PP-HH LADDERS CALCULATIONS FOR NUCLEAR MATTER

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Outline

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CCD energy equation

Energy in the Coupled-Cluster doubles approximation (CCD):

$$E_{CCD} = \sum_{i} \langle i|h|i\rangle + \frac{1}{2}\sum_{ij} \langle ij|v|ij\rangle_{AS} + \frac{1}{4}\sum_{abij} \langle ij|v|ab\rangle_{AS} \langle ab|t|ij\rangle \, .$$

- $i, j, k, \ldots$ denote hole states (occupied in Fermi vacuum),
  $a, b, c, \ldots$ denote particle states (virtual excitations),
  $p, q, r, \ldots$ denote general states (particle or hole)
- $\langle ab|t|ij\rangle$ is the $2p-2h$ Coupled-Cluster amplitude

Physical model and basis states

- Assume we fill a cubic box with an equal number of protons and neutrons
- We can now apply periodic boundary conditions and use plane waves $\exp(i\mathbf{k}\cdot\mathbf{r})$ as basis functions
- Each proton (neturon) is a fermion with spin $s = 1/2$, its z projection $m_s = \pm 1/2$, isospin $t = 1/2$, and its z projection m_t = -1/2 (+1/2)

A single-particle state is now determined by a momentum vector $\mathbf{k}$ together with the quantum numbers m_s and m_t

Conservation of momentum

By symmetry considerations, we can assume that the total momentum of the A-particle system of nucleons is

$$\langle \mathbf{K} \rangle = 0.$$

The Hamiltonian is diagonal in Center of Mass (CM) momentum, and therefore also diagonal in total momentum. In other words, the Hamiltonian conserves the total momentum and $[\mathbf{K}, \hat{H}] = 0$.

Conservation of momentum

From the assumptions above it follows that the total wave function Ψ must be an eigenstate of the momentum operator $\hat{\mathbf{K}}$ with the eigenvalue $\langle \mathbf{K}_0 \rangle = 0$. For the Coupled-Cluster ansatz, we can write

$$\hat{\mathbf{K}}\Psi = \hat{\mathbf{K}} \left(\Phi_0 + \sum_{ia} t_i^a \Phi_i^a + \frac{1}{4} \sum_{ijab} t_{ij}^{ab} \Phi_{ij}^{ab} + \frac{1}{2} \sum_{ia} \sum_{jb} t_i^a t_j^b \Phi_{ij}^{ab} + \dots \right)$$

By definition,

$$\hat{\mathbf{K}}\Phi_i^a = \left(\mathbf{K}_0 + \mathbf{k}_a - \mathbf{k}_i\right) \Phi_i^a,$$
$$\hat{\mathbf{K}}\Phi_{ij}^{ab} = \left(\mathbf{K}_0 + \mathbf{k}_a + \mathbf{k}_b - \mathbf{k}_i - \mathbf{k}_j\right) \Phi_{ij}^{ab}.$$

In order to get $\hat{\mathbf{K}}\Psi = \mathbf{K}_0\Psi$, the coefficients t_i^a must be zero, and we have also the restriction

$$\mathbf{k}_a + \mathbf{k}_b = \mathbf{k}_i + \mathbf{k}_j,$$

among other. Thus, CCSD is equal to CCD for this periodic system.

CCD correlation energy

The CCD correlation energy can be written in the momentum basis as

$$\Delta E_{CCD} = \frac{1}{4} \sum_{abij} \langle ij|v|ab\rangle_{AS} \langle ab|t|ij\rangle$$

$$= \frac{1}{4} \sum_{\substack{|\mathbf{k}_i|\leq k_F \\ m_{s_i} m_{t_i}}} \sum_{\substack{|\mathbf{k}_j|\leq k_F \\ m_{s_j} m_{t_j}}} \sum_{\substack{|\mathbf{k}_a|\leq k_F \\ m_{s_a} m_{t_a}}} \sum_{\substack{|\mathbf{k}_b|\leq k_F \\ m_{s_b} m_{t_b}}} \langle \mathbf{k}_i \mathbf{k}_j|v|\mathbf{k}_a \mathbf{k}_b\rangle_{AS} \langle \mathbf{k}_a \mathbf{k}_b|t|\mathbf{k}_i \mathbf{k}_j\rangle$$

The infinity limit

We keep the number of particles per volume unit, $\rho \equiv A/\Omega$, constant and let the side lenght of the box, L, go towards infinity. In that limit, the sums over momenta can be replaced by integrals

$$\sum_{\mathbf{k}} \rightarrow \frac{\Omega}{(2\pi)^3} \int d\mathbf{k}$$

Countinuous spectrum of momenta

The CCD correlation energy can now be written

$$\Delta E_{CCD} = \frac{1}{4}\left(\frac{\Omega}{(2\pi)^3}\right)^4 \sum_{m_{s_i} m_{t_i}} \sum_{m_{s_j} m_{t_j}} \sum_{m_{s_a} m_{t_a}} \sum_{m_{s_b} m_{t_b}}$$
$$\times \int d\mathbf{k}_i \int d\mathbf{k}_j \int d\mathbf{k}_a \int d\mathbf{k}_b \left\langle \mathbf{k}_i \mathbf{k}_j | v | \mathbf{k}_a \mathbf{k}_b \right\rangle_{AS} \left\langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_i \mathbf{k}_j \right\rangle$$
$$\times \theta(k_F - |\mathbf{k}_i|)\theta(k_F - |\mathbf{k}_j|)\theta(|\mathbf{k}_a| - k_F)\theta(|\mathbf{k}_b| - k_F),$$

where $\theta(x)$ is the Heaviside step function.

The step functions ensure that a given momentum variable is either a hole state ($|\mathbf{k}_h| < k_F$) or a particle state ($|\mathbf{k}|_p > k_F$). Let us call the first pair of Heaviside step functions a *hole-hole Pauli exclusion operator*, and the second pair a *particle-particle Pauli exclusion operator*.

Coordinate system – lab or relative?

The expressions of most of the commonly used nuclear interaction potentials are given in a relative - Center of Mass (RCM) momentum basis.

Two alternatives:

1. We can do a transformation of the potential to laboratory momentum coorinates. This transformation is computationally feasible only if the transformation converges reasonably fast as a function of the relative angular momenta. Unfortunately, the convergence is slow, which makes this method computationally difficult.
2. Another option is to try to formulate the Coupled-Cluster equations directly in RCM coordinates. In this case, the CC equations become more complicated, but hopefully this method can give computationally doable calculations. This is the approach we are going to pursue.

Transformation of coordinates

Let us define the transformation from laboratory to relative - Center of Mass coordinates (RCM)

$$\begin{aligned}
\mathbf{k} &= \left(\mathbf{k}_i - \mathbf{k}_j\right)/2, \\
\mathbf{P} &= \mathbf{k}_i + \mathbf{k}_j, \\
\mathbf{k}' &= \left(\mathbf{k}_a - \mathbf{k}_b\right)/2, \\
\mathbf{P}' &= \mathbf{k}_a + \mathbf{k}_b.
\end{aligned}$$

We also assume that the potential in RCM coordinates is related to the potential in lab coordinates through

$$\left\langle \mathbf{k}_i \mathbf{k}_j | v | \mathbf{k}_a \mathbf{k}_b \right\rangle = \frac{(2\pi)^3}{\Omega} \left\langle \mathbf{k} | v | \mathbf{k}' \right\rangle \delta_{\mathbf{P}\mathbf{P}'}.$$

Earlier we showed that conservation of total momentum leads to the conservation relation in the CC doubles amplitudes

$$\mathbf{k}_a + \mathbf{k}_b = \mathbf{k}_i + \mathbf{k}_j.$$

Therefore, the amplitude t_{ij}^{ab} is diagonal in CM momentum:

$$\langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_i \mathbf{k}_j \rangle = \langle \mathbf{k}' | t(\mathbf{P}) | \mathbf{k} \rangle .$$

For our system, we may do the replacement

$$\delta_{\mathbf{PP}'} \rightarrow \frac{(2\pi)^3}{\Omega} \delta^{(3)}(\mathbf{P} - \mathbf{P}'),$$

where $\delta^{(3)}(\mathbf{x})$ is the 3-dimensional Kronecker delta distribution.

Energy in RCM coordinates

We can now express the CCD correlation energy in RCM coordinates:

$$\Delta E_{CCD} = \frac{1}{4}\left(\frac{\Omega}{(2\pi)^3}\right)^2 \sum_{m_{s_i} m_{t_i}} \sum_{m_{s_j} m_{t_j}} \int d\mathbf{k} \int d\mathbf{k}' \int d\mathbf{P}$$
$$\times \left\langle \mathbf{k}|v|\mathbf{k}'\right\rangle_{AS} \left\langle \mathbf{k}'|t(\mathbf{P})|\mathbf{k}\right\rangle$$
$$\times \theta(k_F - |\mathbf{k} + \mathbf{P}/2|)\theta(k_F - |-\mathbf{k} + \mathbf{P}/2|)$$
$$\times \theta(\left|\mathbf{k}' + \mathbf{P}/2\right| - k_F)\theta(\left|-\mathbf{k}' + \mathbf{P}/2\right| - k_F).$$

Angular momentum quantum numbers

Definitions:

$l =$ quantum number of the orbital angular momentum operator $\hat{l}^2$ related to relative coordinates

$m_l =$ quantum number of the operator $\hat{l}_z$, which is the z projection of $\hat{l}$

$S =$ quantum number of the total two-particle spin operator $\hat{S}^2$ $(S = |s_1 - s_2|, |s_1 - s_2| + 1, \ldots, s_1 + s_2)$

$M_S =$ quantum number of the operator $\hat{S}_z$, which is the z projection of $\hat{S}$

$\mathcal{J} =$ quantum number of the operator $\hat{\mathcal{J}}^2$, where $\hat{\mathcal{J}} = \hat{l} + \hat{S}$

$m_{\mathcal{J}} =$ quantum number of the operator $\hat{\mathcal{J}}_z$, which is the z projection of $\hat{\mathcal{J}}$

Interaction matrix elements

The nuclear interaction potentials are usually given in a relative momentum basis with an expansion in angular momentum quantum numbers:

$$\left\langle k(lS)\mathcal{J}M_T|v|k'(l'S)\mathcal{J}M_T\right\rangle \delta_{\mathcal{J}\mathcal{J}'}\delta_{m_{\mathcal{J}}m'_{\mathcal{J}}}\delta_{SS'}\delta_{M_TM'_T}$$

The interaction matrix elements are expressed in a basis where the relative orbital angular momentum l is coupled with the total two-particle spin S to get $\mathcal{J}$.

Furthermore, the total spin S, the total relative angular momentum $\mathcal{J}$, its z projection $m_{\mathcal{J}}$, and the z projection of the coupled two-particle isospin M_T are all conserved in the interaction.

Angular momentum algebra

Consider the following relations:

$$\sum_{lm_l} |lm_l\rangle \langle lm_l| = 1$$

$$\langle \hat{\mathbf{k}}|lm_l\rangle \equiv Y_{lm_l}(\hat{\mathbf{k}})$$

$$\int d\hat{\mathbf{k}}\, Y^*_{lm_l}(\hat{\mathbf{k}})\, Y_{l'm'_l}(\hat{\mathbf{k}}) = \delta_{ll'}\delta_{m_l m'_l}$$

$$\sum_{SM_S} |SM_S\rangle \langle SM_S| = 1$$

$$|lm_l SM_S\rangle = \sum_{\mathcal{J}m_{\mathcal{J}}} \langle lm_l SM_S|\mathcal{J}m_{\mathcal{J}}\rangle\, |\mathcal{J}m_{\mathcal{J}}(lS)\rangle$$

Here $\hat{\mathbf{k}} \equiv (\theta_{\mathbf{k}}, \phi_{\mathbf{k}})$ denotes the angles of $\mathbf{k}$ and the bracket in the last equation is a Clebsch-Gordan coefficient. $Y_{lm_l}(\hat{\mathbf{k}})$ is a spherical harmonics function.

CCD energy with exact Pauli exclusion operators

Using the relations on the previous page, we can write the CCD correlation energy in the basis in which the interaction is given:

$$\Delta E_{CCD} = \frac{1}{4}\left(\frac{\Omega}{(2\pi)^3}\right)^2 \sum_{S}\sum_{TM_T}\sum_{ll'}\sum_{l''l'''}\sum_{\mathcal{J}m_{\mathcal{J}}}\sum_{\mathcal{J}''m_{\mathcal{J}''}}\sum_{\mathcal{J}'''m_{\mathcal{J}'''}}$$
$$\times \int_0^{k_F} k^2 dk \int_0^{\infty} k'^2 dk' \int_0^{2k_F} P^2 dP \int_{-1}^{1} d\cos\theta_P \int_0^{2\pi} d\phi_P$$
$$\times \left\langle k(lS)\mathcal{J}M_T|v|k'(l'S)\mathcal{J}M_T\right\rangle_{AS} \left\langle k'(l''S)\mathcal{J}''m_{\mathcal{J}''}|t(\mathbf{P})|k(l'''S)\mathcal{J}'''m_{\mathcal{J}'''}\right\rangle$$
$$\times Q_{hh}(l'''\mathcal{J}'''m_{\mathcal{J}'''}, l\mathcal{J}m_{\mathcal{J}}; STkP\theta_P\phi_P)$$
$$\times Q_{pp}(l'\mathcal{J}m_{\mathcal{J}}, l''\mathcal{J}''m_{\mathcal{J}''}; STk'P\theta_P\phi_P)$$

Exact Pauli exclusion operators

In the previous energy expression, we have used the definitions

$$Q_{hh}(l'''\mathcal{J}'''m_{\mathcal{J}'''}, l\mathcal{J}m_{\mathcal{J}}; STkP\theta_P\Phi_P) = \sum_{m_l m_{l'''}} \sum_{M_S} \int d\hat{\mathbf{k}}\, Y^*_{l'''m_{l'''}}(\hat{\mathbf{k}})\, Y_{lm_l}(\hat{\mathbf{k}}) \times \langle lm_l SM_S|\mathcal{J}m_{\mathcal{J}}\rangle \langle l'''m_{l'''}SM_S|\mathcal{J}'''m_{\mathcal{J}'''}\rangle \times \theta(k_F - |\mathbf{k}+\mathbf{P}/2|)\theta(k_F - |-\mathbf{k}+\mathbf{P}/2|)$$

and

$$Q_{pp}(l'\mathcal{J}m_{\mathcal{J}}, l''\mathcal{J}''m_{\mathcal{J}''}; STk'P\theta_P\phi_P) = \sum_{m_{l'} m_{l''}} \sum_{M'_S} \int d\hat{\mathbf{k}}'\, Y^*_{l'm_{l'}}(\hat{\mathbf{k}}')\, Y_{l''m_{l''}}(\hat{\mathbf{k}}') \times \langle l'm_{l'}SM'_S|\mathcal{J}m_{\mathcal{J}}\rangle \langle l''m_{l''}SM'_S|\mathcal{J}''m_{\mathcal{J}''}\rangle \times \theta(|\mathbf{k}'+\mathbf{P}/2| - k_F)\theta(|-\mathbf{k}'+\mathbf{P}/2| - k_F)$$

in a similar way as was introduced in a G-matrix calculation by K. Suzuki *et al.* (Nucl. Phys. A 665 (2000) 92–104).

A simpler expression of Q_{pp}

Suzuki *et al.* have derived an expression for Q_{pp} which avoids the complicated integration limits in the first definition:

$$\begin{aligned} Q_{pp}(l\mathcal{J}m_{\mathcal{J}}, l'\mathcal{J}'m_{\mathcal{J}'}; STkP\theta_P\phi_P) = f_{lST}f_{l'ST}\sum_L(-1)^{S+m_{\mathcal{J}}}\frac{\sqrt{4\pi}\hat{l}\hat{l}'\hat{\mathcal{J}}\hat{\mathcal{J}}'}{\hat{L}} \\ \times \langle l0l'0|L0\rangle \langle \mathcal{J} - m_{\mathcal{J}}\mathcal{J}'m_{\mathcal{J}'}|LM_L\rangle \\ \times Y_{LM_L}(\theta_P,\phi_P)W(l\mathcal{J}l'\mathcal{J}'; SL)\int_0^{x_{pp}} P_L(x)dx, \end{aligned}$$

where $f_{lST} = (1-(-1)^{l+S+T})/2$ is an antisymmetrization factor, $\hat{x} \equiv \sqrt{2x+1}$, $P_L(x)$ is the Legendre polynomial, and $W(l\mathcal{J}l'\mathcal{J}'; SL)$ denotes the Racah coefficient. In addition,

$$x_{pp} = \begin{cases} 0 & \text{if } k < \sqrt{k_F^2 - P^2/4}, \\ \frac{k^2 - k_F^2 + P^2/4}{kP} & \text{if } \sqrt{k_F^2 - P^2/4} < k < k_F + P/2, \\ 1 & \text{otherwise.} \end{cases}$$

A simpler expression also for Q_{hh}

One can easily show that the hole-hole matrix element Q_{hh} can be calculated using the same expression as presented on the previous slide for Q_{pp}, given that the integration limit x_{pp} is replaced by

$$x_{hh} = \begin{cases} 0 & \text{if } k > \sqrt{k_F^2 - P^2/4}, \\ -\frac{k^2 - k_F^2 + P^2/4}{kP} & \text{if } k_F - P/2 < k < \sqrt{k_F^2 - P^2/4}, \\ 1 & \text{otherwise.} \end{cases}$$

Outline

The T_2 amplitude equation

The Coupled-Cluster T_2 amplitude equation only with doubles coefficients t_{ij}^{ab} is defined in laboratory coordinates as

$$
\begin{aligned}
0 = & \langle ab|v|ij\rangle_{AS} + \sum_c \left(\langle b|f|c\rangle \langle ac|t|ij\rangle - \langle a|f|c\rangle \langle bc|t|ij\rangle\right) \\
& - \sum_k \left(\langle ab|t|ik\rangle \langle k|f|j\rangle - \langle ab|t|jk\rangle \langle k|f|i\rangle\right) + \frac{1}{2}\sum_{kl} \langle ab|t|kl\rangle \langle kl|v|ij\rangle_{AS} \\
& + \frac{1}{2}\sum_{cd} \langle ab|v|cd\rangle_{AS} \langle cd|t|ij\rangle + P(ij)P(ab)\sum_{kc} \langle ac|t|ik\rangle \langle kb|v|cj\rangle_{AS} \\
& + \frac{1}{2}P(ij)P(ab)\sum_{klcd} \langle ac|t|ik\rangle \langle db|t|lj\rangle \langle kl|v|cd\rangle_{AS} \\
& + \frac{1}{4}\sum_{klcd} \langle ab|t|kl\rangle \langle kl|v|cd\rangle_{AS} \langle cd|t|ij\rangle \\
& + P(ab)\frac{1}{2}\sum_{klcd} \langle ac|t|ij\rangle \langle bd|t|kl\rangle \langle kl|v|cd\rangle_{AS} \\
& - P(ij)\frac{1}{2}\sum_{klcd} \langle ab|t|ik\rangle \langle kl|v|cd\rangle_{AS} \langle cd|t|jl\rangle \,.
\end{aligned}
$$

The single-particle operator

Here the single-particle matrix elements are defined as

$$\langle p|f|q\rangle = \langle p|t_0|q\rangle + \sum_i \langle pi|v|qi\rangle_{AS} \,,$$

where t_0 is the kinetic energy operator.

We model nuclear matter as a two-component *homogeneous, translationally invariant* Fermi liquid. Based on these assumptions, we choose plane waves as our single-particle basis.

In the momentum basis, the kinetic energy matrix elements $\langle p|t_0|q\rangle$ are trivially diagonal. From the fact that the interaction v conserves the total momentum, we find that also the matrix elements $\sum_i \langle pi|v|qi\rangle_{AS}$ are diagonal in the momentum basis. Accordingly, the matrix elements $\langle p|f|q\rangle$ are diagonal in the momentum basis.

Generally, a basis which diagonalizes an operator consists of egienfunctions of that operator (see f.ex. Liboff p. 485). From the facts that the matrix elements $\langle p|f|q\rangle$ are diagonal in the plane wave basis and the plane wave basis is orthonormal, it follows that the plane waves are eigenfunctions of the Hartree-Fock equation

$$\langle p|f|q\rangle = \varepsilon_q \langle p|q\rangle$$

or

$$\langle p|t_0|q\rangle + \sum_i [\langle pi|v|qi\rangle - \langle pi|v|iq\rangle] = \varepsilon_q \langle p|q\rangle ,$$

which fulfill the necessary the constraint

$$\langle p|q\rangle = \delta_{pq}.$$

Since both the single-particle and the two-particle operators conserve the total momentum, we may conclude that all the Slater determinants in a many-body wavefunction ansatz should have the same total momentum $\langle \mathbf{K}_0 \rangle = 0$.

If we replace sums with integrals and use the diagonality of the single-particle matrix elements, the T_2 amplitude equation can be written in laboratory momentum coordinates as (all interaction matrix elements are antisymmetric)

$$
\begin{aligned}
0 = & \langle \mathbf{k}_a \mathbf{k}_b | v | \mathbf{k}_i \mathbf{k}_j \rangle + \left(\langle \mathbf{k}_a | f | \mathbf{k}_a \rangle + \langle \mathbf{k}_b | f | \mathbf{k}_b \rangle - \langle \mathbf{k}_i | f | \mathbf{k}_i \rangle - \langle \mathbf{k}_j | f | \mathbf{k}_j \rangle \right) \langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_i \mathbf{k}_j \rangle \\
& + \frac{1}{2} \left(\frac{\Omega}{(2\pi)^3} \right)^2 \int d\mathbf{k}_k \int d\mathbf{k}_l \, \langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_k \mathbf{k}_l \rangle \langle \mathbf{k}_k \mathbf{k}_l | v | \mathbf{k}_i \mathbf{k}_j \rangle \, \theta(k_F - |\mathbf{k}_k|) \theta(k_F - |\mathbf{k}_l|) \\
& + \frac{1}{2} \left(\frac{\Omega}{(2\pi)^3} \right)^2 \int d\mathbf{k}_c \int \mathbf{k}_d \, \langle \mathbf{k}_a \mathbf{k}_b | v | \mathbf{k}_c \mathbf{k}_d \rangle \langle \mathbf{k}_c \mathbf{k}_d | t | \mathbf{k}_i \mathbf{k}_j \rangle \, \theta(|\mathbf{k}_c| - k_F) \theta(|\mathbf{k}_d| - k_F) \\
& + P(ij) P(ab) \left(\frac{\Omega}{(2\pi)^3} \right)^2 \int d\mathbf{k}_k \int d\mathbf{k}_c \, \langle \mathbf{k}_a \mathbf{k}_c | t | \mathbf{k}_i \mathbf{k}_k \rangle \langle \mathbf{k}_k \mathbf{k}_b | v | \mathbf{k}_c \mathbf{k}_j \rangle \\
& \times \theta(k_F - |\mathbf{k}_k|) \theta(|\mathbf{k}_c| - k_F) \\
& + \frac{1}{2} P(ij) P(ab) \left(\frac{\Omega}{(2\pi)^3} \right)^4 \int d\mathbf{k}_k \int d\mathbf{k}_l \int d\mathbf{k}_c \int d\mathbf{k}_d \\
& \times \langle \mathbf{k}_a \mathbf{k}_c | t | \mathbf{k}_i \mathbf{k}_k \rangle \langle \mathbf{k}_d \mathbf{k}_b | t | \mathbf{k}_l \mathbf{k}_j \rangle \langle \mathbf{k}_k \mathbf{k}_l | v | \mathbf{k}_c \mathbf{k}_d \rangle \\
& \times \theta(k_F - |\mathbf{k}_k|) \theta(k_F - |\mathbf{k}_l|) \theta(|\mathbf{k}_c| - k_F) \theta(|\mathbf{k}_c| - k_F)
\end{aligned}
$$

$$+\frac{1}{4}\left(\frac{\Omega}{(2\pi)^3}\right)^4\int d\mathbf{k}_k\int d\mathbf{k}_l\int d\mathbf{k}_c\int d\mathbf{k}_d\,\langle\mathbf{k}_a\mathbf{k}_b|t|\mathbf{k}_k\mathbf{k}_l\rangle\,\langle\mathbf{k}_k\mathbf{k}_l|v|\mathbf{k}_c\mathbf{k}_d\rangle$$
$$\times\left\langle\mathbf{k}_c\mathbf{k}_d|t|\mathbf{k}_i\mathbf{k}_j\right\rangle\theta(k_F-|\mathbf{k}_k|)\theta(k_F-|\mathbf{k}_l|)\theta(|\mathbf{k}_c|-k_F)\theta(|\mathbf{k}_d|-k_F)$$
$$+\frac{1}{2}P(ab)\left(\frac{\Omega}{(2\pi)^3}\right)^4\int d\mathbf{k}_k\int d\mathbf{k}_l\int d\mathbf{k}_c\int d\mathbf{k}_d\,\left\langle\mathbf{k}_a\mathbf{k}_c|t|\mathbf{k}_i\mathbf{k}_j\right\rangle\langle\mathbf{k}_b\mathbf{k}_d|t|\mathbf{k}_k\mathbf{k}_l\rangle$$
$$\times\langle\mathbf{k}_k\mathbf{k}_l|v|\mathbf{k}_c\mathbf{k}_d\rangle\,\theta(k_F-|\mathbf{k}_k|)\theta(k_F-|\mathbf{k}_l|)\theta(|\mathbf{k}_c|-k_F)\theta(|\mathbf{k}_d|-k_F)$$
$$-\frac{1}{2}P(ij)\left(\frac{\Omega}{(2\pi)^3}\right)^4\int d\mathbf{k}_k\int d\mathbf{k}_l\int d\mathbf{k}_c\int d\mathbf{k}_d\,\langle\mathbf{k}_a\mathbf{k}_b|t|\mathbf{k}_i\mathbf{k}_k\rangle\,\langle\mathbf{k}_k\mathbf{k}_l|v|\mathbf{k}_c\mathbf{k}_d\rangle$$
$$\times\left\langle\mathbf{k}_c\mathbf{k}_d|t|\mathbf{k}_j\mathbf{k}_l\right\rangle\theta(k_F-|\mathbf{k}_k|)\theta(k_F-|\mathbf{k}_l|)\theta(|\mathbf{k}_c|-k_F)\theta(|\mathbf{k}_d|-k_F).$$

Approximation with pp and hh ladders

As a first approximation we include only a few of the diagrams in the T_2 approximation:

$$
\begin{aligned}
0 = & \left\langle \mathbf{k}_a \mathbf{k}_b | v | \mathbf{k}_i \mathbf{k}_j \right\rangle + \left(\varepsilon(\mathbf{k}_a) + \varepsilon(\mathbf{k}_b) - \varepsilon(\mathbf{k}_i) - \varepsilon(\mathbf{k}_j) \right) \left\langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_i \mathbf{k}_j \right\rangle \\
& + \frac{1}{2} \left(\frac{\Omega}{(2\pi)^3} \right)^2 \int d\mathbf{k}_k \int d\mathbf{k}_l \left\langle \mathbf{k}_a \mathbf{k}_b | t | \mathbf{k}_k \mathbf{k}_l \right\rangle \left\langle \mathbf{k}_k \mathbf{k}_l | v | \mathbf{k}_i \mathbf{k}_j \right\rangle \\
& \times \theta(k_F - |\mathbf{k}_k|) \theta(k_F - |\mathbf{k}_l|) \\
& + \frac{1}{2} \left(\frac{\Omega}{(2\pi)^3} \right)^2 \int d\mathbf{k}_c \int \mathbf{k}_d \left\langle \mathbf{k}_a \mathbf{k}_b | v | \mathbf{k}_c \mathbf{k}_d \right\rangle \left\langle \mathbf{k}_c \mathbf{k}_d | t | \mathbf{k}_i \mathbf{k}_j \right\rangle \\
& \times \theta(|\mathbf{k}_c| - k_F) \theta(|\mathbf{k}_d| - k_F),
\end{aligned}
$$

where we have used the definition $\varepsilon(\mathbf{k}) \equiv \langle \mathbf{k} | f | \mathbf{k} \rangle$. Let us call this the *particle-particle (pp) and hole-hole (hh) ladders approximation*.

Relative-CM momentum coordinates

Let us define the relative and CM momentum coordinates

$$\mathbf{k} = (\mathbf{k}_i - \mathbf{k}_j)/2, \qquad \mathbf{K} = \mathbf{k}_i + \mathbf{k}_j$$
$$\mathbf{k}' = (\mathbf{k}_a - \mathbf{k}_b)/2, \qquad \mathbf{K}' = \mathbf{k}_a + \mathbf{k}_b$$
$$\mathbf{h} = (\mathbf{k}_k - \mathbf{k}_l)/2, \qquad \mathbf{H} = \mathbf{k}_k + \mathbf{l}$$
$$\mathbf{p} = (\mathbf{k}_c - \mathbf{k}_d)/2, \qquad \mathbf{P} = \mathbf{k}_c + \mathbf{k}_d$$

with the corresponding inverse relations

$$\mathbf{k}_i = \mathbf{k} + \mathbf{K}/2, \qquad \mathbf{k}_j = -\mathbf{k} + \mathbf{K}/2$$
$$\mathbf{k}_a = \mathbf{k}' + \mathbf{K}'/2, \qquad \mathbf{k}_b = -\mathbf{k} + \mathbf{K}'/2$$
$$\mathbf{k}_k = \mathbf{h} + \mathbf{H}/2, \qquad \mathbf{k}_l = -\mathbf{h} + \mathbf{H}/2$$
$$\mathbf{k}_c = \mathbf{p} + \mathbf{P}/2, \qquad \mathbf{k}_d = -\mathbf{p} + \mathbf{P}/2$$

pp-hh ladders equation in RCM coordinates

We can then write the pp-hh ladders equation in relative coordinates

$$
\begin{aligned}
0 = & \langle \mathbf{k}' | v | \mathbf{k} \rangle + \left(\varepsilon(|\mathbf{k}' + \mathbf{K}/2|) + \varepsilon(|-\mathbf{k}' + \mathbf{K}/2|) \right. \\
& \left. - \varepsilon(|\mathbf{k} - \mathbf{K}/2|) - \varepsilon(|-\mathbf{k} + \mathbf{K}/2|) \right) \langle \mathbf{k}' | t | \mathbf{k} \rangle \\
& + \frac{1}{2} \int d\mathbf{h} \, \langle \mathbf{k}' | t(\mathbf{K}) | \mathbf{h} \rangle \, \langle \mathbf{h} | v | \mathbf{k} \rangle \\
& \times \theta(k_F - |\mathbf{h} + \mathbf{K}/2|) \theta(k_F - |-\mathbf{h} + \mathbf{K}/2|) \\
& + \frac{1}{2} \int d\mathbf{p} \, \langle \mathbf{k}' | v | \mathbf{p} \rangle \, \langle \mathbf{p} | t(\mathbf{K}) | \mathbf{k} \rangle \\
& \times \theta(|\mathbf{p} + \mathbf{K}/2| - k_F) \theta(|-\mathbf{p} + \mathbf{K}/2| - k_F)
\end{aligned}
$$

Angular-average approximations for sp energy

Let us define

$$\Delta\tilde{\varepsilon}(k,k',K) \equiv \varepsilon(\overline{|\mathbf{k}+\mathbf{K}/2|}) + \varepsilon(\overline{|-\mathbf{k}+\mathbf{K}/2|}) - \varepsilon(\overline{|\mathbf{k}'+\mathbf{K}/2|}) - \varepsilon(\overline{|-\mathbf{k}'+\mathbf{K}/2|}),$$

where the single-particle energies on the right hand side are angular-average approximations. From now on we are going to use only angular-averaged approximations of the single-particle energy $\varepsilon(\mathbf{k},\mathbf{K})$.

Unity operators

Remember the following relations:

$$\int d\mathbf{k}\, |\mathbf{k}\rangle \langle \mathbf{k}| = 1$$

$$\sum_{lm_l} |lm_l\rangle \langle lm_l| = 1$$

$$\langle \hat{\mathbf{k}}|lm_l\rangle \equiv Y_{lm_l}(\hat{\mathbf{k}})$$

$$\int d\hat{\mathbf{k}}\, Y^*_{lm_l}(\hat{\mathbf{k}})\, Y_{l'm'_l}(\hat{\mathbf{k}}) = \delta_{ll'}\delta_{m_l m'_l}$$

$$\sum_{SM_S} |SM_S\rangle \langle SM_S| = 1$$

$$|lm_l SM_S\rangle = \sum_{\mathcal{J}m_{\mathcal{J}}} \langle lm_l SM_S|\mathcal{J}m_{\mathcal{J}}\rangle\, |\mathcal{J}m_{\mathcal{J}}(lS)\rangle$$

Here $\hat{\mathbf{k}} \equiv (\theta_{\mathbf{k}}, \phi_{\mathbf{k}})$ denotes the angles of $\mathbf{k}$ and the bracket in the last equation is a Clebsch-Gordan coefficient. $Y_{lm_l}(\hat{\mathbf{k}})$ is a spherical harmonics function.

Unity operators

Using the relations on the previous page, one can derive the following unity operator:

$$
\begin{aligned}
1 = & \sum_{\mathcal{J} m_{\mathcal{J}}} \sum_{\mathcal{J}' m_{\mathcal{J}'}} \sum_{S M_S} \sum_{\substack{l m_l \\ l' m_l'}} \int k^2 dk \int d\hat{\mathbf{k}} Y^*_{l m_l}(\hat{\mathbf{k}}) Y_{l' m_l'}(\hat{\mathbf{k}}) \\
& \times \langle l m_l S M_S | \mathcal{J} m_{\mathcal{J}} \rangle \langle l' m_{l'} S M_S | \mathcal{J}' m_{\mathcal{J}'} \rangle \\
& \times | k(lS) \mathcal{J} m_{\mathcal{J}} \rangle \langle k(l' S) \mathcal{J}' m_{\mathcal{J}'} | .
\end{aligned}
$$

The pp-hh ladders equation

We can now use the relations on the previous two pages to derive the pp-hh ladders approximation of the Coupled-Cluster T_2 amplitude equation with exact Pauli exclusion operators

$$
\begin{aligned}
&\Delta\tilde{\varepsilon}(k,k',K)\left\langle k'(l'S)\mathcal{J}'m_{\mathcal{J}'}|t(\mathbf{K})|k(lS)\mathcal{J}m_{\mathcal{J}}\right\rangle \\
&= \left\langle k'(l'S)\mathcal{J}'m_{\mathcal{J}'}|v|k(lS)\mathcal{J}m_{\mathcal{J}}\right\rangle \delta_{\mathcal{J}\mathcal{J}'}\delta_{m_{\mathcal{J}}m_{\mathcal{J}'}} \\
&+ \frac{1}{2}\sum_{\mathcal{J}''m_{\mathcal{J}''}}\sum_{l''l'''}\int_0^{k_F} h^2dh\left\langle k'(l'S)\mathcal{J}'m_{\mathcal{J}'}|t(\mathbf{K})|h(l''S)\mathcal{J}''m_{\mathcal{J}''}\right\rangle \\
&\times \left\langle h(l'''S)\mathcal{J}m_{\mathcal{J}}|v|k(lS)\mathcal{J}m_{\mathcal{J}}\right\rangle \\
&\times Q_{hh}(l''\mathcal{J}''m_{\mathcal{J}''},l'''\mathcal{J}m_{\mathcal{J}};STh K\theta_K\phi_K) \\
&+ \frac{1}{2}\sum_{\mathcal{J}''m_{\mathcal{J}''}}\sum_{l''l'''}\int_0^{\infty} p^2dp\left\langle k'(l'S)\mathcal{J}'m_{\mathcal{J}'}|v|p(l''S)\mathcal{J}'m_{\mathcal{J}'}\right\rangle \\
&\times \left\langle p(l'''S)\mathcal{J}''m_{\mathcal{J}''}|t(\mathbf{K})|k(lS)\mathcal{J}m_{\mathcal{J}}\right\rangle \\
&\times Q_{pp}(l''\mathcal{J}'m_{\mathcal{J}'},l'''\mathcal{J}''m_{\mathcal{J}''};STpK\theta_K\phi_K).
\end{aligned}
$$

Here we have the interaction matrix elements in the right form.

Exact Pauli exclusion operators

In the previous energy expression, we have used the definitions

$$Q_{hh}(l'''\mathcal{J}'''m_{\mathcal{J}'''}, l\mathcal{J}m_{\mathcal{J}}; STkP\theta_P\Phi_P) = \sum_{m_l m_{l'''}} \sum_{M_S} \int d\hat{\mathbf{k}}\, Y^*_{l'''m_{l'''}}(\hat{\mathbf{k}})\, Y_{lm_l}(\hat{\mathbf{k}}) \times \langle lm_l SM_S|\mathcal{J}m_{\mathcal{J}}\rangle \langle l'''m_{l'''}SM_S|\mathcal{J}'''m_{\mathcal{J}'''}\rangle \times \theta(k_F - |\mathbf{k}+\mathbf{P}/2|)\theta(k_F - |-\mathbf{k}+\mathbf{P}/2|)$$

and

$$Q_{pp}(l'\mathcal{J}m_{\mathcal{J}}, l''\mathcal{J}''m_{\mathcal{J}''}; STk'P\theta_P\phi_P) = \sum_{m_{l'} m_{l''}} \sum_{M'_S} \int d\hat{\mathbf{k}}'\, Y^*_{l'm_{l'}}(\hat{\mathbf{k}}')\, Y_{l''m_{l''}}(\hat{\mathbf{k}}') \times \langle l'm_{l'}SM'_S|\mathcal{J}m_{\mathcal{J}}\rangle \langle l''m_{l''}SM'_S|\mathcal{J}''m_{\mathcal{J}''}\rangle \times \theta(|\mathbf{k}'+\mathbf{P}/2| - k_F)\theta(|-\mathbf{k}'+\mathbf{P}/2| - k_F)$$

in a similar way as was introduced in a G-matrix calculation by K. Suzuki *et al.* (Nucl. Phys. A 665 (2000) 92–104).

Outline

Angular-average approximation $\overline{Q}_{hh}$

It is a commonly used approximation to do the replacement

$$Q_{hh}(l\mathcal{J}m_{\mathcal{J}}, l'\mathcal{J}'m_{\mathcal{J}'}; STHK\theta_K\phi_K) \to \overline{Q}_{hh} \equiv \frac{1}{4\pi}\int d\hat{\mathbf{K}} Q_{hh}(l\mathcal{J}m_{\mathcal{J}}, l'\mathcal{J}'m_{\mathcal{J}'}; STHK\theta_K\phi_K)$$
$$= f_{lST}x_{hh}\delta_{ll'}\delta_{\mathcal{J}\mathcal{J}'}\delta_{m_{\mathcal{J}}m_{\mathcal{J}'}},$$

where

$$x_{hh} = \begin{cases} 0 & \text{if } k \geq \sqrt{k_F^2 - P^2/4}, \\ -\frac{k^2 - k_F^2 + P^2/4}{kP} & \text{if } k_F - P/2 < k < \sqrt{k_F^2 - P^2/4}, \\ 1 & \text{otherwise.} \end{cases}$$

This is the *angular-average approximation of the hole-hole Pauli exclusion operator*.

Angular-average approximation $\overline{Q}_{pp}$

We can do a similar replacement for the particel-particle operator:

$$Q_{pp}(l\mathcal{J}m_{\mathcal{J}}, l'\mathcal{J}'m_{\mathcal{J}'}; STThK\theta_K\phi_K) \rightarrow \overline{Q}_{pp} \equiv \frac{1}{4\pi}\int d\hat{\mathbf{K}} Q_{pp}(l\mathcal{J}m_{\mathcal{J}}, l'\mathcal{J}'m_{\mathcal{J}'}; STThK\theta_K\phi_K)$$
$$= f_{lST}x_{pp}\delta_{ll'}\delta_{\mathcal{J}\mathcal{J}'}\delta_{m_{\mathcal{J}}m_{\mathcal{J}'}},$$

where

$$x_{pp} = \begin{cases} 0 & \text{if } k \leq \sqrt{k_F^2 - P^2/4}, \\ \frac{k^2 - k_F^2 + P^2/4}{kP} & \text{if } \sqrt{k_F^2 - P^2/4} < k < k_F + P/2, \\ 1 & \text{otherwise.} \end{cases}$$

This is the *angular-average approximation of the particle-particle Pauli exclusion operator*.

pp-hh ladders with angular-average approximation

When using the angular-average approximation, the pp-hh ladders equations simplify considerably:

$$
\begin{aligned}
&\Delta\tilde{\varepsilon}(k,k',K)\left\langle k'(l'S)\mathcal{J}|t(K)|k(lS)\mathcal{J}\right\rangle \\
&= \left\langle k'(l'S)\mathcal{J}|v|k(lS)\mathcal{J}\right\rangle \\
&+ \frac{1}{2}\sum_{l''}\int_0^{k_F} h^2 dh \left\langle k'(l'S)\mathcal{J}|t(K)|h(l''S)\mathcal{J}\right\rangle \left\langle h(l''S)\mathcal{J}|v|k(lS)\mathcal{J}\right\rangle \overline{Q}_{hh}(h,K) \\
&+ \frac{1}{2}\sum_{l''}\int_0^{\infty} p^2 dp \left\langle k'(l'S)\mathcal{J}|v|p(l''S)\mathcal{J}\right\rangle \left\langle p(l''S)\mathcal{J}|t(K)|k(lS)\mathcal{J}\right\rangle \overline{Q}_{pp}(p,K).
\end{aligned}
$$

Observe that the t-amplitude is diagonal in $\mathcal{J}$, and independent of $m_{\mathcal{J}}$ and the CM momentum angles θ_K and ϕ_K.

CCD energy in angular-average approximation

The CCD energy becomes in the angular-average approximation

$$\Delta E_{CCD} = \pi \frac{\Omega}{(2\pi)^3} \sum_{S} \sum_{TM_T} \sum_{ll'} \sum_{\mathcal{J}} (2\mathcal{J}+1)$$
$$\times \int_0^{\sqrt{k_F^2 - P^2/4}} k^2 dk \int_{\sqrt{k_F^2 - P^2/4}}^{\infty} k'^2 dk' \int_0^{2k_F} K^2 dK$$
$$\times \left\langle k(lS)\mathcal{J}|v|k'(l'S)\mathcal{J}\right\rangle \left\langle k'(l'S)\mathcal{J}|t(K)|k(lS)\mathcal{J}\right\rangle$$
$$\times \overline{Q}_{hh}(k,K)\overline{Q}_{pp}(k',K).$$

Outline

How large matrices do we get?

The CCD energy and amplitude equations are solved most efficiently using matrix-matrix multiplications. How large will the matrices in these equations be? Let us estimate the memory requirements for the t-amplitude matrix, which is the largest matrix here.

A reasonable setting for the number of quadratre grid points in the numerical integration is

$$n_k = n_{k'} = n_K = 80, \qquad n_{\theta_K} = n_{\phi_K} = 20,$$

and a realistic condition for the total relative angular momentum is $0 \leq \jmath \leq 6$. With these settings, the approximate size of the total t-matrix becomes

angular-averaged approximation: 660 MB

exact Pauli exclusion operator: 110 TB

Independence of ϕ_K

The required memory use for the exact t-amplitude matrix is clearly too much even for normal supercomputers today. To do calculations with the exact Pauli operator, we need to optimize the memory use.

As given in Eq. (2.11) in K. Suzuki *et al.* (Nucl. Phys. A 665 (2000) 92–104, the Pauli operators can be written

$$Q(l\mathcal{J}m_{\mathcal{J}}, l'\mathcal{J}'m_{\mathcal{J}'}; STkK\theta_K\phi_K) = Q(l\mathcal{J}m_{\mathcal{J}}, l'\mathcal{J}'m_{\mathcal{J}'}; STkK\theta_K\phi_K = 0) \times e^{i(m_{\mathcal{J}'} - m_{\mathcal{J}})\phi_K}.$$

Using this relation, we find that the variable ϕ_K can be separated out from the t-matrix equation. Consequently, the memory use of the t-matrix decreases by a factor of 20 to

exact Pauli exclusion operator: 5.4 TB

This is still too much.

Using the rotation matrix

Similarly as was done by Suzuki *et al.*, we can calculate the t-amplitude matrix in a coordinate system where $\theta_K = \phi_K = 0$, and then use the rotation operator $\hat{D}(\alpha, \beta, \gamma)$ to get the matrix for other CM momentum angles.

Definition (*Wigner D-function*):

$$\left\langle \mathcal{J} m_{\mathcal{J}} | \hat{D}(\alpha, \beta, \gamma) | \mathcal{J}' m_{\mathcal{J}'} \right\rangle = \delta_{\mathcal{J}\mathcal{J}'} D^{\mathcal{J}}_{m_{\mathcal{J}} m_{\mathcal{J}'}}(\alpha, \beta, \gamma),$$

where $\hat{D}(\alpha, \beta, \gamma)$ is the rotation operator.

α, β, and γ are Euler angles defined e.g. in D. A. Varshalovich *et al.*, *Quantum theory of Angular Momentum* (World Scientific, Singapore, 1988).

Rotation of vectors

The ket vector can be rotated as

$$\left|k(l'''S)\mathcal{J}'''m_{\mathcal{J}'''}\mathbf{K}\right\rangle = \sum_{m_{\mathcal{J}'}} D^{\mathcal{J}'''*}_{m_{\mathcal{J}'''}m_{\mathcal{J}'}}(\phi_K,\theta_K,0)\left|k(l'''S)\mathcal{J}'''m_{\mathcal{J}'}K00\right\rangle$$

and the bra vector as

$$\left\langle k'(l''S)\mathcal{J}''m_{\mathcal{J}''}\mathbf{K}\right| = \sum_{m_{\mathcal{J}}} D^{\mathcal{J}''}_{m_{\mathcal{J}''}m_{\mathcal{J}}}(\phi_K,\theta_K,0)\left\langle k'(l''S)\mathcal{J}''m_{\mathcal{J}}K00\right|.$$

Rotation of matrix

The t-matrix can be rotated according to

$$\begin{aligned}
&\left\langle k'(l''S)\mathcal{J}''m_{\mathcal{J}''}|t(\mathbf{K})|k(l'''S)\mathcal{J}'''m_{\mathcal{J}'''}\right\rangle \\
&= \sum_{m_{\mathcal{J}}m_{\mathcal{J}'}} D^{\mathcal{J}''}_{m_{\mathcal{J}''}m_{\mathcal{J}}}(\phi_K,\theta_K,0)D^{\mathcal{J}'''*}_{m_{\mathcal{J}'''}m_{\mathcal{J}'}}(\phi_K,\theta_K,0) \\
&\times \left\langle k'(l''S)\mathcal{J}''m_{\mathcal{J}}|t(K)|k(l'''S)\mathcal{J}'''m_{\mathcal{J}'}\right\rangle .
\end{aligned}$$

In the special case with only pp and hh ladders, the t-amplitude becomes diagonal in $m_{\mathcal{J}}$ when $\phi_k = 0$. In this case we get

$$\begin{aligned}
&\left\langle k'(l''S)\mathcal{J}''m_{\mathcal{J}''}|t(\mathbf{K})|k(l'''S)\mathcal{J}'''m_{\mathcal{J}'''}\right\rangle \\
&= \sum_{m_{\mathcal{J}'}} D^{\mathcal{J}''}_{m_{\mathcal{J}''}m_{\mathcal{J}'}}(\phi_K,\theta_K,0)D^{\mathcal{J}'''*}_{m_{\mathcal{J}'''}m_{\mathcal{J}'}}(\phi_K,\theta_K,0) \\
&\times \left\langle k'(l''S)\mathcal{J}''m_{\mathcal{J}'}|t(K)|k(l'''S)\mathcal{J}'''m_{\mathcal{J}'}\right\rangle .
\end{aligned}$$

We get acceptable memory use

When using the rotation matrix, we have a t-matrix which does not depend on the angles of the CM momentum, (θ_K, ϕ_K). In the pp-hh ladders approximation, the t-matrix is also diagonal in $m_{\mathcal{J}}$. This simplification decreases the memory use further by a factor of around 200.

The memory requirements for the t-matrix becomes now

exact Pauli exclusion operator: 26 GB

This is a matrix size we can handle with. The total RAM memory use becomes around 100 GB, which is acceptable with current resources.

CCD energy with rotation matrices

Let us express the Wigner D-function as

$$D^J_{MM'}(\alpha,\beta,\gamma) = e^{-iM\alpha} d^J_{MM'}(\beta) e^{-iM'\gamma}.$$

The CCD correlation energy can then be written

$$\begin{aligned}
\Delta E_{CCD} = \frac{\pi}{2}\left(\frac{\Omega}{(2\pi)^3}\right)^2 & \sum_S \sum_{TM_T} \sum_{ll'} \sum_{l''l'''} \sum_{\mathcal{J}m_{\mathcal{J}}} \sum_{\mathcal{J}''m_{\mathcal{J}''}} \sum_{\mathcal{J}'''m_{\mathcal{J}'''}} \sum_{m_{\mathcal{J}'}} \\
& \times \int_0^{k_F} k^2 dk \int_0^{\infty} k'^2 dk' \int_0^{2k_F} K^2 dK \int_{-1}^{1} d\cos\theta_K \\
& \times d^{\mathcal{J}''}_{m_{\mathcal{J}''}, m_{\mathcal{J}'}}(\theta_K) d^{\mathcal{J}'''}_{m_{\mathcal{J}'''}, m_{\mathcal{J}'}}(\theta_K) \\
& \times \left\langle k(lS)\mathcal{J}|v|k'(l'S)\mathcal{J}\right\rangle \left\langle k'(l''S)\mathcal{J}''m_{\mathcal{J}'}|t(K)|k(l'''S)\mathcal{J}'''m_{\mathcal{J}'}\right\rangle \\
& \times Q_{hh}(l'''\mathcal{J}'''m_{\mathcal{J}'''}, l\mathcal{J}m_{\mathcal{J}}; STkK\theta_K) \\
& \times Q_{pp}(l'\mathcal{J}m_{\mathcal{J}}, l''\mathcal{J}''m_{\mathcal{J}''}; STk'K\theta_K).
\end{aligned}$$

Outline

Definition of matrices

Assume we have the matrices $T^{S\mathcal{J}M_T K}$, $V^{S\mathcal{J}M_T}$, Q^K_{hh}, and Q^K_{pp}, where the corresponding matrix elements are defined by

$$
\begin{aligned}
t^{S\mathcal{J}M_T K}(k'l', kl) &\equiv \left\langle k'(l'S)\mathcal{J}|t(K)|k(lS)\mathcal{J}\right\rangle, \\
v^{S\mathcal{J}M_T}(kl, k'l') &\equiv \left\langle k(lS)\mathcal{J}|v|k'(l'S)\mathcal{J}\right\rangle, \\
q^K_{hh}(kl, k'l') &\equiv k^2\omega_k Q_{hh}(k, K)\delta_{k,k'}\delta_{ll'}, \\
q^K_{pp}(kl, k'l') &\equiv k^2\omega_k Q_{pp}(k, K)\delta_{k,k'}\delta_{ll'}.
\end{aligned}
$$

Implementation of energy expression

We can then write the energy expression using numerical quadrature integration and matrix-matrix multiplications:

$$\Delta E_{CCD} = \pi \frac{\Omega}{(2\pi)^3} \sum_{S} \sum_{TM_T} \sum_{\mathcal{J}} (2\mathcal{J}+1) \sum_{i} \omega_{K_i} K_i^2 \mathrm{Tr}\left[V^{S\mathcal{J}M_T} Q_{pp}^{K_i} T^{S\mathcal{J}M_T K_i} Q_{hh}^{K_i} \right],$$

where

$$\mathrm{Tr}[A] = \text{trace of the matrix A.}$$

Implementation of pp-hh ladders equation

Using the same definitions as above, we can write the amplitude equation in the angular-average pp-hh ladders approximation

$$T^{S\mathcal{J}M_T K} = V^{S\mathcal{J}M_T} + \frac{1}{2}\tilde{T}^{S\mathcal{J}M_T K} Q^K_{hh} V^{S\mathcal{J}M_T} + \frac{1}{2} V^{S\mathcal{J}M_T} Q^K_{pp} \tilde{T}^{S\mathcal{J}M_T},$$

where the matrix elemenets of the matrix $\tilde{T}^{S\mathcal{J}M_T}$ are defined as

$$\left(\tilde{T}^{S\mathcal{J}M_T}\right)_{(k'l',kl)} = t^{S\mathcal{J}M_T K}(k'l', kl)/\Delta\tilde{\varepsilon}(k, k', K).$$

Results – Angular-average approximation

,

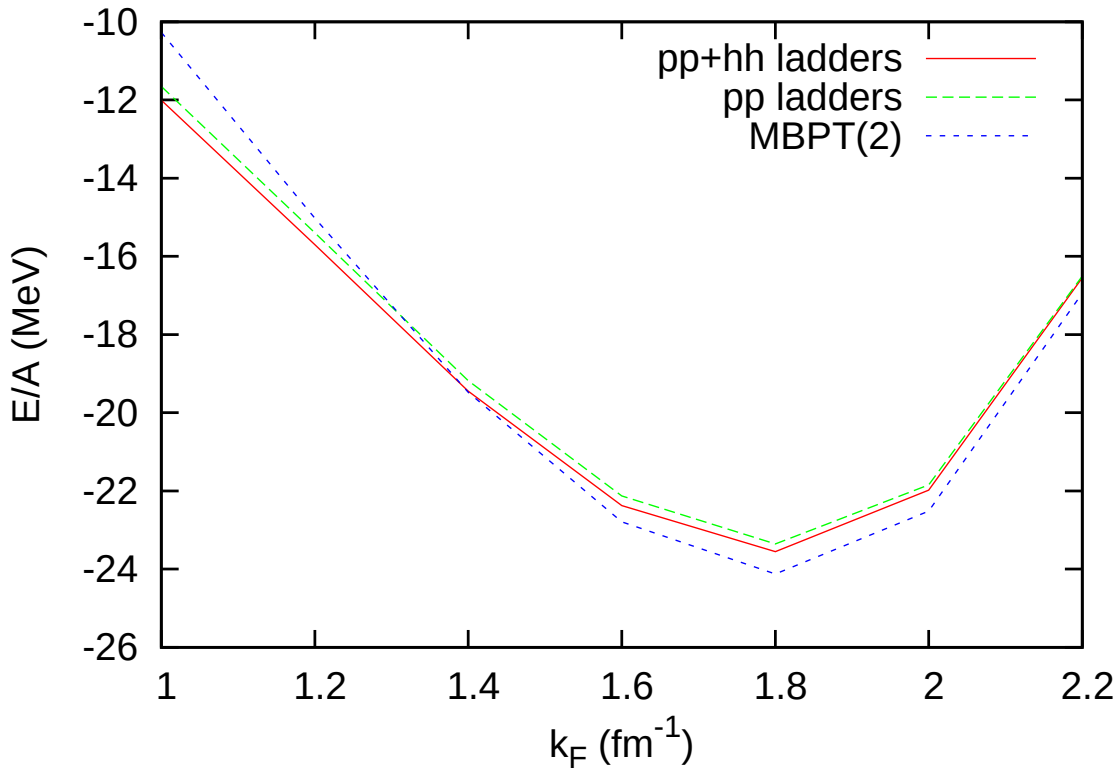

Figure: Binding energy of symmertic nuclear matter. Here we have used the angular-average approximation and a two-particle interaction derived from Chiral Perturbation Theory.

Outline

Definition of matrices

We define for the calculation with exact Pauli operator the matrices $T^{SM_T K \mathcal{J} m_{\mathcal{J}} \mathcal{J}'}$, $V^{SM_T \mathcal{J}}$, $Q_{hh}^{SM_T K \mathcal{J} m_{\mathcal{J}} \mathcal{J}' m_{\mathcal{J}'}}$, and $Q_{pp}^{SM_T K \mathcal{J} m_{\mathcal{J}} \mathcal{J}' m_{\mathcal{J}'}}$ with the corresponding matrix elements

$$
\begin{aligned}
t^{SM_T K \mathcal{J} m_{\mathcal{J}} \mathcal{J}'}(kl, kl') &\equiv \left\langle k(lS)\mathcal{J} m_{\mathcal{J}} | t(K) | k'(l'S)\mathcal{J}' m_{\mathcal{J}} \right\rangle, \\
v^{SM_T \mathcal{J}}(kl, k'l') &\equiv \left\langle k(lS)\mathcal{J} | v | k'(l'S)\mathcal{J} \right\rangle, \\
q_{hh}^{SM_T K \mathcal{J} m_{\mathcal{J}} \mathcal{J}' m_{\mathcal{J}'}}(kl, kl') &\equiv k^2 \omega_k Q_{hh}(l\mathcal{J} m_{\mathcal{J}}, l'\mathcal{J}' m_{\mathcal{J}'}; SM_T k K \theta_K \phi_K = 0), \\
q_{pp}^{SM_T K \mathcal{J} m_{\mathcal{J}} \mathcal{J}' m_{\mathcal{J}'}}(kl, kl') &\equiv k^2 \omega_k Q_{pp}(l\mathcal{J} m_{\mathcal{J}}, l'\mathcal{J}' m_{\mathcal{J}'}; SM_T k K \theta_K \phi_K = 0).
\end{aligned}
$$

Implementation of energy expression

We can then write the energy expression with exact Pauli operators using numerical quadrature integration and matrix-matrix multiplications:

$$\Delta E_{pp-hh} = \frac{\pi}{2}\left(\frac{\Omega}{(2\pi)^3}\right)^2 \sum_{S}\sum_{TM_T}\sum_{\mathcal{J}m_{\mathcal{J}}}\sum_{\mathcal{J}''m_{\mathcal{J}}''}\sum_{\mathcal{J}'''m_{\mathcal{J}}'''}\sum_{m_{\mathcal{J}}'}$$
$$\times \sum_{P_i} P_i^2 \omega_{P_i} \sum_{\theta_j} \sin\theta_j \omega_{\theta_j} d^{\mathcal{J}''}_{m_{\mathcal{J}}'', m_{\mathcal{J}}'}(\theta_j) d^{\mathcal{J}'''}_{m_{\mathcal{J}}''', m_{\mathcal{J}}'}(\theta_j)$$
$$\times \mathrm{Tr}\left[V^{SM_T\mathcal{J}} Q_{pp}^{SM_T P_i \mathcal{J} m_{\mathcal{J}} \mathcal{J}'' m_{\mathcal{J}}''} T^{SM_T P_i \mathcal{J}'' m_{\mathcal{J}}', \mathcal{J}'''} Q_{hh}^{SM_T P_i \mathcal{J}''' m_{\mathcal{J}}''', \mathcal{J} m_{\mathcal{J}}} \right],$$

where θ_j is the discrete counterpart of θ_P and

$$\mathrm{Tr}[A] = \text{trace of the matrix A.}$$

Implementation of pp-hh ladders equation

Using the same definitions as above, we can write the amplitude equation in the pp-hh ladders approximation with exact Pauli operator

$$
\begin{aligned}
T^{SM_T P\mathcal{J}' m_{\mathcal{J}} \mathcal{J}} &= V^{SM_T \mathcal{J}} \delta_{\mathcal{J}\mathcal{J}'} \\
&+ \frac{1}{2} \sum_{\mathcal{J}''} \tilde{T}^{SM_T P\mathcal{J}' m_{\mathcal{J}} \mathcal{J}''} Q_{hh}^{SM_T P\mathcal{J}'' m_{\mathcal{J}} \mathcal{J} m_{\mathcal{J}}} V^{SM_T \mathcal{J}} \\
&+ \frac{1}{2} \sum_{\mathcal{J}''} V^{SM_T \mathcal{J}'} Q_{pp}^{SM_T P\mathcal{J}' m_{\mathcal{J}} \mathcal{J}'' m_{\mathcal{J}}} \tilde{T}^{SM_T P\mathcal{J}'' m_{\mathcal{J}} \mathcal{J}},
\end{aligned}
$$

where the matrix elements of the matrix $\tilde{T}^{SM_T P\mathcal{J} m_{\mathcal{J}} \mathcal{J}'}$ are defined as

$$
\left(\tilde{T}^{SM_T P\mathcal{J} m_{\mathcal{J}} \mathcal{J}'}\right)_{(k'l',kl)} = t^{SM_T P\mathcal{J} m_{\mathcal{J}} \mathcal{J}' m_{\mathcal{J}}}(k'l', kl)/\Delta\tilde{\varepsilon}(k, k', P).
$$