Lecture II: Renormalization of the Nucleon-Nucleon Interaction

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Outline

1. Renormalization of the NN force
   - Perturbation Theory
   - Model Space and Interactions
   - G-matrix
   - No-Core Shell-Model Calculations
   - Momentum-space truncations and effective interactions
   - Final Effective two-body Hamiltonians

What do we want to do?

- An effective interaction for the shell model based on an NN or even NNN nuclear force.
- We need then to understand how to define model spaces for various nuclear systems and their link to large-scale shell-model calculations
- We need to renormalize the repulsive part of the NN force (maybe also NNN force).
- This leads to the first step: computation of the G-matrix, or no-core interaction or $V_{\mathrm{low-k}}$ interactions.
- The next step is the computation of a model space effective interaction and/or operator. Such interactions are normally of two-body character. There are calculations with three-body forces also, standard shell-model, no-core shell-model , coupled-cluster and Green's function Monte Carlo for light nuclei.
- Finally, applications to nuclear systems using the shell model, Green's function methods, many-body perturbation theory, Coupled Cluster etc..

This is what we typically want to do

Find the lowest ($\approx$ 10–50) solution of the eigenvalue problem

$$H\left|\Psi_m(A)\right\rangle = (T+V)\left|\Psi_m(A)\right\rangle = E_m\left|\Psi_m(A)\right\rangle$$

Derivation of a valence shell effective Hamiltonian:

$$H = H_0 + H_1, \quad H_0 = T + U, \quad H_1 = V - U.$$

Valence P–space and excluded Q–space:

$$P = \sum_{i=1}^{n} \left|\psi_i\right\rangle \left\langle\psi_i\right|, \quad Q = \sum_{i=n+1}^{\infty} \left|\psi_i\right\rangle \left\langle\psi_i\right|.$$

and model space Hamiltonian

$$PH_{eff}\,P\left|\Psi_m\right\rangle = P\left(\widetilde{H}_0 + (H_1)_{eff}\right)P\left|\Psi_m\right\rangle = E_m P\left|\Psi_m\right\rangle$$

Approaches to effective interactions

- Extract interactions from spectra
- Parameterize given interactions from say many-body theory so as to reproduce data of selected nuclei. Examples are the interactions for the *sd*-shell and *fp*-shell interactions.
- Take an effective interaction from many-body theory and correct the monopole terms. Strasbourg group has developed a recipe based on a fitted single-particle energies of $A \pm 1$ nuclei. The effective monopole interaction can be rewritten as a global term, one-body term, two-body term etc. The one-body term can be extracted from fitted single-particle energies and used to corrected the energy-centroids. Cures for example problem with closure in ^{48}Ca.
- Fiddle with certain matrix elements which cause problems

A Microscopic Approach

From the NN-interaction to an effective interaction, many-body approach. This encompasses both no-core shell-model calcs, standard effective interactions and Coupled cluster inspired approaches

- NN-interaction fitted to world scattering data, Lecture I.
- Construct a two-body interaction which renormalizes the bare interaction, Lecture II.
- Sum large classes of diagrams with a selected model space, Lecture III.
- Resummation of selected classes of one and two-body diagrams, , Lecture III.
- Inclusion of effective three-body diagrams, , Lecture III.
- Combined with a shell-model code this recipes allows for the possibility to retrace various problems in theory, , Lecture IV.

Model Space and Hamiltonians

$$P = \sum_{i=1}^{D} |\psi_i\rangle \langle\psi_i| ,$$

and

$$Q = \sum_{i=D+1}^{\infty} |\psi_i\rangle \langle\psi_i| ,$$

with D being the dimension of the model space, and $PQ = 0$, $P^2 = P$, $Q^2 = Q$ and $P + Q = I$. The wave functions $|\psi_i\rangle$ are eigenfunctions of the unperturbed hamiltonian $H_0 = T + U$ (with eigenvalues ε_i), where T is the kinetic energy and U an appropriately chosen one-body potential, normally that of the harmonic oscillator (h.o.). The full hamiltonian is then rewritten as $H = H_0 + H_1$ with $H_1 = V - U$, V being e.g. the nucleon-nucleon (NN) interaction

Wave Operator I

We define the projection of the exact wave function $|\Psi_\alpha\rangle$ of a state α, i.e. the solution to the full Schrödinger equation

$$H|\Psi_\alpha\rangle = E_\alpha|\Psi_\alpha\rangle,$$

as $P|\Psi_\alpha\rangle = |\Psi_\alpha^M\rangle$ and a wave operator Ω which transforms all the model states back into the corresponding exact states as $|\Psi_\alpha\rangle = \Omega|\Psi_\alpha^M\rangle$. The latter statement is however not trivial, it actually means that there is a one-to-one correspondence between the d exact states and the model functions. We will now assume that the wave operator Ω has an inverse. Use a similarity transformation of the hamiltonian

$$\Omega^{-1}H\Omega\Omega^{-1}|\Psi_\alpha\rangle = E_\alpha\Omega^{-1}|\Psi_\alpha\rangle.$$

Wave Operator II

Recall also that $|\Psi_\alpha\rangle = \Omega \left|\Psi_\alpha^M\right\rangle$, which means that $\Omega^{-1} |\Psi_\alpha\rangle = \left|\Psi_\alpha^M\right\rangle$ insofar as the inverse of Ω exists. Let us define the transformed hamiltonian $\mathcal{H} = \Omega^{-1} H \Omega$, which can be rewritten in terms of the operators P and Q ($P + Q = I$) as

$$\mathcal{H} = P\mathcal{H}P + P\mathcal{H}Q + Q\mathcal{H}P + Q\mathcal{H}Q.$$

The eigenvalues of $\mathcal{H}$ are the same as those of H, since a similarity transformation does not affect the eigenvalues.

$$\mathcal{H} \left|\Psi_\alpha^M\right\rangle = E_\alpha \left|\Psi_\alpha^M\right\rangle,$$

with the operator Q, one can show the so-called decoupling condition

$$Q\mathcal{H}P = 0.$$

Wave Operator III

The last equation is an important relation which states that the eigenfunction $P|\Psi_\alpha\rangle$ is a *pure model space eigenfunction*. This implies that we can define an *effective model space hamiltonian*

$$H_{\text{eff}} = P\mathcal{H}P = P\Omega^{-1}H\Omega P,$$

or equivalently

$$H\Omega P = \Omega P H_{\text{eff}} P,$$

which is the Bloch equation. This equation can be used to determine the wave operator Ω.
The wave operator is often expressed as

$$\Omega = 1 + \chi,$$

where χ is known as the correlation operator.

Wave Operator IV

The wave operator Ω can be ordered in terms of the number of interactions with the perturbation H_1

$$\Omega = 1 + \Omega^{(1)} + \Omega^{(2)} + \dots,$$

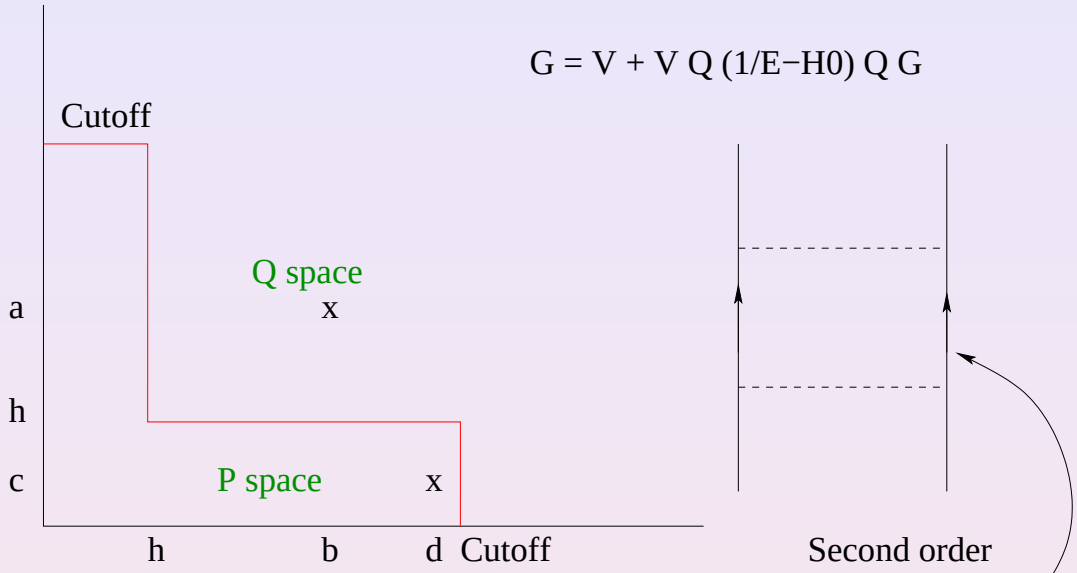
where $\Omega^{(n)}$ means that we have n H_1 terms. Explicitly, the above equation reads

$$\begin{aligned}\Omega \left|\psi_\alpha\right\rangle = \quad \left|\psi_\alpha\right\rangle + \sum_i \frac{\left|i\right\rangle \left\langle i\right| H_1 \left|\psi_\alpha\right\rangle}{\varepsilon_\alpha - \varepsilon_i} + \sum_{ij} \frac{\left|i\right\rangle \left\langle i\right| H_1 \left|j\right\rangle \left\langle j\right| H_1 \left|\psi_\alpha\right\rangle}{(\varepsilon_\alpha - \varepsilon_i)(\varepsilon_\alpha - \varepsilon_j)} \\ - \sum_{\beta i} \frac{\left|i\right\rangle \left\langle i\right| H_1 \left|\psi_\beta\right\rangle \left\langle \psi_\beta\right| H_1 \left|\psi_\alpha\right\rangle}{(\varepsilon_\alpha - \varepsilon_i)(\varepsilon_\alpha - \varepsilon_\beta)} + \dots,\end{aligned}$$

where ε are the unperturbed energies of the P-space

Pauli Operator I

Typical Pauli operator for Nuclear matter



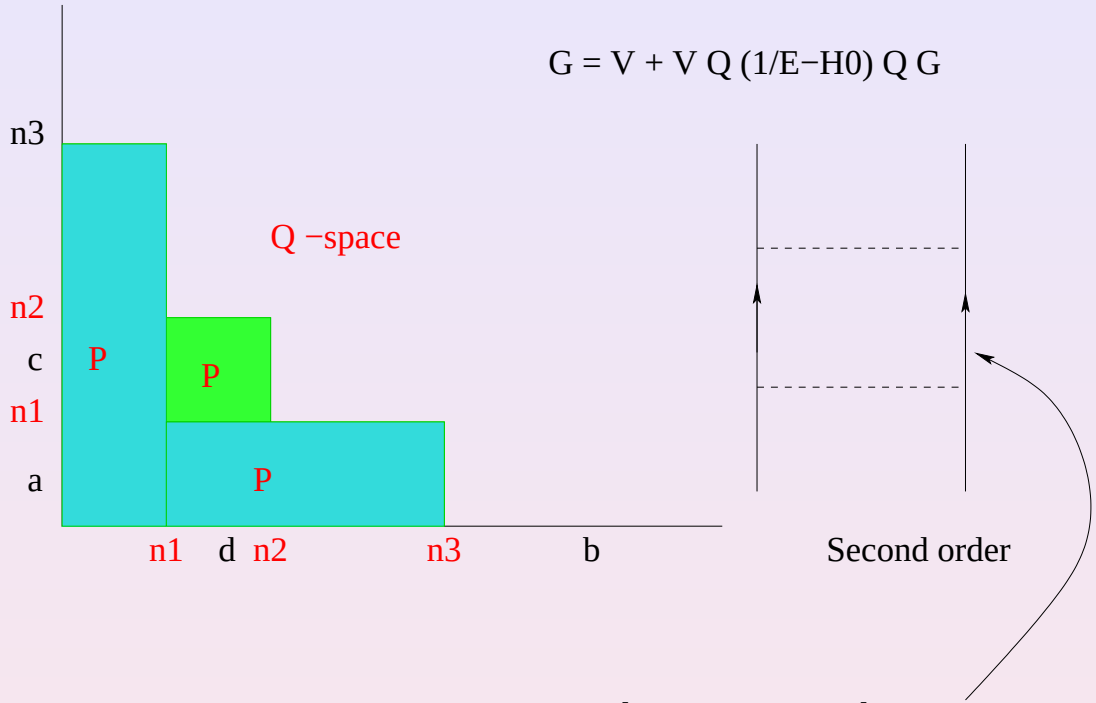
Intermediate states outside P−space

| ab > is in Q−space and included as intermediate state in G

| cd > is not included in G

Pauli Operator II

Typical Pauli operator for finite nuclei



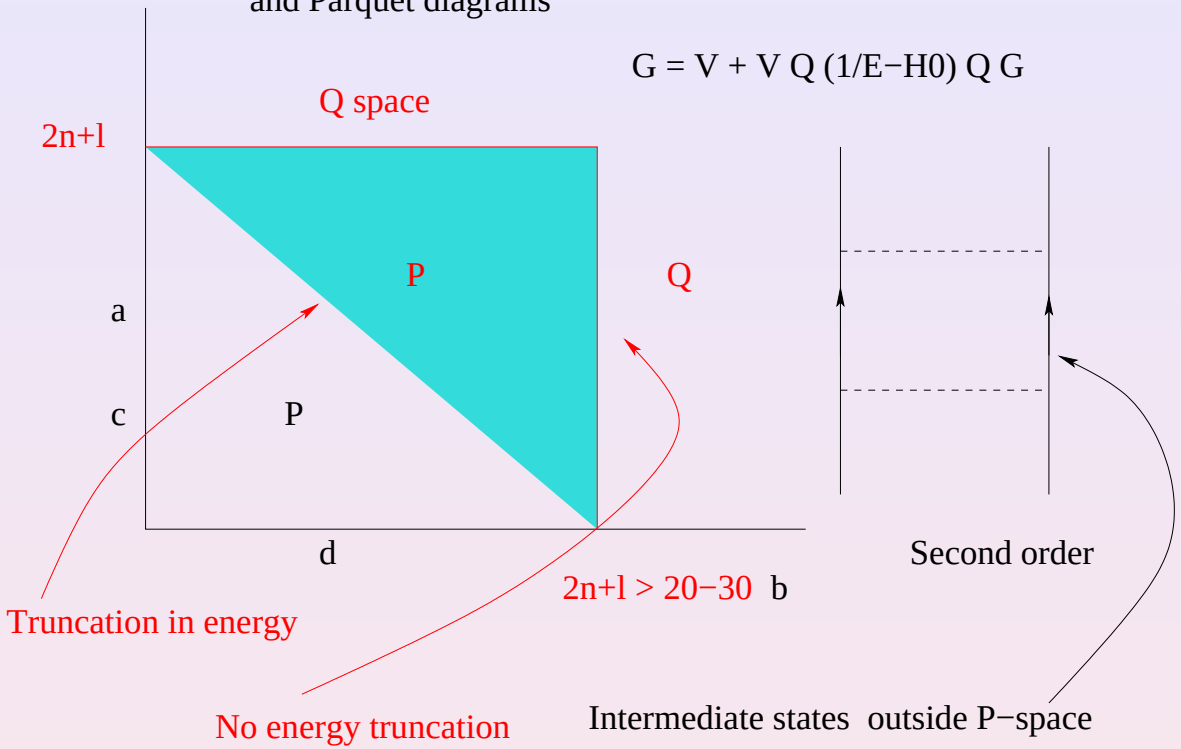
| ab > is in Q−space and included as intermediate state in G

| cd > is not included in G

Pauli Operator III

Pauli operator for no−core calculations and Coupled cluster and Parquet diagrams

G = V + V Q (1/E−H0) Q G



| ab > is in Q−space and included as intermediate state in G

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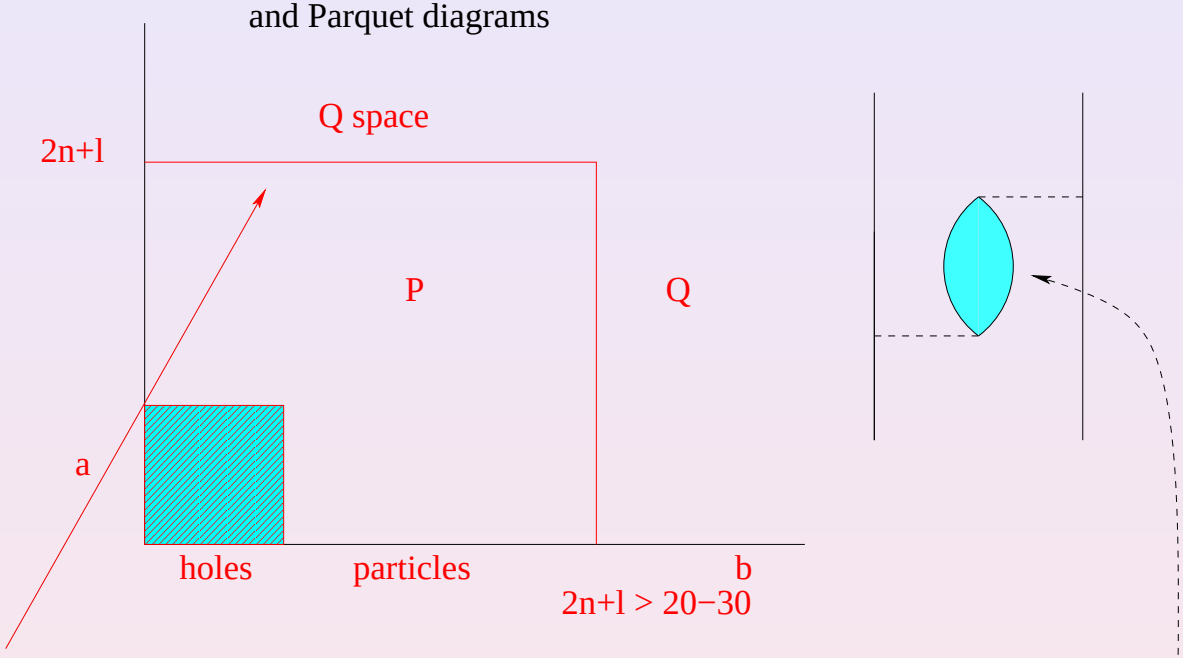
Pauli Operator IV

Pauli operator for no−core calculations and Coupled cluster and Parquet diagrams



Defines new Hilbert space where the bare interaction V has been replaced by an appropriate G−matrix. Many types of basis can be used, oscillator, plane waves etc.

Can generate through Parquet or Coupled cluster diagrams with | hh >, |pp > and | ph > states. However, by definition, configurations like | a b > cannot be included where a is a hole and b a particle state (1p−1h correlations)

G-matrix: Resummation of a Class of Diagrams

- The NN (and also NNN) are strongly repulsive at short distances. This will give large matrix elements for the shell model.
- Construct an interaction which renormalizes the short distance part of the nucleon-nucleon force. Here we can use a G-matrix appropriatey defined for a model space or a no-core interaction.
- For a G-matrix we sum the so-called ladder diagrams, representing highly excited (short distances) two-body states.

G-matrix: Resummation of a Class of Diagrams

- Then we use this renormalized short-range interaction to compute other processes, like core-polarization diagrams etc.
- Note that strictly speaking we are solving a two-body problem. However, for the deuteron (free particles) we can solve Schrödinger's equation exactly. For the many-body problem we need to define a model space and can thus sum only selected classes of physical processes.

Definitions

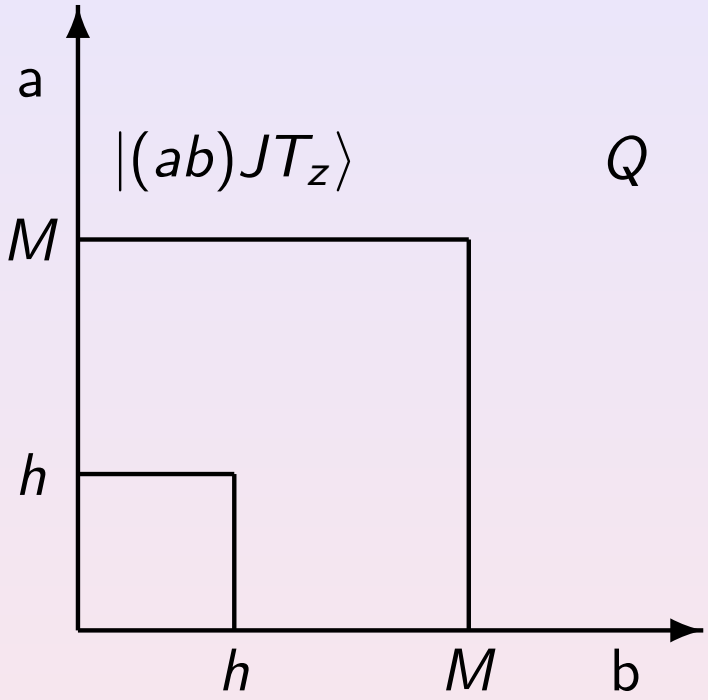
$$\tilde{G}_{ijij} = \tilde{V}_{ijij} + \sum_{mn>k_F} \frac{1}{2} \tilde{V}_{ijmn} \frac{1}{\varepsilon_i + \varepsilon_j - \varepsilon_m - \varepsilon_n} \tilde{G}_{mnij}.$$

Note that $\tilde{G}$ is the antisymmetrized G-matrix since the potential $\tilde{V}$ is also antisymmetrized. This means that $\tilde{G}$ obeys$\tilde{G}_{ijij} = -\tilde{G}_{jiij} = -\tilde{G}_{ijji}$ The $\tilde{G}$-matrix is defined as $\tilde{G}_{ijij} = G_{ijij} - G_{jiij}$,

$$G_{ijij} = V_{ijij} + \sum_{mn>k_F} V_{ijmn} \frac{1}{\varepsilon_i + \varepsilon_j - \varepsilon_m - \varepsilon_n} G_{mnij},$$

$$G_{ijij} = V_{ijij} + \sum_{mn>0} V_{ijmn} \frac{Q(mn)}{\omega - \varepsilon_m - \varepsilon_n} G_{mnij},$$

Effective Hamiltonian and Model Spaces



$$M \leq 2n + l \approx 4 - 20$$

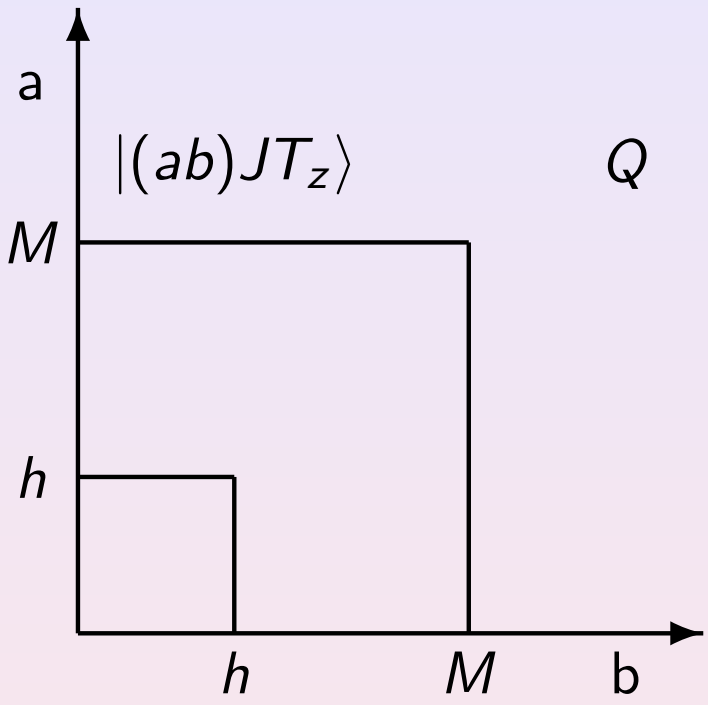
Two-Body Effective Hamiltonian for Large Space

Need to renormalize short-range behavior of V:

$$G_{ijkl} = V_{ijkl} + \sum_{mn \in Q} V_{ijmn} \frac{Q}{\omega - \varepsilon_m - \varepsilon_n} G_{mnkl}$$

- Harmonic oscillator basis.
- Note well energy ω dependence!
- NN interactions + Coulomb.

Effective Hamiltonian and Model Spaces



$$M \leq 2n + l \approx 4 - 20$$

Two-Body Effective Hamiltonian for Large Space

- With G we can in turn include higher-order contributions via Many-body perturbation theory.
- This is defined for a smaller space
- Need to test results as function of smaller space in connection with shell-model calculations.

Computational Procedure I

$$G(\omega) = V + V\frac{Q}{\omega - H_0}G(\omega),$$

or

$$G(\omega) = V + VQ\frac{1}{\omega - QH_0Q}QG(\omega).$$

The former equation applies if the Pauli operator Q commutes with the unperturbed hamiltonian H_0, whereas the latter is needed if $[H_0, Q] \neq 0$. Similarly, the correlated wave function Ψ is given as

$$|\Psi\rangle = |\psi\rangle + \frac{Q}{\omega - H_0}G\,|\psi\rangle\,,$$

or

$$|\Psi\rangle = |\psi\rangle + Q\frac{1}{\omega - QH_0Q}QG\,|\psi\rangle\,.$$

Computational Procedure II

Defining the wave operators

$$\Omega_1 = 1 + \frac{Q_1}{e_1} G_1,$$

and

$$\Omega_2 = 1 + \frac{Q_2}{e_2} G_2,$$

we can rewrite the above G-matrices as

$$G_1 = V_1 \Omega_1,$$

and

$$G_2 = V_2 \Omega_2.$$

Computational Procedure III

Using these relations, we rewrite G_1 as

$$\begin{aligned} G_1 = \quad & G_1 - G_2^\dagger \left(\Omega_1 - 1 - \frac{Q_1}{e_1} G_1 \right) + \left(\Omega_2^\dagger - 1 - G_2^\dagger \frac{Q_2}{e_2} \right) G_1 \\ = \quad & G_2^\dagger + G_2^\dagger \left(\frac{Q_1}{e_1} - \frac{Q_2}{e_2} \right) G_1 + \Omega_2^\dagger G_1 - G_2^\dagger \Omega_1, \end{aligned}$$

we obtain the identity

$$G_1 = G_2^\dagger + G_2^\dagger \left(\frac{Q_1}{e_1} - \frac{Q_2}{e_2} \right) G_1 + \Omega_2^\dagger (V_1 - V_2) \Omega_1.$$

The second term on the rhs. is called the propagator-correction term; it vanishes if G_1 and G_2 have the same propagators. The third term is often referred to as the potential-correction term, and it disappears if G_1 and G_2 have the same potentials.

Computational Procedure IV

Define the correlated wave function Ψ_a

$$G\,|\psi_a\rangle = V\,|\Psi_a\rangle\,,$$

where ψ_a is the unperturbed wave function. Using the definition of the correlated wave function we have

$$|\Psi_a\rangle = |\psi_a\rangle + \frac{Q}{\omega - H_0}\,G\,|\psi_a\rangle = |\psi_a\rangle + \frac{Q}{\omega - H_0}\,V\,|\Psi_a\rangle\,.$$

Note that we have assumed that the Pauli operator Q and the unperturbed Hamiltonian H_0 commute. If we are able to obtain the correlated wave function, we get the G-matrix by

$$\langle\psi_a|\,G\,|\psi_b\rangle = \langle\psi_a|\,V\,|\Psi_b\rangle\,.$$

Computational Procedure V

For computations, there is a handy matrix relation

$$Q\frac{1}{QAQ}Q = \frac{1}{A} - \frac{1}{A}P\frac{1}{PA^{-1}P}P\frac{1}{A},$$

Write

$$G = G_F + \Delta G,$$

where G_F is the free G-matrix (easy to compute) defined as

$$G_F = V + V\frac{1}{\omega - T}G_F.$$

The term ΔG is a correction term defined entirely within the model space P (finite but big) and given by e.g.,

$$\Delta G = -G_F\frac{1}{e}\tilde{P}\frac{1}{P(e^{-1} + e^{-1}G_F e^{-1})P}P\frac{1}{e}G_F,$$

and can be solved by matrix inversion.

Computational Procedure VI

The equation for the free matrix G_F is solved in momentum space and we obtain

$$\langle kKlL\mathcal{J}ST|\, G_F \left|k'Kl'L\mathcal{J}S'T\right\rangle .$$

Transformations from the relative and center-of-mass motion system to the lab system will be discussed below.
To obtain a G-matrix in a h.o. basis, we need the transformation

$$\langle nNlL\mathcal{J}ST|\, G_F \left|n'N'l'L'\mathcal{J}S'T\right\rangle ,$$

with n and N the principal quantum numbers of the relative and center-of-mass motion, respectively.

$$|nlNL\mathcal{J}ST\rangle = \int k^2K^2dkdKR_{nl}(\sqrt{2}\alpha k)R_{NL}(\sqrt{1/2}\alpha K)\,|klKL\mathcal{J}ST\rangle .$$

Computational Procedure VII

The most commonly employed sp basis is the harmonic oscillator, which in turn means that a two-particle wave function with total angular momentum J and isospin T can be expressed as

$$
\begin{aligned}
|(n_a l_a j_a)(n_b l_b j_b) JT\rangle = \quad & \frac{1}{\sqrt{(1+\delta_{12})}} \sum_{\lambda S \mathcal{J}} \sum_{nNlL} F \times \langle ab|\lambda S J\rangle \\
& \times (-1)^{\lambda+\mathcal{J}-L-S} \hat{\lambda} \left\{ \begin{array}{ccc} L & l & \lambda \\ S & J & \mathcal{J} \end{array} \right\} \\
& \times \langle nlNL|n_a l_a n_b l_b\rangle \, |nlNL\mathcal{J}ST\rangle \,,
\end{aligned}
$$

where the term $\langle nlNL|n_a l_a n_b l_b\rangle$ is the familiar Moshinsky bracket.

Computational Procedure VIII

The term $\langle ab|LSJ\rangle$ is a shorthand for the $LS-jj$ transformation coefficient,

$$\langle ab|\lambda SJ\rangle = \hat{j_a}\hat{j_b}\hat{\lambda}\hat{S}\left\{\begin{array}{ccc} l_a & s_a & j_a \\ l_b & s_b & j_b \\ \lambda & S & J \end{array}\right\}.$$

Here we use $\hat{x} = \sqrt{2x+1}$. The factor F is defined as $F = \frac{1-(-1)^{l+S+T}}{\sqrt{2}}$ if $s_a = s_b$.

Computational Procedure IX

The G-matrix in terms of harmonic oscillator wave functions reads

$$\langle (ab)JT|\, G\, |(cd)JT\rangle = \sum_{\lambda\lambda' SS' \mathcal{J}} \sum_{nln'l'NN'L} \frac{\left(1-(-1)^{l+S+T}\right)}{\sqrt{(1+\delta_{ab})(1+\delta_{cd})}}$$

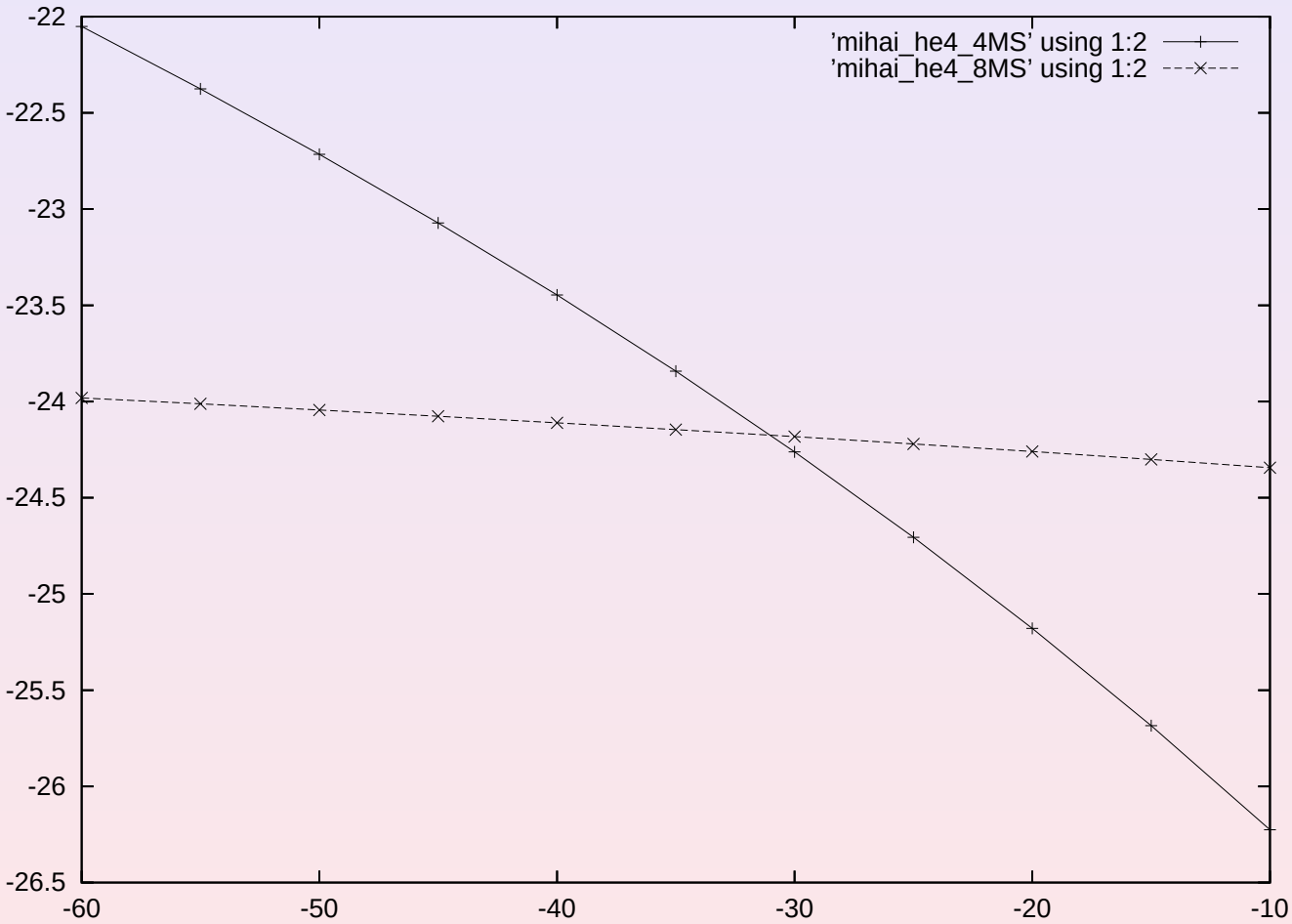
$$\times \langle ab|\lambda SJ\rangle \langle cd|\lambda' S' J\rangle \, \langle nlNL|n_a l_a n_b l_b \lambda\rangle \left\langle n' l' NL|n_c l_c n_d l_d \lambda'\right\rangle$$

$$\times \hat{\mathcal{J}} (-1)^{\lambda+\lambda'+l+l'} \left\{ \begin{array}{ccc} L & l & \lambda \\ S & J & \mathcal{J} \end{array} \right\} \left\{ \begin{array}{ccc} L & l' & \lambda' \\ S & J & \mathcal{J} \end{array} \right\}$$

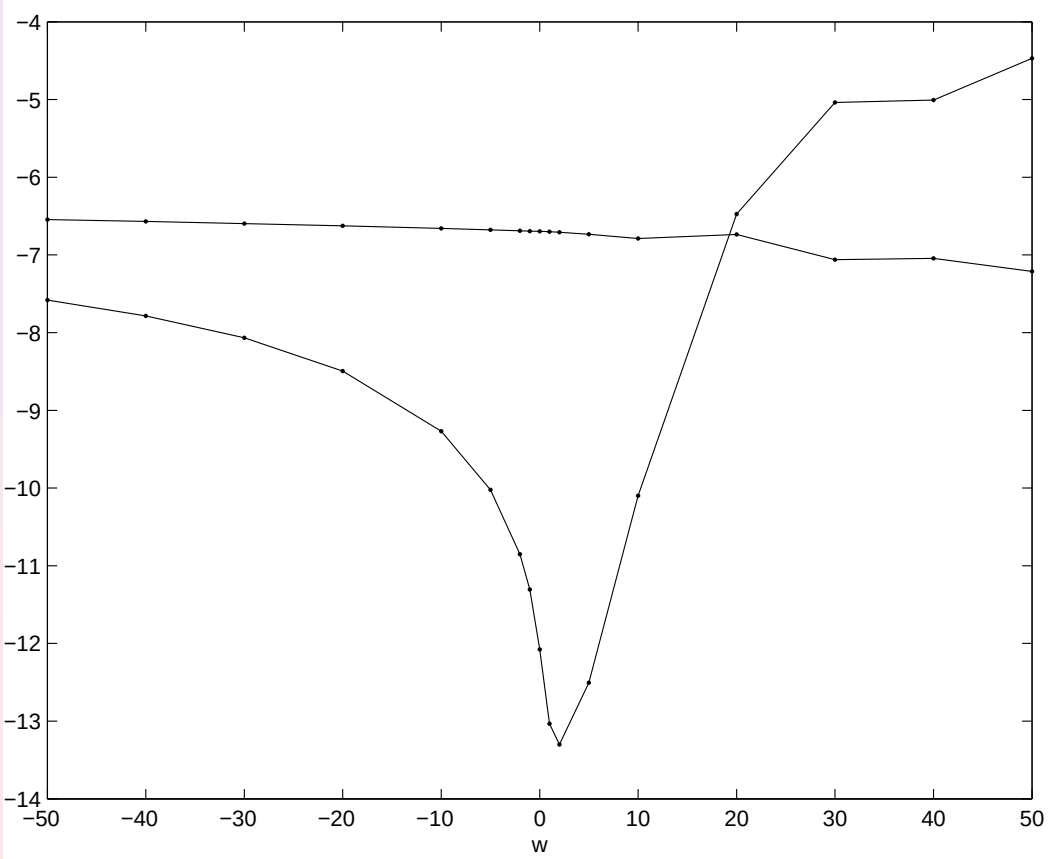
$$\times \left\langle nNlL\mathcal{J}ST|\, G\, \middle| n' N' l' L' \mathcal{J} S' T\right\rangle,$$

where G is the given by the sum $G = G_F + \Delta G$. The label a represents here all the single particle quantum numbers $n_a l_a j_a$.

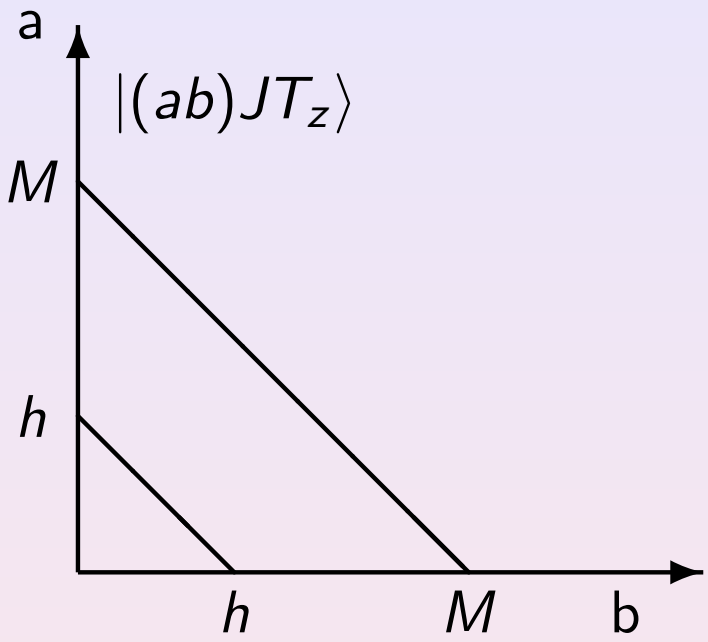
Energy dependence and no-core Shell Model for ^{4}He



Starting energy dependence of G and G_F for $(0s_{1/2})^2 JT_z = 01$



Effective Hamiltonian for Large Spaces II



$$M \leq 2n + l \approx 200$$
$$h \leq 2n + l \approx 4 - 20$$

Similarity Transformation

- Diagonalize

$$H_2^\Omega = \frac{\vec{p}_1^2 + \vec{p}_2^2}{2m} + \frac{1}{2} m\Omega^2 (\vec{r}_1^2 + \vec{r}_2^2)$$

$$+ V(\vec{r}_1 - \vec{r}_2) - \frac{m\Omega^2}{2A} (\vec{r}_1 - \vec{r}_2)^2$$

- Use similarity-transformation to obtain V_{eff} for smaller space.
- No energy dependence! HO basis.

Translationally Invariant Hamiltonian

In deriving and effective interaction with CoM corrections, the following expressions are helpful. The CoM momentum is

$$P = \sum_{i=1}^{A} \vec{p}_i,$$

and we have that

$$\sum_{i=1}^{A} \vec{p}_i^2 = \frac{1}{A}\left[\vec{P}^2 + \sum_{i<j}(\vec{p}_i - \vec{p}_j)^2\right]$$

meaning that

$$\left[\sum_{i=1}^{A} \frac{\vec{p}_i^2}{2m} - \frac{\vec{P}^2}{2mA}\right] = \frac{1}{2mA}\sum_{i<j}(\vec{p}_i - \vec{p}_j)^2.$$

Translationally Invariant Hamiltonian

In a similar fashion we can define the CoM coordinate

$$\vec{R} = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i,$$

which yields

$$\sum_{i=1}^{A}\vec{r}_i^{\,2} = \frac{1}{A}\left[A^2\vec{R}^2 + \sum_{i<j}(\vec{r}_i - \vec{r}_j)^2\right].$$

Translationally Invariant Hamiltonian

If we then introduce the harmonic oscillator one-body Hamiltonian

$$H_0 = \sum_{i=1}^{A} \left(\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} \right),$$

with Ω the oscillator frequency, we can rewrite the latter as

$$H_{\rm HO} = \frac{\vec{P}^2}{2mA} + \frac{mA\Omega^2 \vec{R}^2}{2} + \frac{1}{2mA} \sum_{i<j} (\vec{p}_i - \vec{p}_j)^2 + \frac{m\Omega^2}{2A} \sum_{i<j} (\vec{r}_i - \vec{r}_j)^2.$$

Translationally Invariant Hamiltonian

Or we could write

$$H_{\rm HO} = H_{\rm CoM} + \frac{1}{2mA}\sum_{i<j}(\vec{p}_i - \vec{p}_j)^2 + \frac{m\Omega^2}{2A}\sum_{i<j}(\vec{r}_i - \vec{r}_j)^2,$$

with

$$H_{\rm CoM} = \frac{\vec{P}^2}{2mA} + \frac{mA\Omega^2\vec{R}^2}{2}.$$

Translationally Invariant Hamiltonian

In shell model studies the translationally invariant one- and two-body Hamiltonian reads for an A-nucleon system,

$$H = \left[\sum_{i=1}^{A} \frac{\vec{p}_i^2}{2m} - \frac{\vec{P}^2}{2mA}\right] + \sum_{i<j}^{A} V_{ij} \ ,$$

where V_{ij} the nucleon-nucleon interaction, modified by including the harmonic oscillator potential

$$\sum_{i=1}^{A} \frac{1}{2} m\Omega^2 \vec{r}_i^2 - \frac{m\Omega^2}{2A}\left[\vec{R}^2 + \sum_{i<j}(\vec{r}_i - \vec{r}_j)^2\right] = 0.$$

Translationally Invariant Hamiltonian

We can rewrite the Hamiltonian as

$$H^{\Omega} = \sum_{i=1}^{A} \left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} \right] + \sum_{i<j}^{A} \left[V_{ij} - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right]$$

$$- H_{\mathrm{CoM}}.$$

Translationally Invariant Hamiltonian

Shell-model calculations are carried out in a model space defined by a projector P. The complementary space to the model space is defined by the projector $Q = 1 - P$. Consequently, for the P-space part of the shell-model Hamiltonian we get

$$H_P^\Omega = \sum_{i=1}^{A} P\left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}m\Omega^2\vec{r}_i^{\,2}\right]P + \sum_{i<j}^{A} P\left[V_{ij} - \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2\right]_{\text{eff}} P$$

$$- PH_{\text{CoM}}P.$$

Translationally Invariant Hamiltonian

The effective interaction appearing in the last equation is in general an A-body interaction and if it is determined without any approximations, the model-space Hamiltonian provides an identical description of a subset of states as the full-space Hamiltonian. The intrinsic properties of the many-body system still do not depend on Ω. From among the eigenstates of the Hamiltonian it is necessary to choose only those corresponding to the same CoM energy. This can be achieved by projecting the CoM eigenstates with energies greater than $\frac{3}{2}\hbar\Omega$ upwards in the energy spectrum.

The effective interaction should be determined from H^{Ω}. Calculation of the exact A-body effective interaction is, however, as difficult as finding the full space solution. Usually, the effective interaction is approximated by a two-body effective interaction determined from a two-nucleon problem. The relevant two-nucleon Hamiltonian is then

$$H_2^{\Omega} \equiv H_{02}^{\Omega} + V_2^{\Omega} = \frac{\vec{p}_1^2 + \vec{p}_2^2}{2m} + \frac{1}{2} m\Omega^2 (\vec{r}_1^2 + \vec{r}_2^2) + V(\vec{r}_1 - \vec{r}_2) - \frac{m\Omega^2}{2A} (\vec{r}_1 - \vec{r}_2)^2 \ .$$

With this Hamiltonian we can then compute a starting-energy independent effective interaction or G-matrix corresponding to a two-nucleon model space defined by the projector P_2. This equation is the starting point for a no-core shell-model interaction.

First Step

Start with the two-body equation

$$H_2^\Omega \equiv H_{02}^\Omega + V_2^\Omega = \frac{\vec{p}_1^2 + \vec{p}_2^2}{2m} + \frac{1}{2} m\Omega^2 (\vec{r}_1^2 + \vec{r}_2^2) + V(\vec{r}_1 - \vec{r}_2) - \frac{m\Omega^2}{2A} (\vec{r}_1 - \vec{r}_2)^2 \ .$$

- Define A for the specific nucleus
- Define a large space in terms of the h.o. shells $2n + l \sim 200 - 300$
- Diagonalize exactly the two-body problem.
- Transform to a smaller space with $2n + l \sim 4 - 20$

Second Step: Lee-Suzuki similarity transformation

We wish to construct an effective two-body interaction within the model space, reproducing in the P-space exactly the N_P model space eigenvalues of the full Hamiltonian. This can be accomplished by a similarity transformation

$$\tilde{H} = e^{-\omega} H e^{\omega},$$

where ω is defined by $\omega = Q\omega P$. It follows that $\omega^2 = \omega^3 = ... = 0$ and $e^{\omega} = P + Q + \omega$. The two-body Schrödinger equation can then be rewritten in terms of a 2×2 block structure

$$\begin{pmatrix} P\tilde{H}P & P\tilde{H}Q \\ Q\tilde{H}P & Q\tilde{H}Q \end{pmatrix} \begin{pmatrix} P\psi_n \\ Q\psi_n \end{pmatrix} = E_n \begin{pmatrix} P\psi_n \\ Q\psi_n \end{pmatrix}.$$

If $P\tilde{H}P$ is to be the two-particle effective interaction, the decoupling condition $P\tilde{H}Q = 0$ must be fulfilled. One may show that the decoupling condition becomes

$$QHP + QHQ\omega - \omega PHP - \omega PHQ\omega = 0,$$

with ω acting as a transformation from the model space P to its complement Q, viz.,

$$\langle \tilde{\alpha}_Q | \psi_n \rangle = \sum_{\alpha_P} \langle \tilde{\alpha}_Q | \omega | \alpha_P \rangle \langle \tilde{\alpha}_P | \psi_n \rangle.$$

There is however no unique solution for ω. The effective interaction generated in the model space depends on the N_P exact solutions. This is why the effective interaction generated by the similarity transformation method is often referred to as a state dependent effective interaction. The solution for ω may be obtained as long as the matrix $\langle \tilde{\alpha}_P | \psi_n \rangle$ is invertible and non-singular.

Based on this we choose those N_P exact solutions with the lowest eigenvalues. With the solution ω, the non-symmetric effective interaction R is given by

$$R = P\tilde{H}P - PH_0P = PV_{12}P + PV_{12}Q\omega.$$

It would be preferable to obtain a symmetric effective interaction, in order to take advantage of the anti-symmetrization of the two-particle basis. This may be accomplished by an orthogonal transformation

$$V_{\rm eff} = U^{-1}(H_0 + V_{12})U - H_0,$$

where U is orthogonal and defined by

$$U = \exp(-S), \;\; S = \mathrm{arctanh}(\omega - \omega^T),$$

and

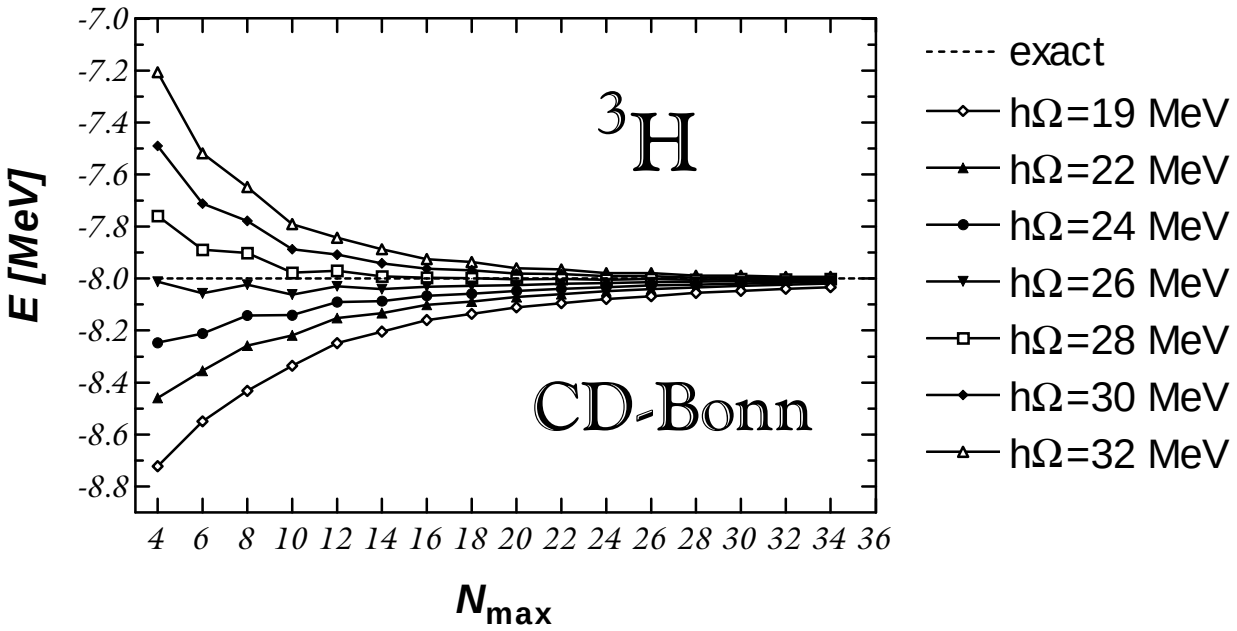
$$U^TU = UU^T = 1, \;\; U^T = U^{-1}.$$

Last Step

We can then define a hermitian effective two-body interaction

$$V_{\rm eff} = (P + \omega^{\rm T}\omega)^{1/2}(PHP + PHQ\omega)(P + \omega^{\rm T}\omega)^{-1/2} - H_0.$$

To determine $V_{\rm eff}$, one has to find the square root of the matrix $A = (P + \omega^{\rm T}\omega)$. In the case of A being real and positive definite the method based on eigenvector decomposition gives generally a stable solution.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E [MeV]
4 6 8 10 12 14 16 18 20 22 24 26 28 30 32 34 36
N_{max}
^{3}H
CD-Bonn
exact
hΩ=19 MeV
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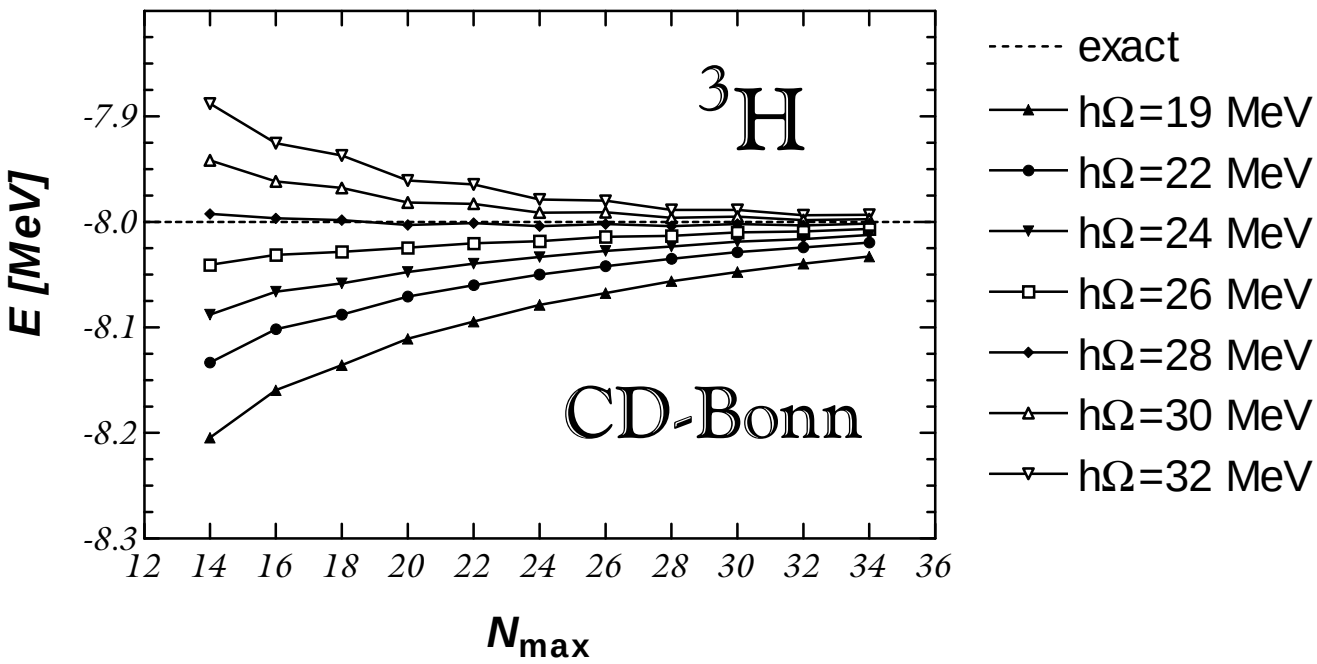
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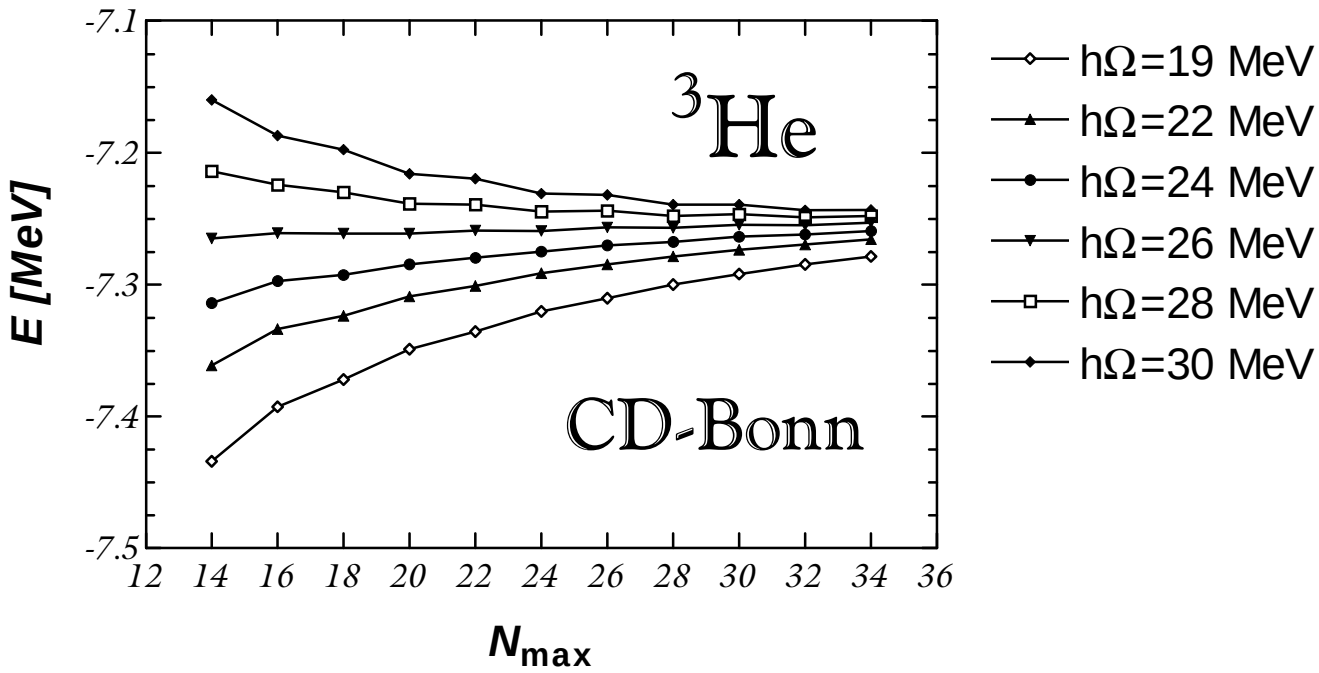
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E [MeV]
12 14 16 18 20 22 24 26 28 30 32 34 36
N_{max}
^{3}He
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hΩ=19 MeV
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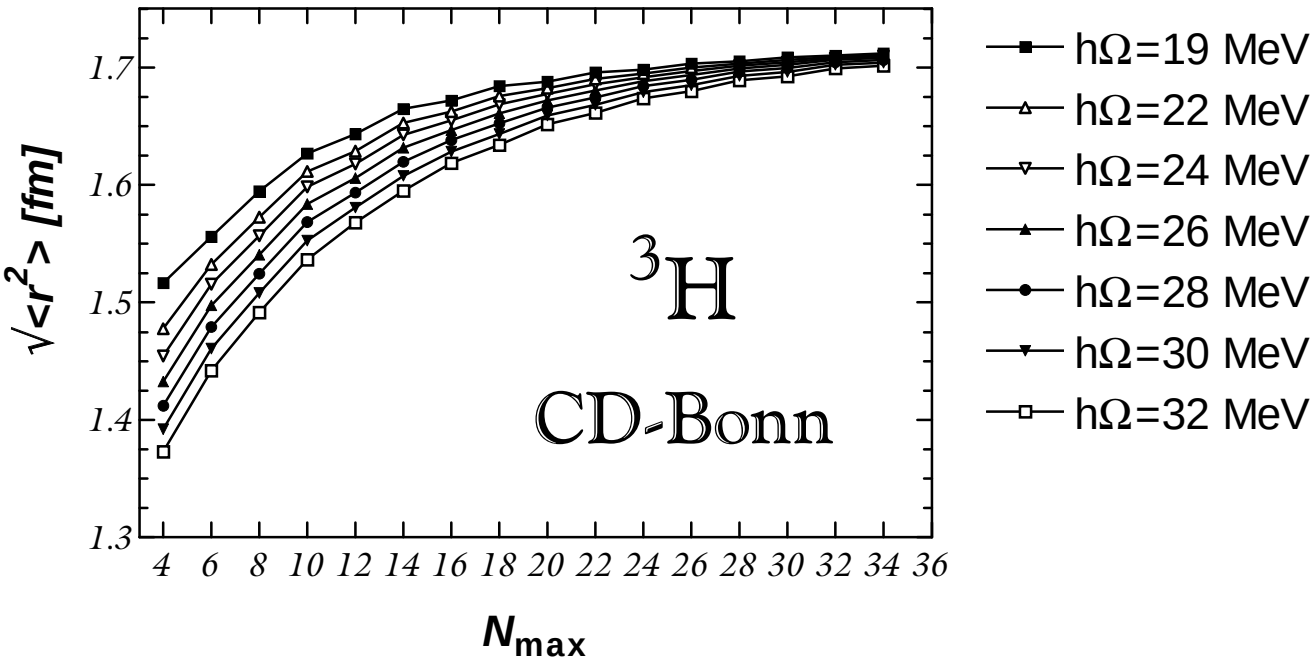
$\sqrt{<r^2>}$ [fm]
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N_{max}
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CD-Bonn
hΩ=19 MeV
hΩ=22 MeV
hΩ=24 MeV
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hΩ=28 MeV
hΩ=30 MeV
hΩ=32 MeV

Algorithm for Low-Momentum Interaction I

A unitary transformation can be parametrized as

$$U = \begin{pmatrix} P(1+\omega^\dagger\omega)^{-1/2}P & -P\omega^\dagger(1+\omega\omega^\dagger)^{-1/2}Q \\ Q\omega(1+\omega^\dagger\omega)^{-1/2}P & Q(1+\omega\omega^\dagger)^{-1/2}Q \end{pmatrix},$$

and the wave operator ω satisfies the condition $\omega = Q\omega P$. The well-known Ōkubo form. Notice that the unitary transformation is by no means unique: in fact one can construct infinitely many different unitary transformations which decouple the P and Q subspaces. The transformation in the above depends only on the operator ω which mixes the P and Q subspaces and is in some sense "the minimal possible" unitary transformation.

Algorithm for Low-Momentum Interaction II

Choose

$$U = (1 + \omega - \omega^\dagger)(1 + \omega\omega^\dagger + \omega^\dagger\omega)^{-1/2}.$$

Using the above operator U, in general, the effective interaction $\tilde{V}$ is defined through

$$\tilde{V} = U^{-1}(H_0 + V)U - H_0,$$

where H_0 is the kinetic energy of the constituent nucleons in the nuclear system, and V is the bare two-body interaction between the nucleons.

Algorithm for Low-Momentum Interaction III

The Low-Momentum NN interaction $V_{\mathrm{low}-k}$ of interest is given by

$$V_{\mathrm{low}-k} = P_{\mathrm{low}-k} \tilde{V} P_{\mathrm{low}-k},$$

where $P_{\mathrm{low}-k}$ is the projection operator onto the low-momentum space for relative two-body states. Need $V_{\mathrm{low}-k}$ in the form of the matrix elements defined by relative coordinate momenta.

Algorithm for Low-Momentum Interaction IV

We first consider an eigenvalue equation for the relative motion of a two-nucleon system as

$$(H_0 + V)|\Psi_n\rangle = E_n|\Psi_n\rangle.$$

The above equation is written also in an integral form concerning relative momenta k and k' as

$$\int_0^\infty \langle k'|H_0 + V|k\rangle\langle k|\Psi_n\rangle k^2 dk = E_n\langle k'|\Psi_n\rangle,$$

where

$$\int_0^\infty |k\rangle\langle k|k^2 dk = 1.$$

Algorithm for Low-Momentum Interaction V

Discretize $k \longrightarrow k_j$ and $k' \longrightarrow k_i$ giving

$$\sum_j \langle \bar{k}_i | H_0 + V | \bar{k}_j \rangle \langle \bar{k}_j | \Psi_n \rangle = E_n \langle \bar{k}_i | \Psi_n \rangle,$$

where $|\bar{k}_i\rangle$ and $|\bar{k}_j\rangle$ represent the plane-wave basis states in the matrices.

$$|\bar{k}_i\rangle = k_i \sqrt{W_i} |k_i\rangle$$

Normalized as $\langle \bar{k}_i | \bar{k}_j \rangle = \delta_{i,j}$.

Algorithm for Low-Momentum Interaction VI

Note that the eigenvectors $|\Psi_n\rangle$ can be expressed as $|\Psi_n\rangle = |\phi_n\rangle + \omega|\phi_n\rangle$ in terms of the operator ω and the P-space components $|\phi_n\rangle = P|\Psi_n\rangle$. Thus, the formal solution of ω is given by $\omega = \sum_n |\Psi_n\rangle\langle\tilde{\phi}_n|$ with the biorthogonal state $\langle\tilde{\phi}_n|$ of $|\phi_n\rangle$.
In order to obtain the matrix elements of ω, we first diagonalizing using the basis states $|\bar{k}_i\rangle$. Then, the matrix elements ω for the basis states $|\bar{k}_p\rangle$ in the P space and $|\bar{k}_q\rangle$ in the Q space are obtained as

$$\langle\bar{k}_q|\omega|\bar{k}_p\rangle = \sum_{n=1}^{d}\langle\bar{k}_q|Q|\Psi_n\rangle\langle\tilde{\phi}_n|P|\bar{k}_p\rangle,$$

where d is the number of the basis states (the integral points) in the P space.

Algorithm for Low-Momentum Interaction VII

In order to obtain the P-space effective interaction, we introduce the eigenvalue equation for $\omega^\dagger\omega$ in the P space as

$$\omega^\dagger\omega|\psi_\alpha\rangle = \mu_\alpha^2|\psi_\alpha\rangle.$$

Using the solutions to the above equation we get

$$\begin{aligned}
&\langle\psi_\alpha|V_{\mathrm{low}-k}|\psi_\beta\rangle \\
&= \frac{\sqrt{(1+\mu_\alpha^2)}\langle\psi_\alpha|R|\psi_\beta\rangle + \sqrt{(1+\mu_\beta^2)}\langle\psi_\alpha|R^\dagger|\psi_\beta\rangle}{\sqrt{(1+\mu_\alpha^2)}+\sqrt{(1+\mu_\beta^2)}},
\end{aligned} \tag{1}$$

where $R = P(V + V\omega)P$ is a low-momentum non-Hermitian effective interaction.

Algorithm for Low-Momentum Interaction VIII

Finally, the matrix elements in a plane-wave basis states $|k_i\rangle$ and $|k_j\rangle$ are

$$\langle k_i|V_{\mathrm{low}-k}|k_j\rangle = \frac{\sum_{\alpha,\beta}\langle \bar{k}_i|\psi_\alpha\rangle\langle\psi_\alpha|V_{\mathrm{low}-k}|\psi_\beta\rangle\langle\psi_\beta|\bar{k}_j\rangle}{k_i k_j\sqrt{W_i W_j}}.$$

Final Recipe

- Diagonalize the two-body Schr$\acute{}$odinger equation in momentum space for all momenta
- Choose a cutoff which defines the model space in terms of relative momenta
- Use exact eigenvalues and momenta to perform a similarity transformation
- Obtain effective interaction in relative momenta
- Integrate to get harmonic oscillator matrix elements for relative quantum numbers
- Transform to lab frame

Potential drawback: no connection with harmonic oscillator cutoff. Interaction stays the same irrespective of the number of shells. May yield wrong saturation for coupled cluster or no-core shell-model calculations.

Input File for Renormalization of the NN interactions

```
# Parameters for renormalization procedure, codes in Fortran 95.
# It reads the variable names and corresponding values as
# variable = something
# You can have as many blank lines as you want.
# to the left is btw the comment sign


# Determine the renormalization procedure you want to do,
# only one at the time
# options are: g-matrix, no-core or vlowk
type_of_renormv  =  vlowk


# Determine if you wish to include the Coulomb interaction or no
# options are: no-coulomb or coulomb
coulomb_included  =  coulomb
```

renorm.ini File for Renormalization of the NN interactions

```
# output_run is prefixed to output file for
# optional printouts, tests etc.
output_run = run1_25march.dat

# output file for the renormalized NN interaction
renorminteraction_file  =  gint52n3lo_10hbar.dat

# output file for the set of single-particle orbits,
# this file can be
# further manipulated by the effective interaction part
spdata_file  =  spdat52n3lo_10hbar.dat
```

renorm.ini File for Renormalization of the NN interactions

```
# Give the number of nucleons, recall that for nocore the
# results depend on A
mass_nucleus = 16

# The oscillator energy in MeV
hbar_omega = 15.

# For the NN interaction you need to define the min and max valu
# of J for the partial waves. Typical values are 0 and 6.
# For the argonne interactions Jmax <= 4.
# For waves greater
# than J_max, the Hamiltonian is set to zero in this version
# of the program.
jmin = 0
jmax = 6
```

renorm.ini File for Renormalization of the NN interactions

```
# specify the type of NN interaction, here you can use
# Idaho-A, Idaho-B, CD-bonn, argonnev18, n3lo, argonnev8
# There is an importan point concerning the different interactio
# Idaho-A and Idaho-B have NO charge-symmetry (CSB) or
# charge-independence breaking terms  (ISB).
# The Argonne potentials run only with full CSB and CIB.
# The N3LO and CD-bonn models allow
# you to run with or without one or both of these terms.
# NO CSB means that for a given set of qauntum numbers
# ( a specific partial wave) the neutron-neutron
# and proton-proton parts are identical
# NO CIB  means that the pp, pn or nn
# interactions are equal. Isospin symmetry.
type_of_pot = n3lo
```

renorm.ini File for Renormalization of the NN interactions

```
# Here you specify if you wish to exclude CSB: options:
# 1) no-csb  2) csb
csb_choice =  csb

# Here you specify if you wish to exclude CIB: options:
# 1) no-cib  2) cib
cib_choice =  cib

# specify the type of model space, three choices: square,
# triangular or wings. For the
# nocore calculation you can only use the triangular choice
pauli_operator  = square
```

renorm.ini File for Renormalization of the NN interactions

```
# define the maximum values of  l and n for the model space.
# For square the model
# space 2n+l is entirely defined by lab_lmax.
lab_lmax =  3
lab_nmax = 1

#  if you do nocore, you need also to specify the cut
#  in 2n+l for the huge space, use 200-300
#  for interactions like cdbonn or argonne  use 300.
max_space = 100
```

renorm.ini File for Renormalization of the NN interactions

```
# If you do the g-matrix you need to specify the number
# of starting energies
# and their corresponding values. Typically you would use
# some 5 or more starting energies and they should all be
# smaller than the binding energy of the deuteron in order
# to avoid poles in the computation of G(w). The present
# code does not allow you to use positive starting
# energies. Typical start
# and end values are listed here.
# Based on the endpoints of the interval, the next values
# are generated by the simple algo
# first_value+  interval*i    where interval   is just
# end-start/number of values.
n_startenergy_g  = 5
first_startingenergy   =   -5.0
last_startingenergy   =   -150.0
```

renorm.ini File for Renormalization of the NN interactions

```
# If you do Vlowk you need to specify the number of mesh points
# for the model  space and the large space. You need also to
# define the cutoff for the
# model in space in fm^- 1 and the in principal infinite
# integration limit
# set it to 20 fm^-1.  Recall that the NN interactions is
# fitted up to 350 MeV.
n_k1 = 50
n_k2 = 50
k_cutoff = 2.1
k_max = 20.0
```

$V_{\mathrm{low}-k}$

The $A-$body Hamiltonian H is defined as

$$H = \frac{1}{2m}\sum_{i=1}^{A}\mathbf{k}_i^2 + \sum_{i<j}^{A} V_{\mathrm{low}-\mathrm{k}}(i,j).$$

The spurious center of mass energy is removed by writing the internal kinetic energy as

$$T_{\mathrm{in}} = T - T_{\mathrm{c.m.}} = \left(1 - \frac{1}{A}\right)\sum_{i=1}^{A}\frac{\mathbf{k}_i^2}{2m} - \sum_{i<j}^{A}\frac{\mathbf{k}_i\cdot\mathbf{k}_j}{mA}.$$

The introduction of an additional two-body term yields a modified two-body interaction

$$H_{\mathrm{I}} = V_{\mathrm{low}-\mathrm{k}} + V_{\mathrm{c.m.}} = \sum_{i<j}^{A}\left(V_{\mathrm{low}-\mathrm{k}}(i,j) - \frac{\mathbf{k}_i\cdot\mathbf{k}_j}{mA}\right).$$

This interaction is in turn written out in terms of harmonic oscillator elements.

G-matrix

The $A-$body Hamiltonian H is defined as for the $V\mathrm{low}_k$ case

$$H = \frac{1}{2m}\sum_{i=1}^{A}\mathbf{k}_i^2 + \sum_{i<j}^{A} G(i,j).$$

The spurious center of mass energy is removed by writing the internal kinetic energy as

$$T_{\mathrm{in}} = T - T_{\mathrm{c.m.}} = \left(1-\frac{1}{A}\right)\sum_{i=1}^{A}\frac{\mathbf{k}_i^2}{2m} - \sum_{i<j}^{A}\frac{\mathbf{k}_i\cdot\mathbf{k}_j}{mA}.$$

The modified two-body interaction

$$H_{\mathrm{I}} = G + V_{\mathrm{c.m.}} = \sum_{i<j}^{A}\left(G(i,j) - \frac{\mathbf{k}_i\cdot\mathbf{k}_j}{mA}\right).$$

This interaction is in turn written out in terms of harmonic oscillator elements.

Both the G-matrix codes and the $V_{\mathrm{low}-k}$ codes list separately G or $V_{\mathrm{low}-k}$ in addition to the term $\frac{\mathbf{k}_i\cdot\mathbf{k}_j}{mA}$. The last term has to be multiplied by $\hbar\omega/A$ in order to be used in derivations of the effective interaction.

No-core

The total Hamiltonian is

$$H_P^\omega = \sum_{i=1}^{A} P\left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}m\omega^2\vec{r}_i^{\,2}\right]P + \sum_{i<j}^{A} P\left[V_{ij} - \frac{m\omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2\right]_{\rm eff} P$$

$$- PH_{\rm CoM}P.$$

The two-body part of the center-of-mass Hamiltonian is listed separately and needs to be multiplied by $\hbar\omega/A$. Since we only give the two-body part, you need to add the Harmonic oscillator single-particle energies to this part and multiply the harmonic oscillator single-particle energies with $\hbar\omega/A$ as well.

Note that the no-core Hamiltonian depends explicitely on the mass number A. The G-matrix and $V_{\rm low-k}$ include only a mass dependence via the term $\frac{\mathbf{k}_i\cdot\mathbf{k}_j}{mA}$. The Coulomb interaction is included in all models.

Momentum Space Basis

Instead of the harmonic oscillator basis we could use plane waves. Two-particle state in the laboratory system is given via transformation from the relative and center of mass system.

$$
\begin{aligned}
|(k_a l_a j_a t_{z_a})(k_b l_b j_b t_{z_b}) J T_z\rangle = & \sum_{lL\lambda S\mathcal{J}} \int k^2 dk \int K^2 dK \left\{ \begin{array}{ccc} l_a & l_b & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_a & j_b & J \end{array} \right\} \\
& \times (-1)^{\lambda+\mathcal{J}-L-S} F \hat{\mathcal{J}} \hat{\lambda}^2 \hat{j}_a \hat{j}_b \hat{S} \left\{ \begin{array}{ccc} L & l & \lambda \\ S & J & \mathcal{J} \end{array} \right\} \\
& \times \langle klKL | k_a l_a k_b l_b \lambda \rangle \, |klKL(\mathcal{J}) S J T_z\rangle \, ,
\end{aligned}
$$

Hartree-Fock Diagram

The HF contribution

$$\mathcal{V}_{HF}(k_a k_c l_a j_a t_{z_a}) = \frac{1}{\hat{j_a}^2} \sum_J \sum_{n_h l_h j_h t_{z_h}} \hat{J}^2 \left\langle (k_a l_a j_a t_{z_a})(n_h l_h j_h t_{z_h}) J T_z \right| H_{\rm I} \left| (k_c l_a j_a t_{z_a})(n_h l_h j_h t_{z_h}) J T_z \right\rangle ,$$

where $\hat{x} = \sqrt{2x+1}$ and $n_h l_h j_h t_{z_h}$ are the quantum numbers of the nucleon hole states. The variables l_a, j_a, t_{z_a} are the orbital angular momentum, total angular momentum and isospin projection ($t_{z_a} = \pm 1/2$) of the incoming/outgoing nucleon, and k_a (k_c) the outgoing (incoming) particle momenta.

Self-Energy

We limit ourselves to the computation of the HF contribution, the expression for the self-energy reads

$$\Sigma(j_a l_a k_a k_c) = \mathcal{V}_{HF}(j_a l_a k_a k_c).$$

This equation is only valid along the real-energy axis. These equations can in turn be useful when we want to move to weakly bound systems and study bound states, resonant states and continuum states on the same footing.

Two-body Matrix Elements I

The renormalized nucleon-nucleon interaction in an arbitrary two-particle basis in the laboratory frame is given by

$$\langle ab|H_{\rm I}|cd\rangle = \langle (n_a l_a j_a t_{z_a})(n_b l_b j_b t_{z_b}) JT_z|\, H_{\rm I}\, |(n_c l_c j_c t_{z_c})(n_d l_d j_d t_{z_d}) JT_z\rangle\,.$$

Here $H_{\rm I}$ can be a G-matrix, it can be a no-core or Vlowk interaction. The two-body state $|ab\rangle$ is implicitly coupled to good angular momentum J. The labels $n_{a\ldots d}$ number all bound, resonant and discretized scattering states with orbital and angular momenta $(l_{a\ldots d}, j_{a\ldots d})$. Here these single-particle states will be the Hartree-Fock states.
In order to efficiently calculate the matrix elements, we introduce a two-particle harmonic oscillator basis completeness relation

$$\sum_{\alpha\leq\beta} |\alpha\beta\rangle\langle\alpha\beta| = \mathbf{1}, \tag{2}$$

where the sum is not restricted in the neutron-proton case. We introduce the greek single particle labels α, β for the single-particle harmonic oscillator states in order to distinguish them from the latin single-particle labels Hartree-Fock states a, b

Two-body Matrix Elements II

The interaction can then be expressed in the complete basis is

$$H_{\mathrm{I}} = \sum_{\alpha \leq \beta} \sum_{\gamma \leq \delta} |\alpha\beta\rangle \langle \alpha\beta | H_{\mathrm{I}} | \gamma\delta \rangle \langle \gamma\delta|,$$

where the sums over two-particle harmonic oscillator states are infinite. The expansion coefficients

$$\langle \alpha\beta | H_{\mathrm{I}} | \gamma\delta \rangle = \left\langle (n_\alpha l_\alpha j_\alpha t_{z_\alpha})(n_\beta l_\beta j_\beta t_{z_\beta}) JT_z \right| H_{\mathrm{I}} \left| (n_\gamma l_\gamma j_\gamma t_{z_\gamma})(n_\delta l_\delta j_\delta t_{z_\delta}) JT_z \right\rangle,$$

represent the interaction H_{I} in an antisymmetrized two-particle harmonic oscillator basis, and may easily be calculated using the well known Moshinsky transformation coefficients.

Two-body Matrix Elements III

The matrix elements are calculated numerically up to N harmonic oscillator two-body states

$$\langle ab|H_{\rm I}|cd\rangle = \sum_{\alpha\leq\beta}^{N}\sum_{\gamma\leq\delta}^{N}\langle ab|\alpha\beta\rangle\langle\alpha\beta|H_{\rm I}|\gamma\delta\rangle\langle\gamma\delta|cd\rangle.$$

The two-particle overlap integrals $\langle ab|\alpha\beta\rangle$ read

$$\langle ab|\alpha\beta\rangle = \frac{\langle a|\alpha\rangle\langle b|\beta\rangle - (-1)^{J-j_\alpha-j_\beta}\langle a|\beta\rangle\langle b|\alpha\rangle}{\sqrt{(1+\delta_{ab})(1+\delta_{\alpha\beta})}} \tag{3}$$

for identical particles (proton-proton or neutron-neutron states) and

$$\langle ab|\alpha\beta\rangle = \langle a|\alpha\rangle\langle b|\beta\rangle \tag{4}$$

for the proton-neutron case.

Exercises Lecture II

(a) Download the codes at the webpage and try to compile the no-core code. Run the no-core code for various harmonic oscillator energies and study the stability of the Deuteron (use $A = 2$) as function of increasing number of harmonic oscillator shells. Try also different nucleon-nucleon interactions.

(b) Set up the Hartree-Fock equations in a harmonic oscillator basis and sketch the algorithm for finding the overlaps $\langle a|\alpha\rangle$.