Lecture II: Renormalization of the Nucleon-Nucleon Interaction

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Outline

1. Renormalization of the NN force
   - Definitions
   - No-Core Shell-Model Calculations
   - Green's function renormalization
   - 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 model-space effective Hamiltonian:

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

Model 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

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

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*

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

or equivalently

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

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

Understanding excitations, model spaces and excluded spaces

We always start with a 'vacuum' reference state, the Slater determinant for the believed dominating configuration of the ground state. Here a simple case of eight particles with single-particle wave functions $\phi_i(\mathbf{x}_i)$

$$\Phi_0 = \frac{1}{\sqrt{8!}} \begin{pmatrix} \phi_1(\mathbf{x}_1) & \phi_1(\mathbf{x}_2) & \dots & \phi_1(\mathbf{x}_8) \\ \phi_2(\mathbf{x}_1) & \phi_2(\mathbf{x}_2) & \dots & \phi_2(\mathbf{x}_8) \\ \phi_3(\mathbf{x}_1) & \phi_3(\mathbf{x}_2) & \dots & \phi_3(\mathbf{x}_8) \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \phi_8(\mathbf{x}_1) & \phi_8(\mathbf{x}_2) & \dots & \phi_8(\mathbf{x}_8) \end{pmatrix}$$

If this is it, we are staying at the Hartree-Fock level. We can however allow for a linear combination of excitations beyond the ground state, viz., we could assume that we include 1p-1h and 2p-2h excitations

$$\Psi_{2p-2h} = (1 + T_1 + T_2)\Phi_0$$

T_1 is a 1p-1h excitation while T_2 is a 2p-2h excitation.

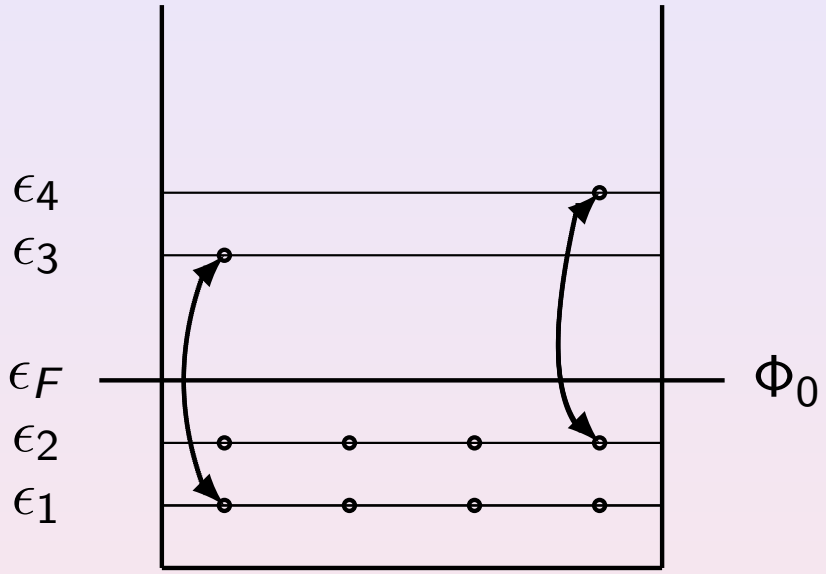
Understanding excitations, model spaces and excluded spaces

The single-particle wave functions of

$$\Phi_0 = \frac{1}{\sqrt{8!}} \begin{pmatrix} \phi_1(\mathbf{x}_1) & \phi_1(\mathbf{x}_2) & \dots & \phi_1(\mathbf{x}_8) \\ \phi_2(\mathbf{x}_1) & \phi_2(\mathbf{x}_2) & \dots & \phi_2(\mathbf{x}_8) \\ \phi_3(\mathbf{x}_1) & \phi_3(\mathbf{x}_2) & \dots & \phi_3(\mathbf{x}_8) \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \phi_8(\mathbf{x}_1) & \phi_8(\mathbf{x}_2) & \dots & \phi_8(\mathbf{x}_8) \end{pmatrix}$$

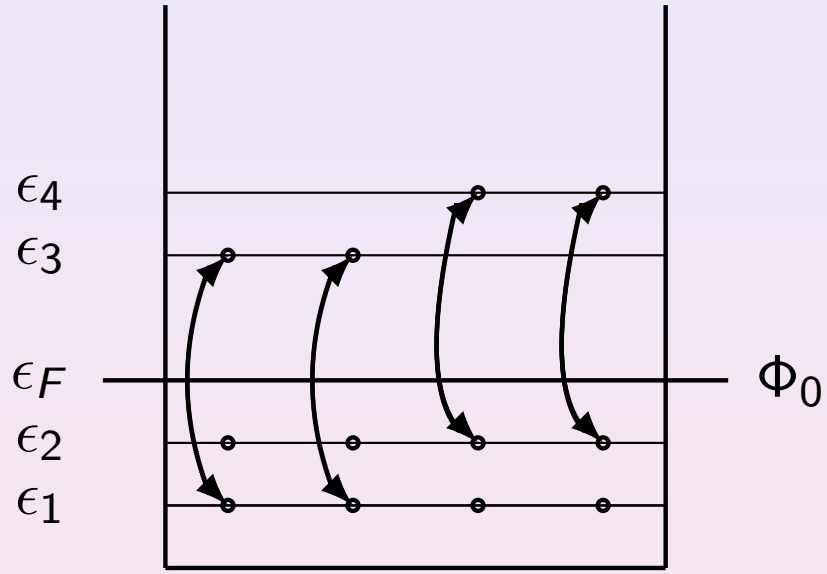
are normally chosen as the solutions of the so-called non-interacting part of the Hamiltonian, H_0. A typical basis is provided by the harmonic oscillator problem.

Excitations in Pictures



From T_1 to T_1^2

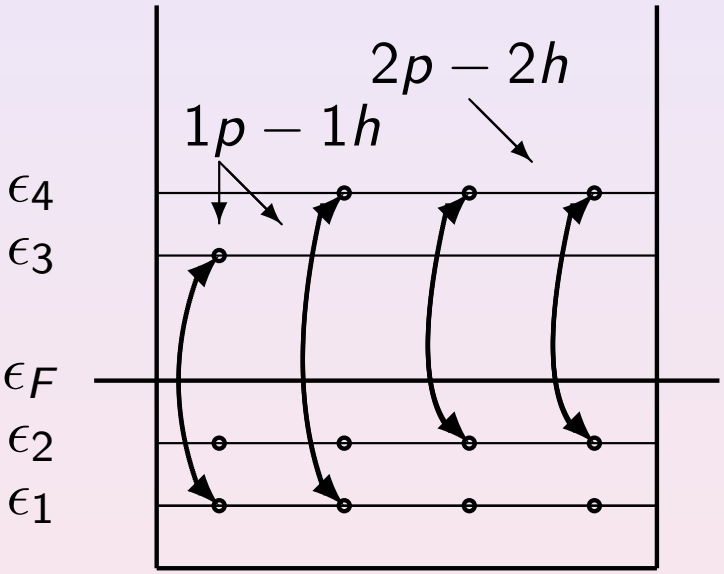
$T_1 \propto a_a^+ a_i$



From T_2 to T_2^2

$T_2 \propto a_a^+ a_b^+ a_j a_i$

Excitations



$T_1^2 T_2$

Shell-Model Truncations

- Truncated shell model with $2p-2h$ has $\Psi_{2p-2h} = (1 + T_1 + T_2)\Phi_0$
- Energy contains then

$$E_{2p-2h} =$$

$$\langle \Phi_0 (1 + T_1^\dagger + T_2^\dagger) | H | (1 + T_1 + T_2)\Phi_0 \rangle$$

- Note that $T_1^2 T_2$ is not in truncated shell model. Important.

Simple Toy Model to illustrate basic principles

Choose a hamiltonian that depends linearly on a strength parameter z

$$H = H_0 + zH_1,$$

with $0 \leq z \leq 1$, where the limits $z = 0$ and $z = 1$ represent the non-interacting (unperturbed) and fully interacting system, respectively. The model is an eigenvalue problem with only two available states, which we label P and Q. Below we will let state P represent the model-space eigenvalue whereas state Q represents the eigenvalue of the excluded space. The unperturbed solutions to this problem are

$$H_0\Phi_P = \epsilon_P\Phi_P$$

and

$$H_0\Phi_Q = \epsilon_Q\Phi_Q,$$

with $\epsilon_P < \epsilon_Q$. We label the off-diagonal matrix elements X, while $X_P = \langle\Phi_P| H_1 |\Phi_P\rangle$ and $X_Q = \langle\Phi_Q| H_1 |\Phi_Q\rangle$.

Simple Two-Level Model

The exact eigenvalue problem

$$\begin{pmatrix} \epsilon_P + zX_P & zX \\ zX & \epsilon_Q + zX_Q \end{pmatrix}$$

yields

$$E(z) = \frac{1}{2}\left\{\epsilon_P + \epsilon_Q + zX_P + zX_Q \pm (\epsilon_Q - \epsilon_P + zX_Q - zX_P) \times \sqrt{1 + \frac{4z^2X^2}{(\epsilon_Q - \epsilon_P + zX_Q - zX_P)^2}}\right\}.$$

A Rayleigh-Schrödinger like expansion for the lowest eigenstate

$$E = \epsilon_P + zX_P + \frac{z^2X^2}{\epsilon_P - \epsilon_Q} + \frac{z^3X^2(X_Q - X_P)}{(\epsilon_P - \epsilon_Q)^2} + \frac{z^4X^2(X_Q - X_P)^2}{(\epsilon_P - \epsilon_Q)^3} - \frac{z^4X^4}{(\epsilon_P - \epsilon_Q)^3} + \ldots,$$

which can be viewed as an effective interaction for state P in which state Q is taken into account to successive orders of the perturbation.

Another look at the problem: Similarity Transformations

We have defined a transformation

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

We rewrite this for later use, introducing $\Omega = e^T$, as

$$H' = e^{-T} H e^T ,$$

and T is constructed so that $QH'P = PH'Q = 0$. The P-space effective Hamiltonian is given by

$$H^{\text{eff}} = PH'P,$$

and has d exact eigenvalues of H.

Another look at the simple 2×2 Case, Jacobi Rotation

We have the simple model

$$\begin{pmatrix} \epsilon_P + zX_P & zX \\ zX & \epsilon_Q + zX_Q \end{pmatrix}$$

Rewrite for simplicity as a symmetric matrix $H \in \mathbb{R}^{2\times 2}$

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}.$$

The standard Jacobi rotation allows to find the eigenvalues via the orthogonal matrix Ω

$$\Omega = e^T = \begin{bmatrix} c & s \\ -s & c \end{bmatrix},$$

with $c = \cos\gamma$ and $s = \sin\gamma$. We have then that $H' = e^{-T} H e^T$ is diagonal.

Simple 2×2 Case, Jacobi Rotation first

To have non-zero nondiagonal matrix H' we need to solve

$$(H_{22} - H_{11})cs + H_{12}(c^2 - s^2) = 0,$$

and using $c^2 - s^2 = \cos(2\gamma)$ and $cs = \sin(2\gamma)/2$ this is equivalent with

$$\tan(2\gamma) = \frac{2H_{12}}{H_{11} - H_{22}}.$$

Solving the equation we have

$$\gamma = \frac{1}{2}\tan^{-1}\left(\frac{2H_{12}}{H_{11} - H_{22}}\right) + \frac{k\pi}{2}, \quad k = \ldots, -1, 0, 1, \ldots, \tag{1}$$

where $k\pi/2$ is added due to the periodicity of the tan function.

Simple 2×2 Case, Jacobi Rotation first

Note that $k = 0$ gives a diagonal matrix on the form

$$H'_{k=0} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}, \tag{2}$$

while $k = 1$ changes the diagonal elements

$$H'_{k=1} = \begin{bmatrix} \lambda_2 & 0 \\ 0 & \lambda_1 \end{bmatrix}. \tag{3}$$

Simple 2×2 system, exercise

Exercise: Find the similarity transformed expression for H'_{11} for a simplepairing model and compare it with the perturbative expansion till fifth order.
Use

$$\begin{pmatrix} -g & -g \\ -g & 2d-g \end{pmatrix}$$

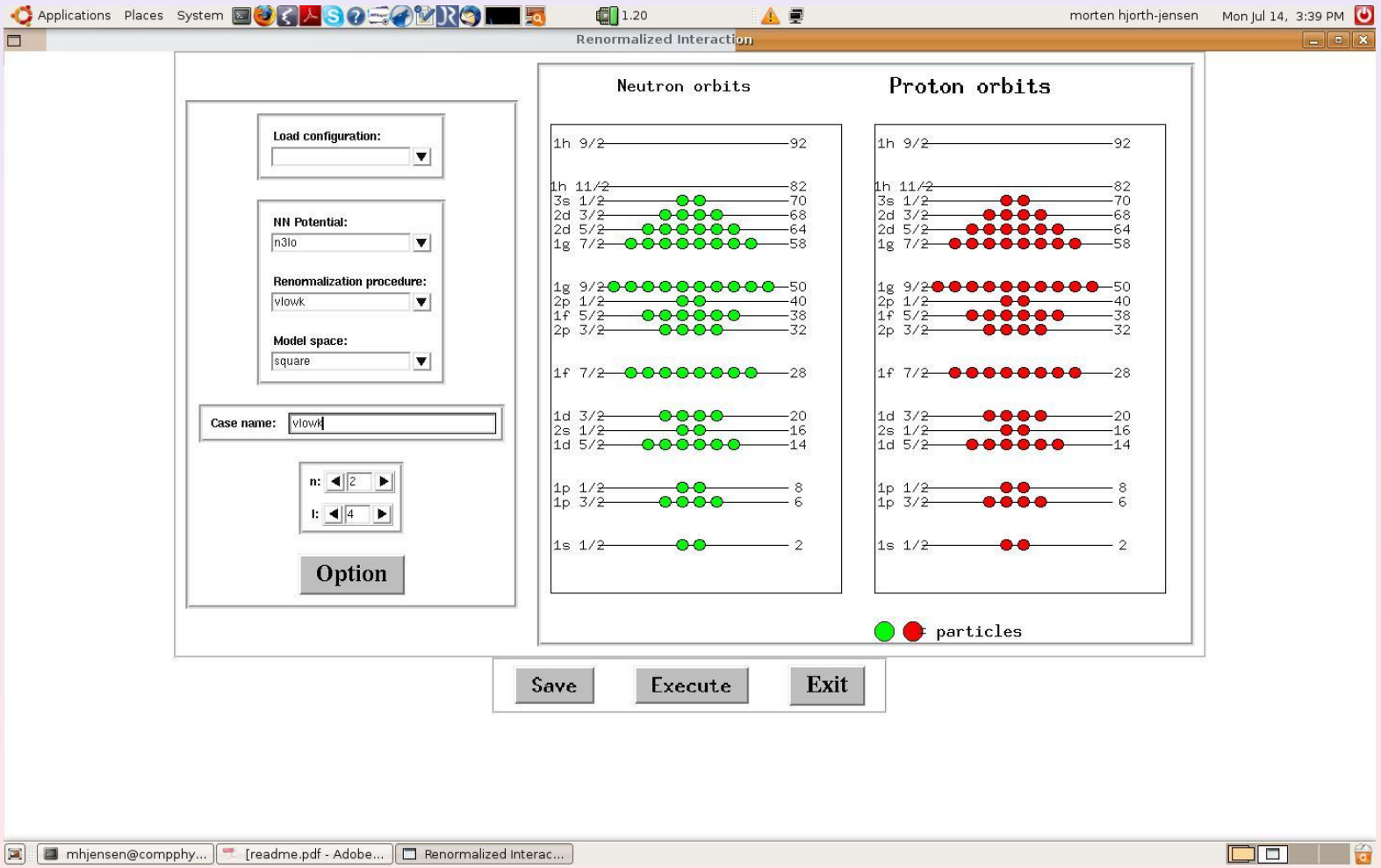
where $\epsilon_P = 0$ and $\epsilon_q = 2d$.

The effective interaction depends on the angles of the rotation matrix!

CENS options

1. Can compute a renormalized two-body interaction using a no-core shell-model prescription
2. Can compute a renormalized two-body interaction using a G-matrix prescription
3. Can compute a renormalized two-body interaction using a Vlowk prescription
4. Can compute a renormalized two-body interaction using a renormalization group prescription in momentum space or in oscillator space (not ideal for shell-model calculations)

CENS image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Renormalized Interaction
Load configuration:
NN Potential:
n3lo
Renormalization procedure:
vlowk
Model space:
square
Case name:
vlowk
n:
2
l:
4
Option
Neutron orbits
Proton orbits
1h 9/2 92
1h 11/2 82
3s 1/2 70
2d 3/2 68
2d 5/2 64
1g 7/2 58
1g 9/2 50
2p 1/2 40
1f 5/2 38
2p 3/2 32
1f 7/2 28
1d 3/2 20
2s 1/2 16
1d 5/2 14
1p 1/2 8
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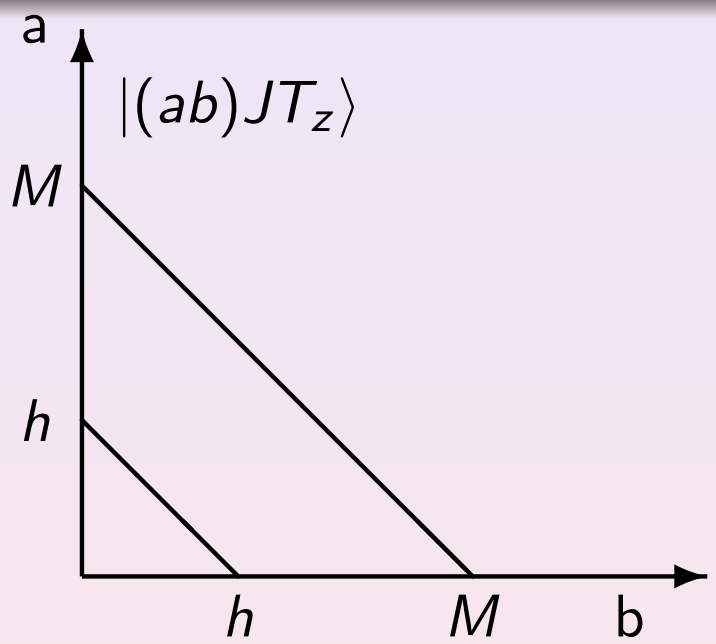
Effective Hamiltonian for Large Spaces, no-core calculations



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

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

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

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

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 $2n + l \sim 4 - 20$

Convergence criteria

See Simen Kvaal: Harmonic oscillator eigenfunction expansions, quantum dots, and effective interactions arxiv:0808.2145.
Accuracy of FCI calculations for quantum dots with harmonic oscillator wave functions for many-body state: For an exact eigenfunction which is k times differentiable we have

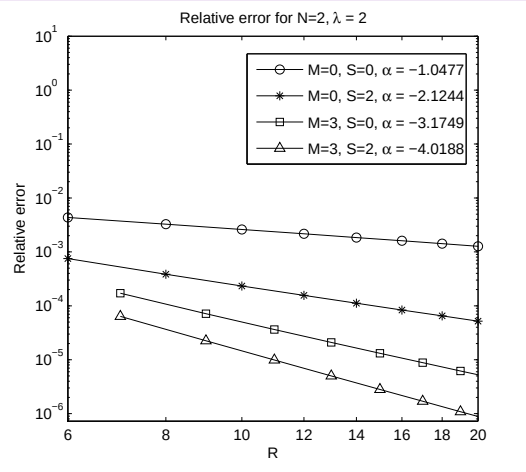
$$\Delta E \leq C R_{\rm cut}^{-(k+\epsilon-1)}$$

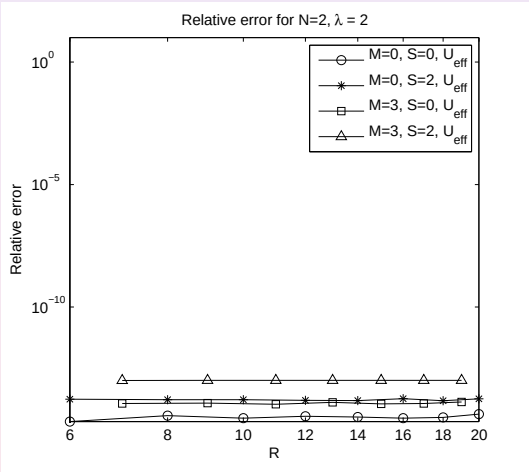
with $0 \leq \epsilon < 1$ and C s a constant. $R_{\rm cut}$ is the shell-energy $2n + l + d/2$.
Ground state has typically $k = 1$ yielding

$$\Delta E \sim R^{-\alpha},$$

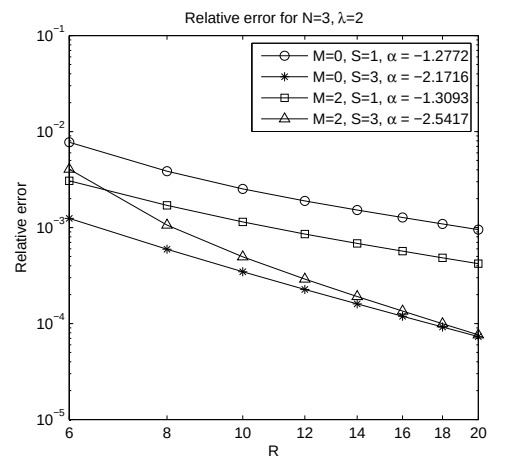
with $\alpha \approx 1$, which is a poor convergence.

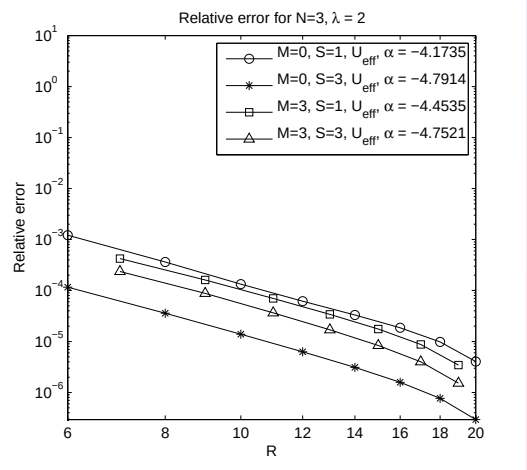
Two electrons QD, Johnson and Payne model, PRL **67**, 1157 (1991)



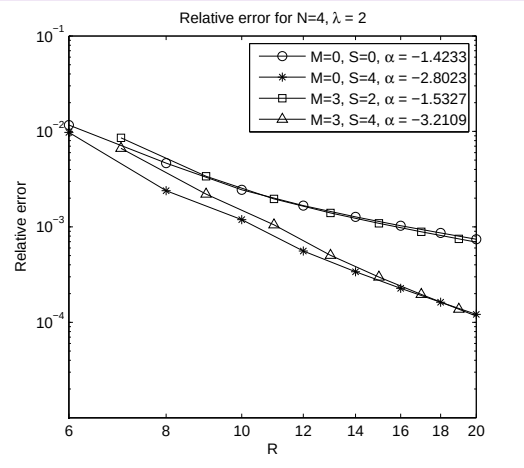


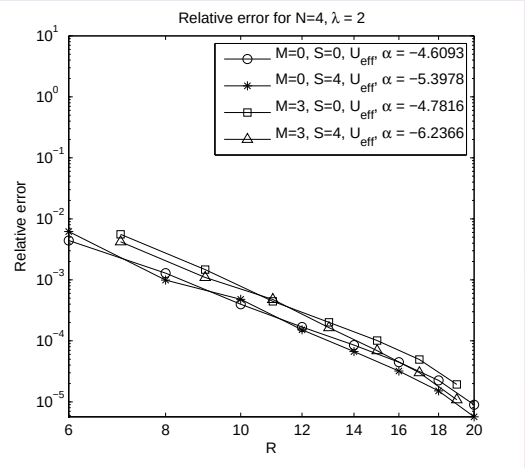
Three electrons QD, Johnson and Payne model, PRL **67**, 1157 (1991)



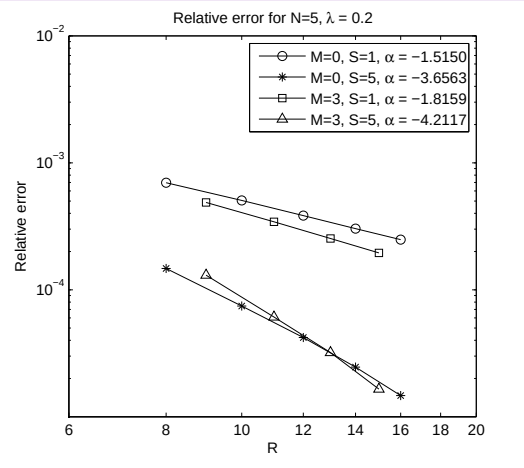


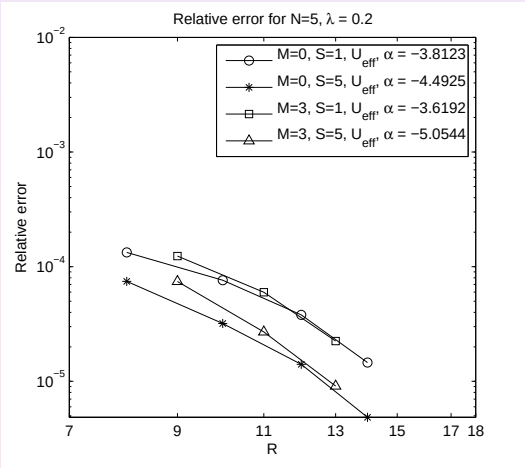
Four electrons QD, Johnson and Payne model, PRL **67**, 1157 (1991)





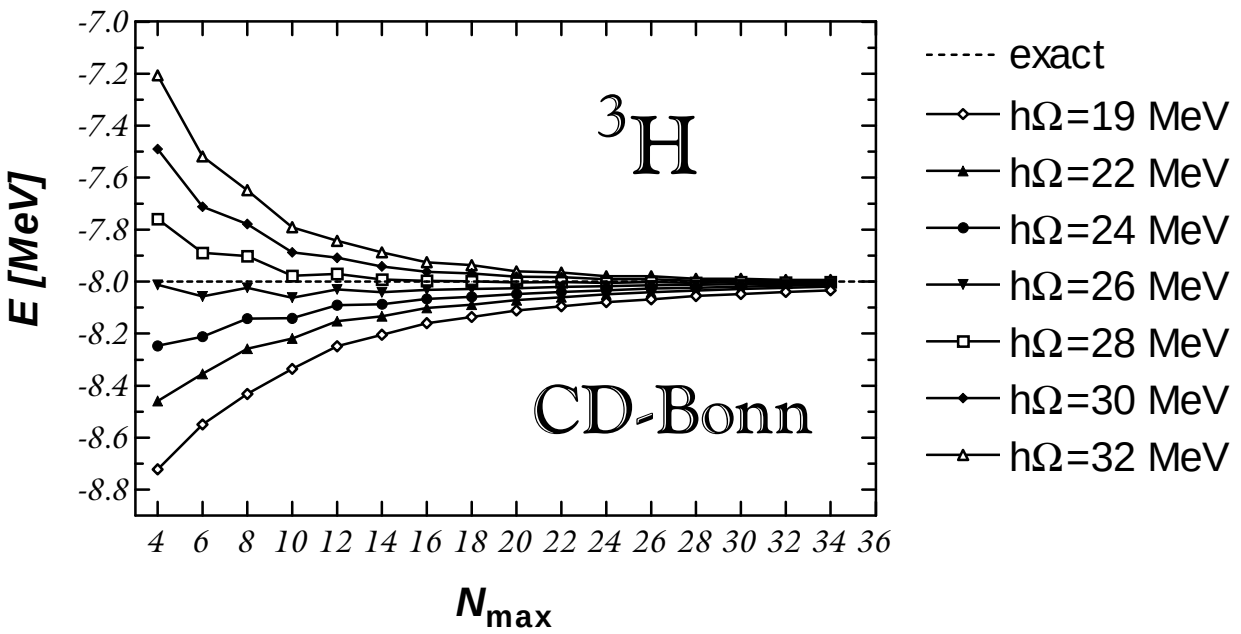
Five electrons QD, Johnson and Payne model, PRL **67**, 1157 (1991)





CENS options

1. You need to fix the the value of $2n + l$ for the maximum size of the huge two-particle space, typically 200-300
2. You need to choose the oscillator energy in MeV
3. The no-core shell-model interaction depends on the number of nucleons, derive one for each nucleus
4. You need to fix $2n + l$ for the model space.
5. Only the triangular model space is available.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-7.2
-7.4
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-7.8
-8.0
-8.2
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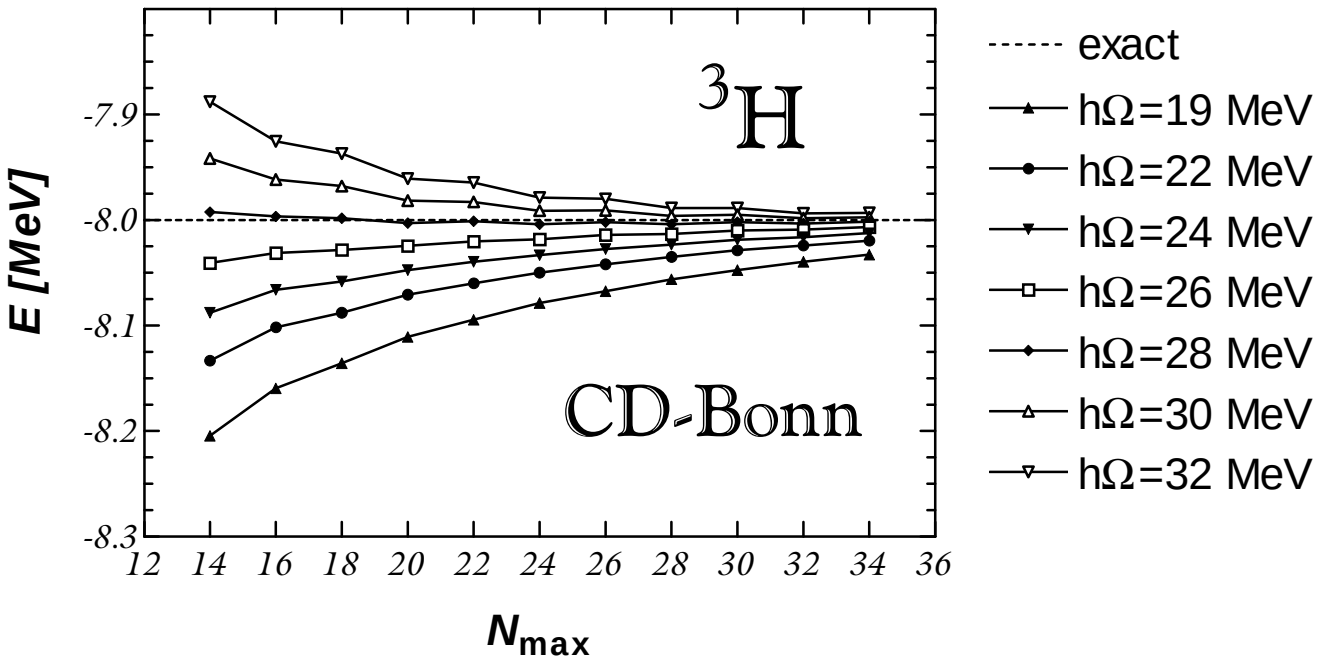
-8.6
-8.8
E [MeV]
4 6 8 10 12 14 16 18 20 22 24 26 28 30 32 34 36
N_{max}
^{3}H
CD-Bonn
exact
hΩ=19 MeV
hΩ=22 MeV
hΩ=24 MeV
hΩ=26 MeV
hΩ=28 MeV
hΩ=30 MeV
hΩ=32 MeV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CD-Bonn
E [MeV]
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-8.0
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N_{max}
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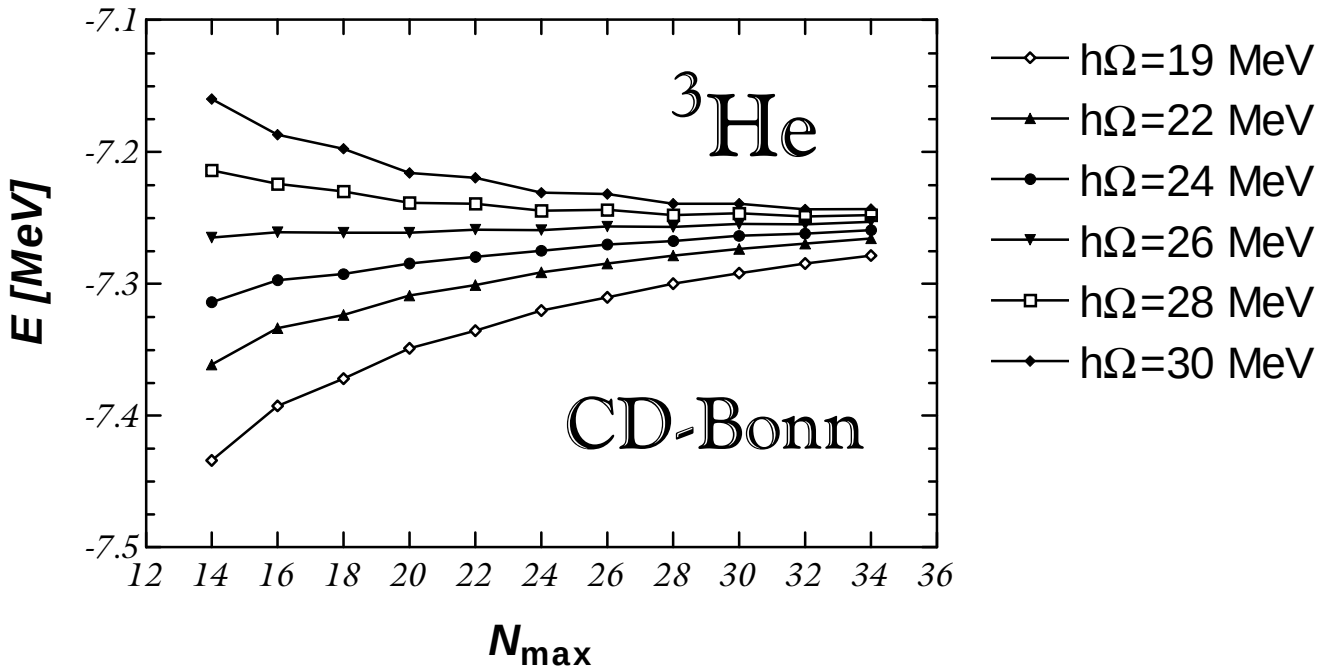
hΩ=32 MeV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E [MeV]
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N_max
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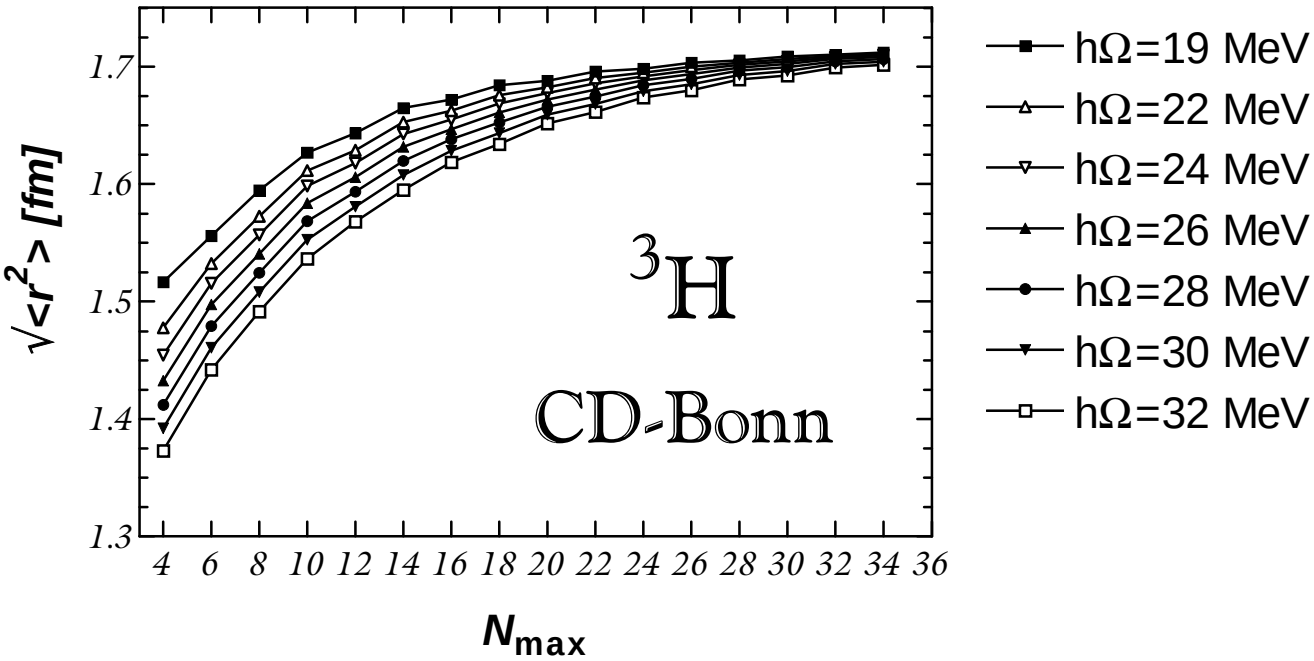
$\sqrt{<r^2>}$ [fm]
1.7
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4 6 8 10 12 14 16 18 20 22 24 26 28 30 32 34 36
N_{max}
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CD-Bonn
hΩ=19 MeV
hΩ=22 MeV
hΩ=24 MeV
hΩ=26 MeV
hΩ=28 MeV
hΩ=30 MeV
hΩ=32 MeV

Decoupling Subspaces and the SVD, a new look at the Lee-Suzuki Method

From Golub and Van Loan (Matrix Computations, chapters 8.6 and 12.4), Shavitt and Redmon (J. Chem. Phys. **73**, 5711 (1980)) and Suzuki (PTP **68**, 246 (1982)). Consider $\omega^\dagger\omega = P\omega^\dagger Q\omega P$, a positive semi-definite (i.e., non-negative definite) operator, acting in the d-dimensional P space only. Since it is symmetric, we may diagonalize it with real eigenvalues $\mu_1^2 \geq \mu_2^2 \geq \cdots \geq \mu_d^2 \geq 0$ and corresponding eigenvectors $|\alpha_k\rangle$, viz,

$$\omega^\dagger\omega\,|\alpha_k\rangle = \mu_k^2\,|\alpha_k\rangle\,, \quad Q\,|\alpha_k\rangle = 0.$$

The eigenvectors $|\alpha_k\rangle$ constitute an ONB for P-space. Observe that we have ordered the eigenvalues in *descending order*, consistent with the interpretation of μ_k as singular values to come.
See Simen Kvaal, PRC **78**, 044330 (2008) for algo.

Decoupling Subspaces and the SVD

Let the dimension of Q-space be n, such that $Q+P$-space is $d+n$-dimensional. It should be clear that in the case that $n < d$, i.e., the Q-space is smaller than the P-space, at least one of the μ_k must be zero. This may of course happen if $n \geq d$ as well.
Let j be the number of zero eigenvalues μ_k^2, i.e.,

$$\mu_d = \mu_{d-1} = \cdots = \mu_{d-j+1} = 0, \quad \mu_{d-j} \neq 0.$$

For each $k \leq d-j$ define $|\nu_k\rangle$ by

$$|\nu_k\rangle := \frac{1}{\mu_k} \omega |\alpha_k\rangle, \quad k \leq d-j.$$

It is readily seen that $P|\nu_k\rangle = 0$, and that

$$\langle \nu_k | \alpha_k | = 0, \quad \langle \nu_k | \nu_\ell | = \delta_{k,\ell}.$$

The vectors $|\nu_k\rangle$ constitute a basis for the *image* of ω. This basis is also orthonormal.

Decoupling Subspaces and the SVD

We can then obtained the SVD of ω in abstract form, viz,

$$\omega = \sum_{k=1}^{d-j} \mu_k \left|\nu_k\right\rangle \left\langle\alpha_k\right| .$$

Recall that the SVD of a matrix loosely can be described as taking an ONB (here the $|\alpha_k\rangle$), stretching it with the singular values (here μ_k), and transforming into a new orthonormal set of vectors (the $|\nu_k\rangle$).

Similarity Transformations

We consider the unitary similarity transform of H given by

$$H' = e^{-T} H e^{T},$$

and T is constructed so that $QH'P = PH'Q = 0$. The P-space effective Hamiltonian is given by

$$H^{\text{eff}} = PH'P,$$

and has d exact eigenvalues of H.

Similarity Transformations

We need to compute $T = \tanh^{-1} X$, with $X = \omega - \omega^\dagger$. This expression is defined through its power series, viz,

$$\tanh^{-1} z = \sum_{n=0}^{\infty} \frac{z^{2n+1}}{2n+1},$$

convergent for all $|z| < 1$. We make a simple observation: Since $\sinh(iy) = i \sin y$ and $\cosh iy = \cos y$, we have $\tanh iy = i \tan y$, and therefore $\tanh^{-1} ix = i \tan^{-1} x$. This is also readily seen from the power series of $\tan^{-1}$:

$$\tan^{-1} z = \sum_{n=0}^{\infty} \frac{(-1)^n z^{2n+1}}{2n+1}.$$

Similarity Transformations

Notice that X is skew-symmetric ($X^\dagger = -X$) and that $PXP = QXQ = 0$. Using the canonical form of ω we have,

$$X = \omega - \omega^\dagger = \sum_{k=1}^{d} \mu_k \left(|\nu_k\rangle \langle \alpha_k| - |\alpha_k\rangle \langle \nu_k| \right).$$

Taking the square of X yields

$$X^2 = -\sum_k \mu_k^2 \left(|\nu_k\rangle \langle \nu_k| + |\alpha_k\rangle \langle \alpha_k| \right),$$

and since $P_k = |\alpha_k\rangle \langle \alpha_k|$ and $Q_k = |\nu_k\rangle \langle \nu_k|$ are projection operators, with $P_k^2 = P_k$, $Q_k^2 = Q_k$, and $P_k Q_k = 0$, we obtain

$$X^{2n} = \sum_k (-1)^n \mu_k^{2n} \left(|\nu_k\rangle \langle \nu_k| + |\alpha_k\rangle \langle \alpha_k| \right).$$

Moreover,

$$X^{2n+1} = \sum_k (-1)^n \mu_k^{2n+1} \left(|\nu_k\rangle \langle \alpha_k| - |\alpha_k\rangle \langle \nu_k| \right).$$

Similarity Transformations

Insertion into the power expansion for $\tanh^{-1} X$, we obtain

$$\tanh^{-1} X = \sum_{n=0}^{\infty} \sum_{k} \frac{(-1)^n \mu_k^{2n+1}}{2n+1} \left(|\nu_k\rangle \langle \alpha_k| - |\alpha_k\rangle \langle \nu_k| \right).$$

We now define

$$\eta_k := \tan^{-1} \mu_k,$$

and by changing the order of the summation readily obtain

$$T = \tanh^{-1} X = \sum_{k} \eta_k \left(|\nu_k\rangle \langle \alpha_k| - |\alpha_k\rangle \langle \nu_k| \right),$$

and note that $T^\dagger = -T$.

Observe how the η_k can be interpreted as *angles*, and that the singular values are simply the tangent of these angles.

Similarity Transformations

The goal here is to compute the exponential exp T, and for that we need all integer powers of T, viz,

$$e^T := \sum_{n=0}^{\infty} \frac{T^n}{n!} = 1 + \sum_{n=1}^{\infty} \frac{T^n}{n!}.$$

By definition, $T^0 = 1$. Computing T^2, then T^{2n} and finally T^{2n+1} is completely analoguous to the computation of the powers of X; it is the same mechanism but "different μ_k" in the summation over k. We simply state the result:

$$T^{2n} = \sum_k (-1)^n \eta_k^{2n} \left(|\alpha_k\rangle \langle \alpha_k| + |\nu_k\rangle \langle \nu_k| \right),$$

$$T^{2n+1} = \sum_k (-1)^n \eta_k^{2n+1} \left(|\nu_k\rangle \langle \alpha_k| + |\alpha_k\rangle \langle \nu_k| \right).$$

Similarity Transformations

The power expansion of exp T splits into a cosine part and a sine part:

$$e^T = 1 + \sum_k (c_k - 1)\left(|\alpha_k\rangle\langle\alpha_k| + |\nu_k\rangle\langle\nu_k|\right) + \sum_k s_k\left(|\nu_k\rangle\langle\alpha_k| + |\alpha_k\rangle\langle\nu_k|\right),$$

where for brevity we have defined

$$s_k := \sin\eta_k, \quad c_k := \cos\eta_k.$$

Thus, exp T is manifestly a multi-dimensional rotation in the basis of $P+Q$-space given by $|\alpha_k\rangle$, $|\nu_k\rangle$.
The unitarity of exp T is readily checked.

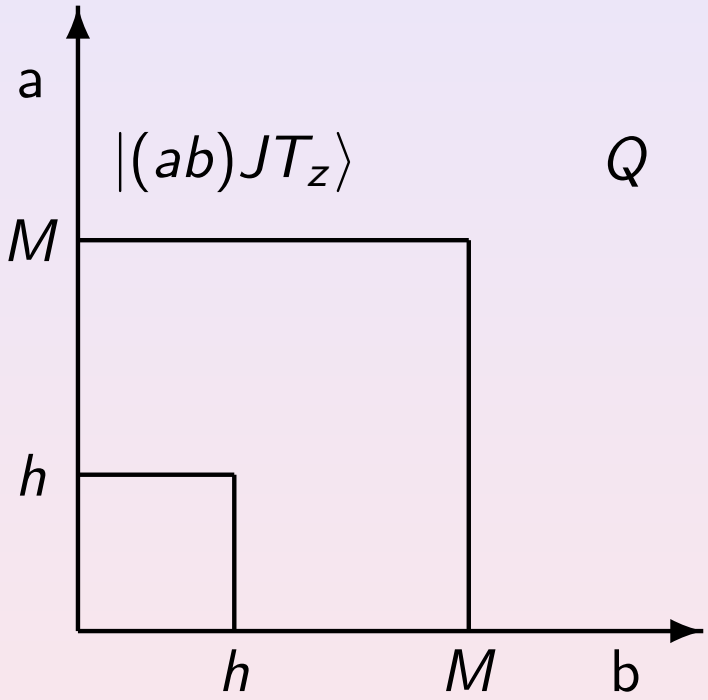
G-matrix: Resummation of a Class of Diagrams

- 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.

Effective Hamiltonian and Model Spaces



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

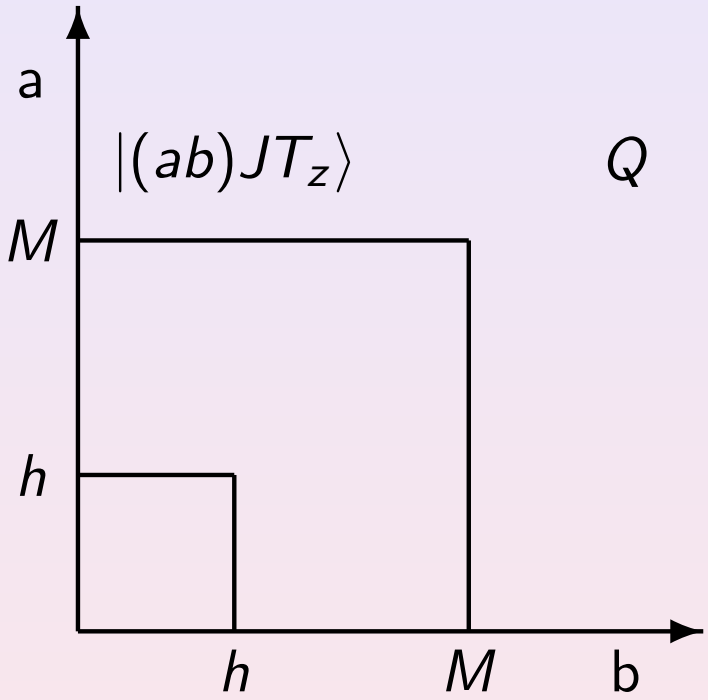
Two-Body Effective Hamiltonian for Large Space

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

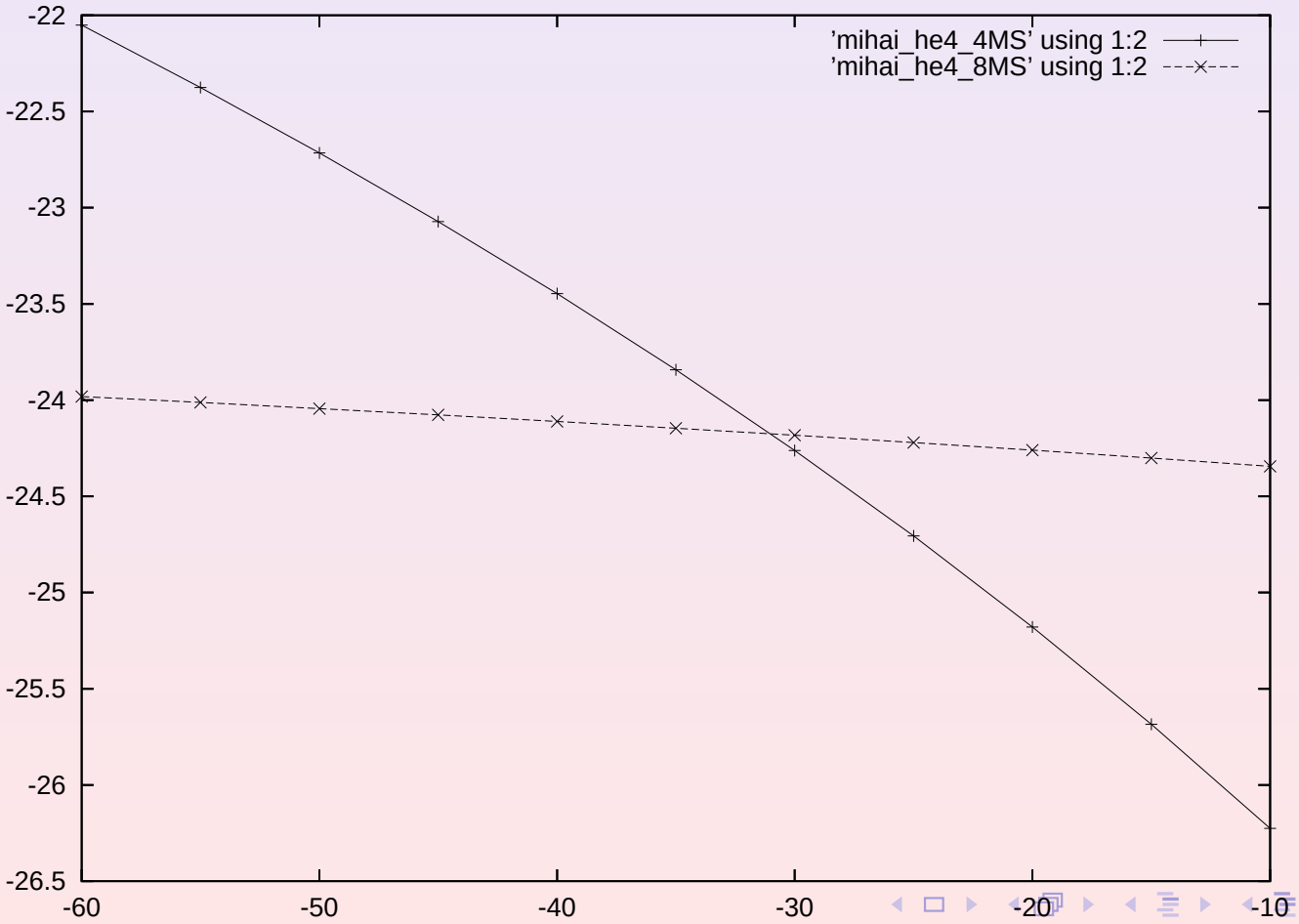
$$\times \langle ab|\lambda SJ\rangle \langle cd|\lambda' S' J\rangle \, \langle nlNL|n_a l_a n_b l_b \lambda\rangle \left\langle n' l' NL|n_c l_c n_d l_d \lambda'\right\rangle$$

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

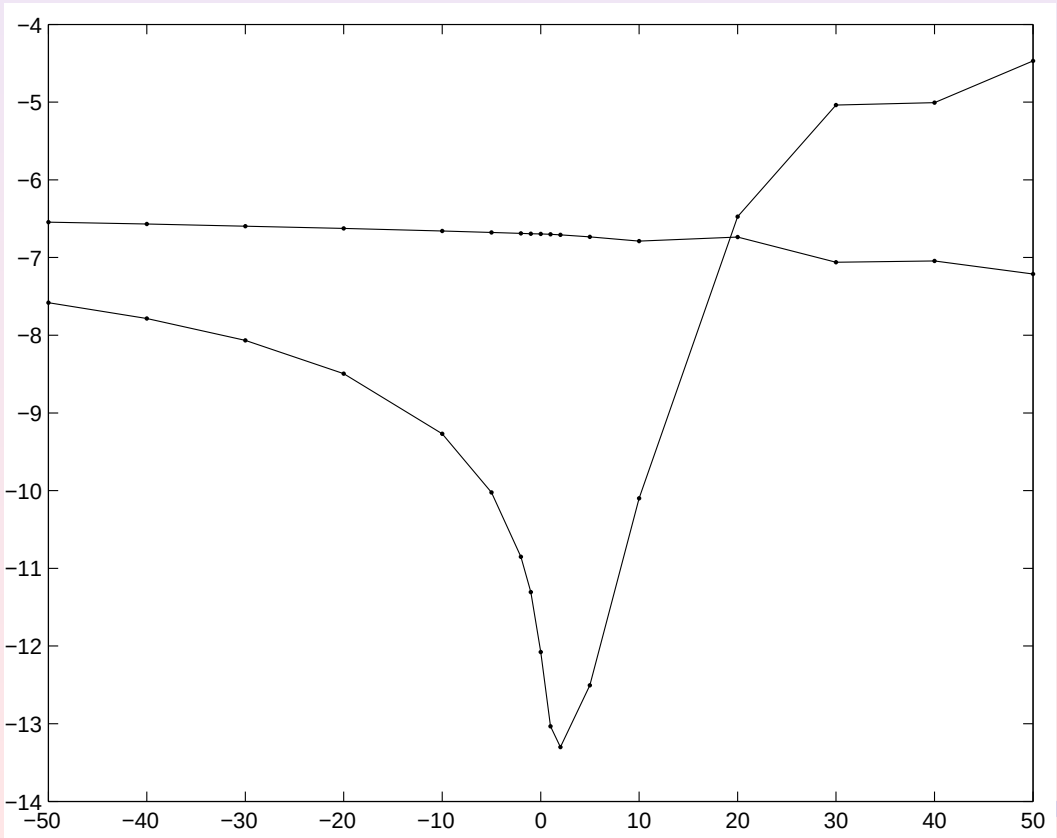
$$\times \left\langle nNlL\mathcal{J}ST|\, G\, \middle| n' N' l' L' \mathcal{J} S' T \right\rangle,$$

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 $(0s_{1/2})^2 JT_z = 01$



CENS options

1. You need to fix the number of starting energies, default is 5 and the energies run from -5 to -140 MeV
2. You need to choose the oscillator energy in MeV
3. The G-matrix does not depend on number of nucleons.
4. You can use square, triangular or wings as options for the model space.
5. You need to fix the size of the model space

Recipe for Vlowk

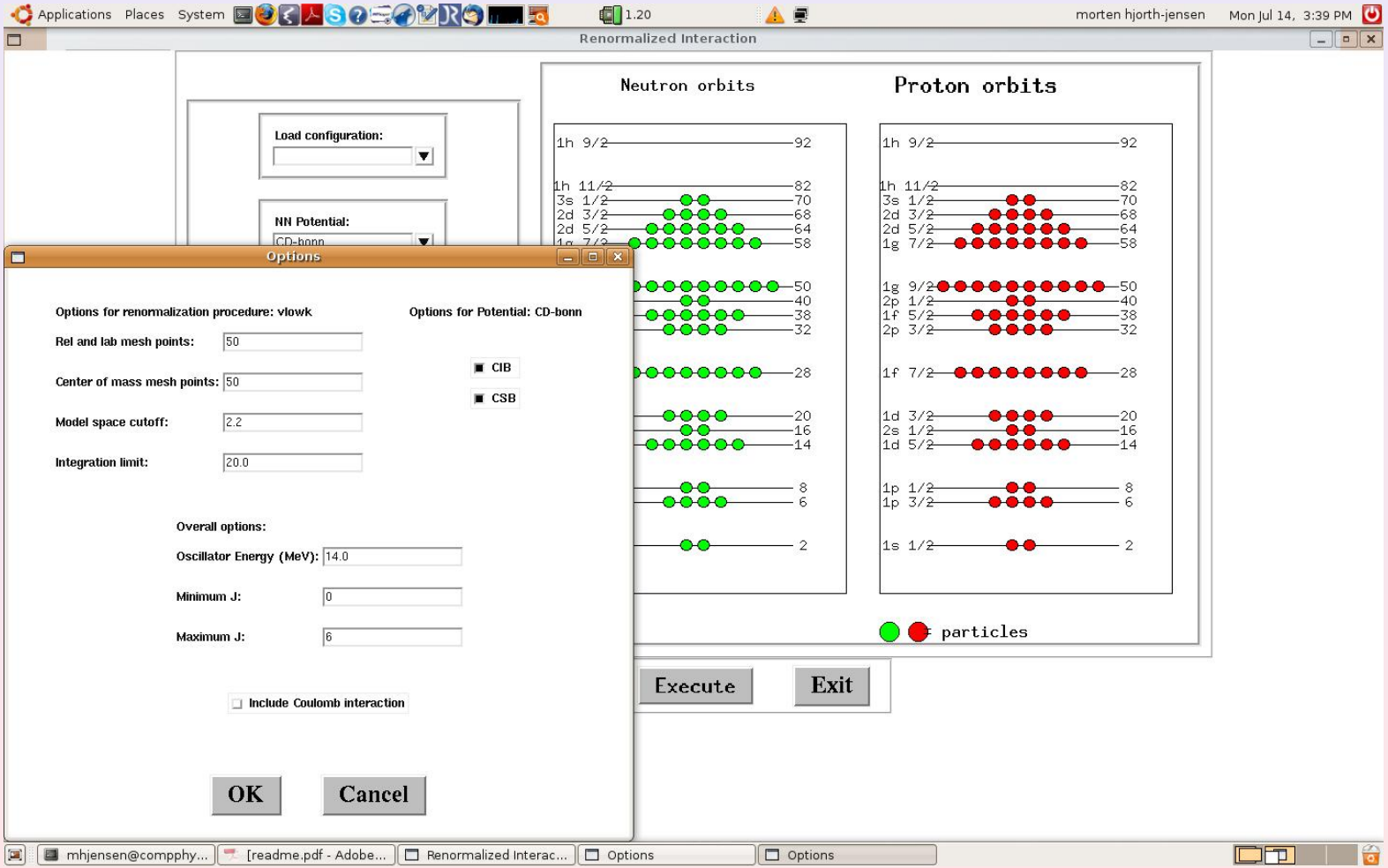
- Diagonalize the two-body Schrödinger equation in momentum space for all momenta
- Choose a cutoff which defines the model space in terms of relative momenta
- Use exact eigenvalues and momenta to perform a similarity transformation
- Obtain effective interaction in relative momenta
- Integrate to get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

Potential drawback: no connection with harmonic oscillator cutoff. Results are cutoff dependent and one needs cutoff dependent many-body forces as well.

CENS options

1. You need to fix the the cutoff for model space in momentum space, and the infinite space.
2. Fix number of integration points for the model space and the huge space
3. You need to choose the oscillator energy in MeV
4. You need to fix $2n + l$ for the model space.
5. You can use square, triangular and wings as options for the model space in an oscillator representation.

CENS image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CD-bonn
Neutron orbits
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1h 11/2 82
3s 1/2 70
2d 3/2 68
2d 5/2 64
1g 7/2 58
50
40
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32
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16
14
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1f 7/2
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2s 1/2
1d 5/2
1p 1/2
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Integration limit: 20.0
CIB
CSB
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Maximum J: 6
Include Coulomb interaction
OK
Cancel
mhjensen@compphy...
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Options
Options

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

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 can be included in all models.

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

$$\sum_{\alpha\leq\beta} |\alpha\beta\rangle\langle\alpha\beta| = \mathbf{1}, \tag{4}$$

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

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

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

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

represent the interaction $H_{\rm I}$ 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

$$\langle ab|\alpha\beta\rangle = \frac{\langle a|\alpha\rangle\langle b|\beta\rangle - (-1)^{J-j_\alpha-j_\beta}\langle a|\beta\rangle\langle b|\alpha\rangle}{\sqrt{(1+\delta_{ab})(1+\delta_{\alpha\beta})}} \tag{5}$$

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

$$\langle ab|\alpha\beta\rangle = \langle a|\alpha\rangle\langle b|\beta\rangle \tag{6}$$

for the proton-neutron case.