho_k$ of the occupied s.p. states $k = 1, \dots, F$.

Example 2: ground state kinetic energy $\langle T \rangle_{g.s.}$

kin. energy operator in occup. # representation

$$\hat{T} = \sum_{k,\ell=1}^{\infty} \langle k| \underset{\substack{\uparrow \\ \text{s.p. operator}}}{t} |\ell\rangle\, \hat{c}_k^{+} \hat{c}_\ell \qquad (23)$$

Consider the s.p. matrix element

$$\langle k|t|\ell\rangle = \int dx\ \varphi_k^{*}(x)\, t(x)\, \varphi(x) \qquad \text{with } x = (\vec{r}, s_z, t_z)$$

$$\langle k|t|l\rangle \rightarrow \int d^3r \sum_{s_z}\sum_{t_z} \varphi_k^*(\vec{r}, s_z, t_z)\left(-\frac{\hbar^2}{2m}\nabla^2\right)\varphi_l(\vec{r}, s_z, t_z) \tag{24}$$

The g.s. kinetic energy is defined as the expectation value

$$\langle T\rangle_{g.s.} = \langle \phi_{g.s.}|\hat{T}|\phi_{g.s.}\rangle \overset{(23)}{=}$$

$$= \sum_{k,l=1}^{\infty} \langle k|t|l\rangle \underbrace{\langle \phi_{g.s.}|\hat{c}_k^+\hat{c}_l|\phi_{g.s.}\rangle}_{=\rho_{lk}}$$

Again, in the HF ground state, one obtains from eq. (21):

$$\langle T\rangle_{g.s.}^{HF} = \sum_{k,l=1}^{\infty} \langle k|t|l\rangle \delta_{kl}\,\theta(\varepsilon_F - \varepsilon_k)$$

$$= \sum_{k=1}^{\infty} \langle k|t|k\rangle\,\theta(\varepsilon_F - \varepsilon_k) = \sum_{k=1}^{F} \langle k|t|k\rangle$$

Inserting expression (24) for s.p. matrix element, we obtain

$$\boxed{\langle T\rangle_{g.s.}^{HF} = \sum_{k=1}^{F} \int d^3r \sum_{s_z}\sum_{t_z} \varphi_k^*(\vec{r}, s_z, t_z)\left(-\frac{\hbar^2}{2m}\nabla^2\right)\varphi_k(\vec{r}, s_z, t_z)} \tag{25}$$

We use partial integration of the form

$$\int_V u\,v'\,dx = u\,v\Big|_B - \int_V u'\,v\,dx$$

to re-write the kin. energy term:

$$\left(-\frac{\hbar^2}{2m}\right)\int d^3r\, \varphi_k^*\,(\nabla\cdot\nabla)\,\varphi_k \rightarrow \left(+\frac{\hbar^2}{2m}\right)\int d^3r\,\{\nabla\varphi_k^*\cdot\nabla\varphi_k\},$$

and the surface term vanishes because we integrate to ∞.

Defining the <u>kinetic energy density</u>

$$\boxed{\tau(\vec{r}) = \sum_{s_z=\pm\frac{1}{2}} \sum_{t_z=\pm\frac{1}{2}} \sum_{k=1}^{F} |\nabla\varphi_k(\vec{r}, s_z, t_z)|^2} \qquad (26a)$$

we obtain

$$\boxed{\langle T\rangle^{HF}_{g.s.} = \int d^3r \left[\frac{\hbar^2}{2m}\tau(\vec{r})\right]} \qquad (26b)$$

This is an important expression for the g.s. kinetic energy of any nuclear many-body problem.

Two-body operators in occupation # representation

<u>Ref</u>: Fetter & Walecka, p. chapter 1

In <u>coordinate space</u>, a <u>two-body operator</u> is defined as

$$\boxed{B = \frac{1}{2}\sum_{i,j=1}^{N} B(x_i, x_j)} \qquad (27a)$$

<u>Examples</u>: a) Coulomb potential between protons

$$V^{(2)}_{Coul} = \frac{1}{2}\sum_{i,j=1}^{Z} v_{ij}^{(2)\,Coul}(x_i, x_j) = \frac{1}{2}\sum_{i,j=1}^{Z}\frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

b) 2-body strong nuclear interaction

$$V^{(2)}_{nucl} = \frac{1}{2}\sum_{i,j=1}^{A} v_{ij}^{(2)\,nucl}(x_i, x_j)$$

$\downarrow$

e.g. Argonne $v-18$ potential for N-N

In occupation # representation, the 2-body operator becomes

$$\boxed{\hat{B} = \frac{1}{2} \sum_{k,l,m,n=1}^{\infty} \langle k\,l | B | m n \rangle \, \hat{c}_k^{+} \hat{c}_l^{+} \hat{c}_n \hat{c}_m} \tag{27b}$$

note sequence!

with the 2-body matrix element

$$\boxed{\langle k\,l | B | m n \rangle = \int dx \int dx' \, \varphi_k^*(x)\, \varphi_l^*(x')\, B(x,x')\, \varphi_m(x)\, \varphi_n(x')} \tag{27c}$$

Three-body operators

In coordinate space:

$$C = \frac{1}{6} \sum_{i,j,k=1}^{N} C(x_i, x_j, x_k)$$

Example: 3-body N-N-N interaction

$$V^{(3)}_{nucl} = \frac{1}{6} \sum_{i,j,k=1}^{A} v_{ijk}^{(3)\,nucl}(x_i, x_j, x_k)$$

In occupation # repr., the 3-body operator becomes

$$\boxed{\hat{C} = \frac{1}{6} \sum_{i,j,k,l,m,n=1}^{\infty} \langle i j k | C | l m n \rangle \, \hat{c}_i^{+} \hat{c}_j^{+} \hat{c}_k^{+} \hat{c}_n \hat{c}_m \hat{c}_l} \tag{28}$$

note sequence!

We are now in a position to write down the nuclear many-body Hamiltonian in occupation # space:

$$\hat{H} = \sum_{i,j=1}^{\infty} \langle i|t|j\rangle \hat{c}_i^+ \hat{c}_j + \frac{1}{2} \sum_{i,j,k,l=1}^{\infty} \langle ij| V_{Coul}^{(2)} + V_{nucl}^{(2)} |kl\rangle *$$

$$* \hat{c}_i^+ \hat{c}_j^+ \hat{c}_l \hat{c}_k + \frac{1}{6} \sum_{i,j,k,l,m,n=1}^{\infty} \langle ijk| V_{nucl}^{(3)} | lmn\rangle *$$

$$* \hat{c}_i^+ \hat{c}_j^+ \hat{c}_k^+ \hat{c}_n \hat{c}_m \hat{c}_l \qquad (29)$$

The ground-state energy of the nucleus is given by

$$E_{g.s.} = E_{binding} = \langle \phi_{g.s.} | \hat{H} | \phi_{g.s.} \rangle \qquad (30a)$$

~~or~~ ~~or~~ more explicitly by

$$\boxed{\begin{aligned} E_{g.s.} &= \sum_{i,j=1}^{\infty} \langle i|t|j\rangle \langle \phi_{g.s.} | \hat{c}_i^+ \hat{c}_j | \phi_{g.s.} \rangle \\ &+ \frac{1}{2} \sum_{i,j,k,l=1}^{\infty} \langle ij| V_{Coul}^{(2)} + V_{nucl}^{(2)} |kl\rangle \langle \phi_{g.s.} | \hat{c}_i^+ \hat{c}_j^+ \hat{c}_l \hat{c}_k | \phi_{g.s.} \rangle \\ &+ \frac{1}{6} \sum_{i,j,k,l,m,n=1}^{\infty} \langle ijk| V_{nucl}^{(3)} | lmn\rangle \langle \phi_{g.s.} | \hat{c}_i^+ \hat{c}_j^+ \hat{c}_k^+ \hat{c}_n \hat{c}_m \hat{c}_l | \phi_{g.s.} \rangle \qquad (30b) \end{aligned}}$$

The expressions $\langle \phi_{g.s.} | \hat{c}_i^+ \dots \hat{c}_l | \phi_{g.s.} \rangle$ depend on the structure of the ground state; in general, they can be evaluated using "Wick's theorem". $\rightarrow$ Details see Phys. 365 lecture notes!