Lecture II: Renormalization of the Nucleon-Nucleon Interaction

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Lectures at Universitad Complutense Madrid

Outline

Renormalization of the NN force
- Definitions
- 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..

From yesterday: Before we proceed...some philosophical thoughts...

We wish to interpret data. To do so we need to define what we mean with the concept of an **OBSERVABLE**.

- How do you define an observable;
- Make then a list of observables;
- and possible links to theoretical descriptions
- and more for today: how do we define a closed-shell core and
- and single-particle states?

Where are we from a many-body point view?

- Exact or virtually exact solutions available for: $A = 3$: solution of Faddeev equation. $A = 4$: solvable via Faddeev-Yakubowski approach.
- Light nuclei (up to $A = 12$ at present): Green's function Monte Carlo (GFMC); virtually exact; limited to certain forms of interactions. Highly accurate approximate solutions available for:
- Light nuclei (up to $A = 16$ at present): No-core Shell model (NCSM); truncation in model space.
- Light and medium mass region ($A = 4$, 16, 40, 48 56 and 60 at present): Coupled cluster theory, truncations in model space and correlations.

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

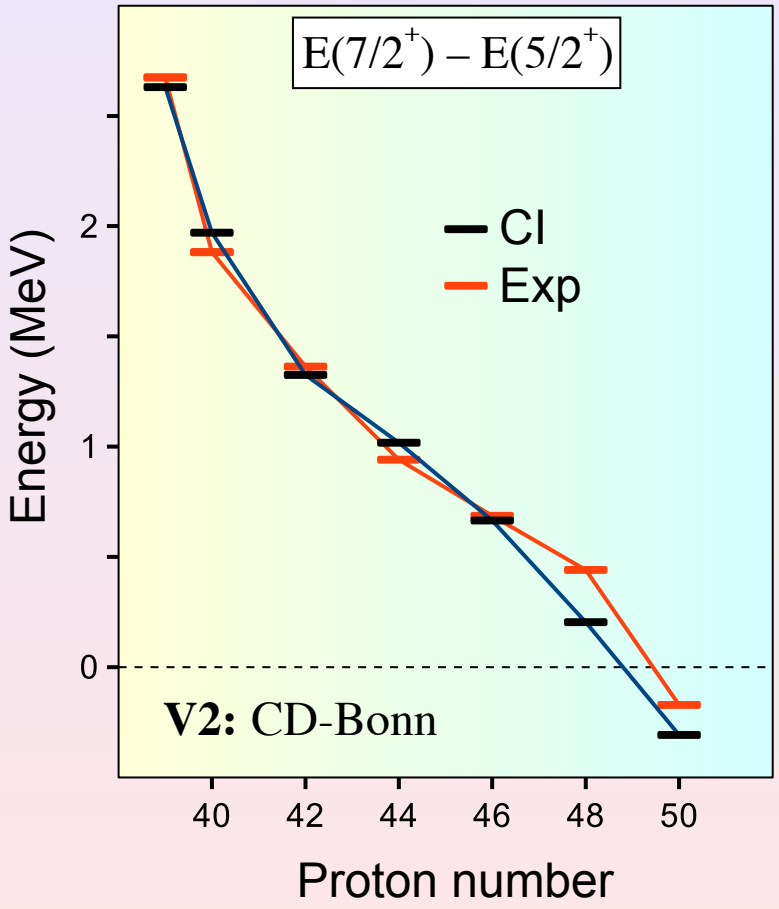
$$P = \sum_{i=1}^{D} |\psi_i\rangle \langle\psi_i| ,$$

and

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

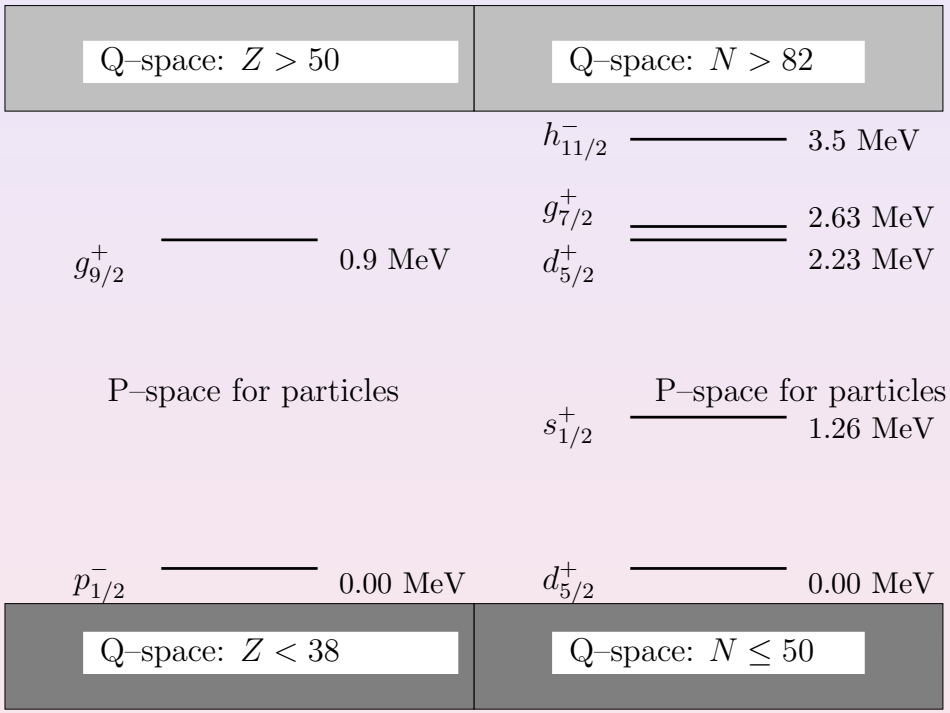
with D being the dimension of the model space, and $PQ = 0$, $P^2 = P$, $Q^2 = Q$ and $P + Q = I$. The wave functions $|\psi_i\rangle$ are eigenfunctions of the unperturbed hamiltonian $H_0 = T + U$ (with eigenvalues ε_i), where T is the kinetic energy and U an appropriately chosen one-body potential, 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

Our story: Ground state of ^{101}Sn, Darby *et al*, PRL105, 2010



- Shell-model calculation with ^{88}Sr as core.
- How do we define this model space?
- And how do we define interactions?

Closed Shell **Core**: ^{88}Sr, Model Space Example



Dimensionalities

Solution of the Schrödinger eq. for N nucleons in a valence P–space $\Longrightarrow$ Numerous to infinite degrees of freedom. Number of basic states for the shell model calculation in the Sn isotopes with the single–particle orbits and using the m-scheme: $1d_{5/2}$, $0g_{7/2}$, $1d_{3/2}$, $2s_{1/2}$ and $0h_{11/2}$

System	Dimension	System	Dimension
^{102}Sn	36	^{110}Sn	1 853 256
^{103}Sn	245	^{111}Sn	3 608 550
^{104}Sn	1 504	^{112}Sn	6 210 638
^{105}Sn	7 451	^{113}Sn	9 397 335
^{106}Sn	31 124	^{114}Sn	12 655 280
^{107}Sn	108 297	^{115}Sn	15 064 787
^{108}Sn	323 682	^{116}Sn	16 010 204
^{109}Sn	828 422		

More on Dimensionalities

Using ^{100}Sn as closed shell core as soon as we add protons the dimension grows dramatically

System	Dimension	System	Dimension
^{104}Sn	$\approx 1.5 \cdot 10^3$	^{112}Sn	$\approx 6.2 \cdot 10^6$
^{108}Sn	$\approx 3.2 \cdot 10^5$	^{116}Sn	$\approx 1.6 \cdot 10^7$
^{104}Sb	$\approx 6.5 \cdot 10^3$	^{112}Sb	$\approx 1.1 \cdot 10^8$
^{108}Sb	$\approx 3.2 \cdot 10^6$	^{116}Sb	$\approx 1.9 \cdot 10^9$

Even more on Dimensionalities

Huge dimensionalities in brute force no-core shell-model calcs

System	4 major shells	7 major shells
^{4}He	4E4	9E6
^{8}B	4E8	5E13
^{12}C	6E11	4E19
^{16}O	3E14	9E24

Shell-model codes can today reach dimensionalities of $d \sim 10^{10}$ basis states. Monte Carlo based shell-model codes can attack problems with $d \sim 10^{15}$.

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 $\phi_i(\mathbf{x}_i)$

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

We can 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.

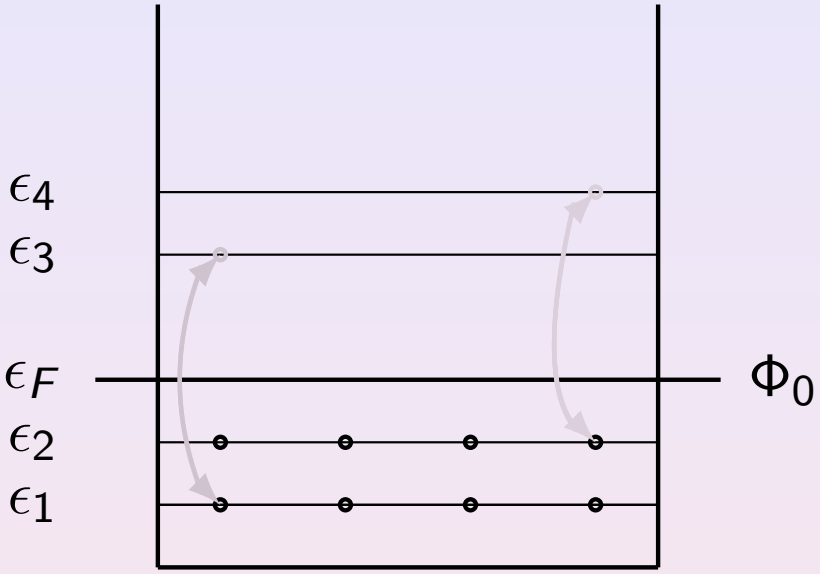
Understanding excitations, model spaces and excluded spaces

The single-particle wave functions of

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

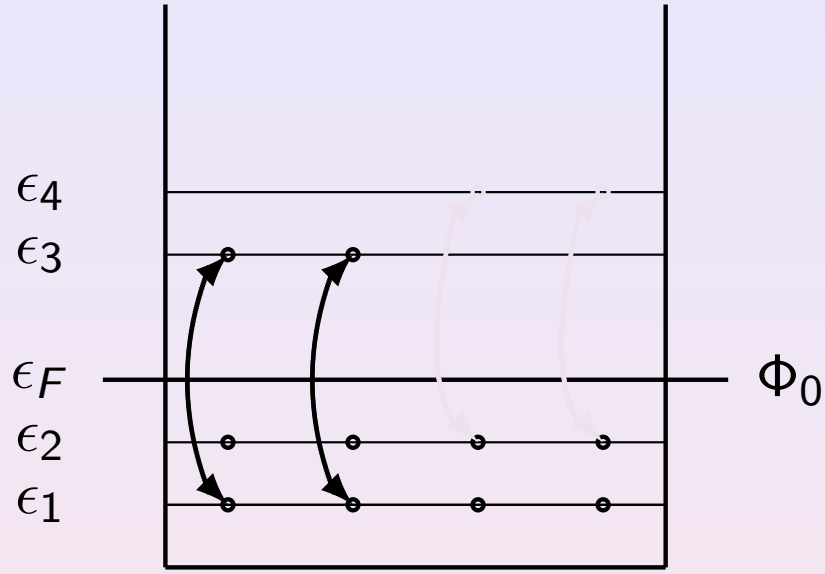
are normally chosen as the solutions of the so-called non-interacting part of the Hamiltonian, H_0. A typical basis is provided by the harmonic oscillator problem.

Excitations in Pictures



From T_1 to T_1^2

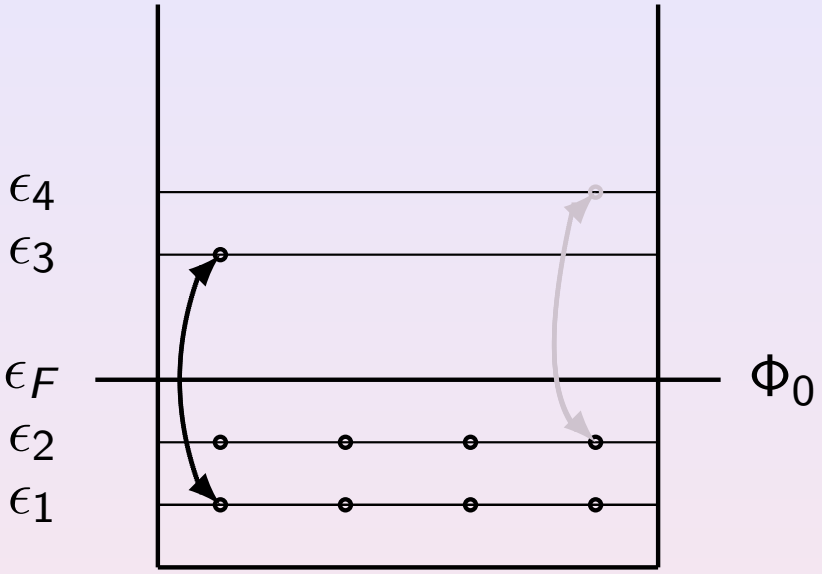
$T_1 \propto a_a^+ a_i$



From T_2 to T_2^2

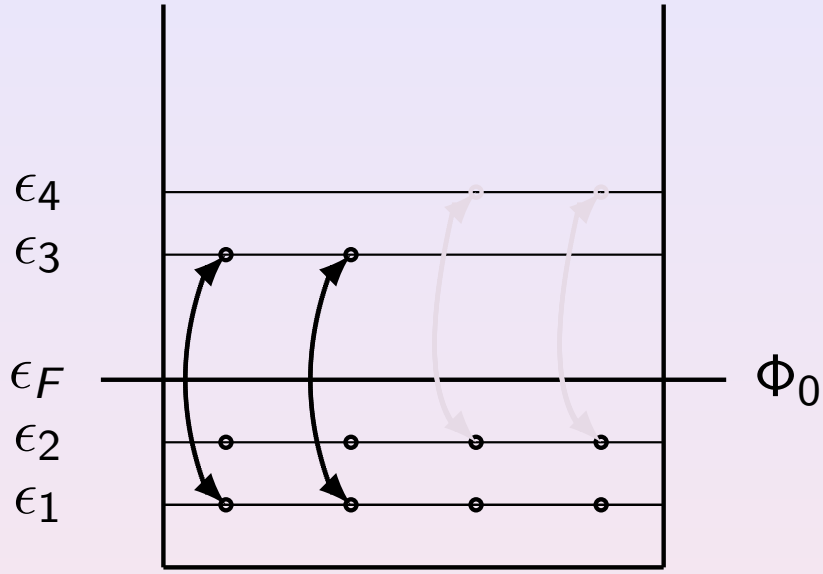
$T_2 \propto a_a^+ a_b^+ a_j a_i$

Excitations in Pictures



From T_1 to T_1^2

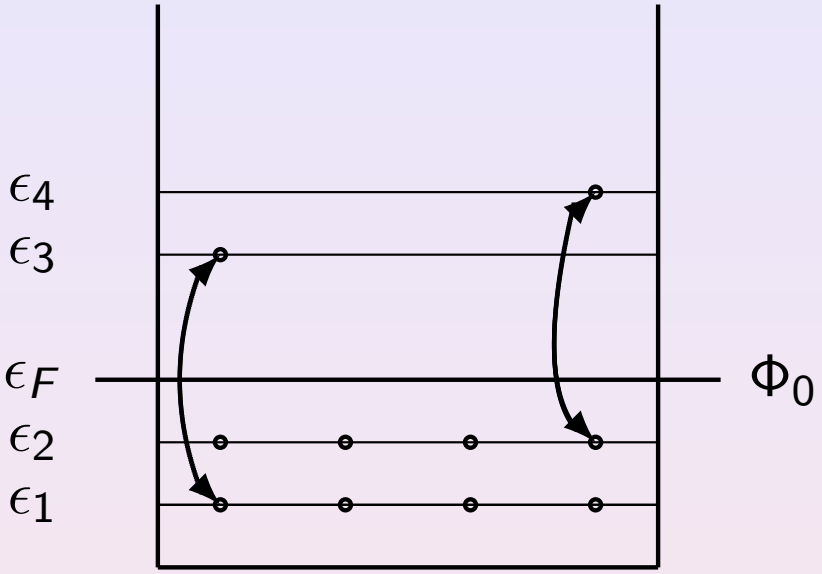
$T_1 \propto a_a^+ a_i$



From T_2 to T_2^2

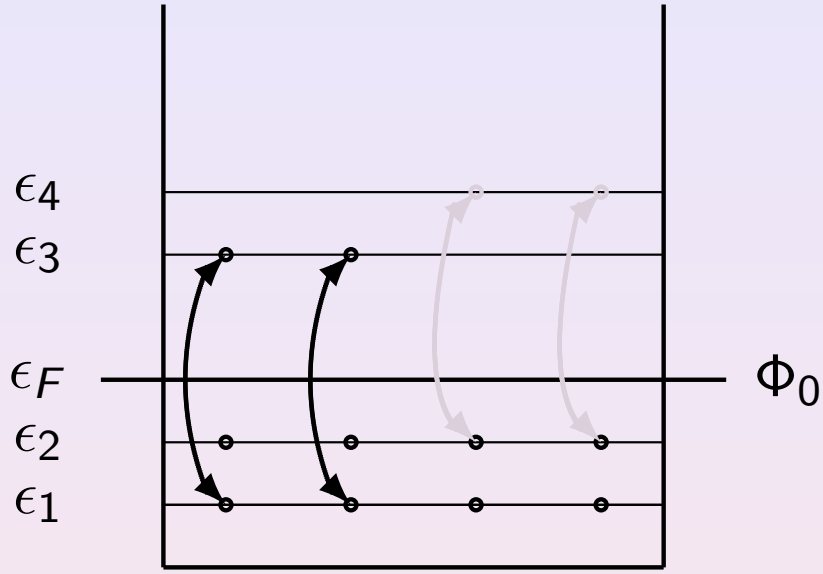
$T_2 \propto a_a^+ a_b^+ a_j a_i$

Excitations in Pictures



From T_1 to T_1^2

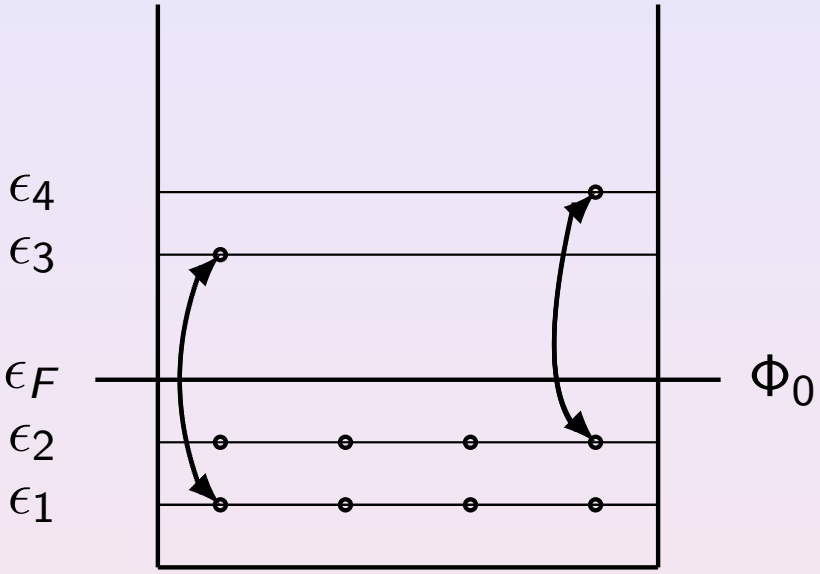
$T_1 \propto a_a^+ a_i$



From T_2 to T_2^2

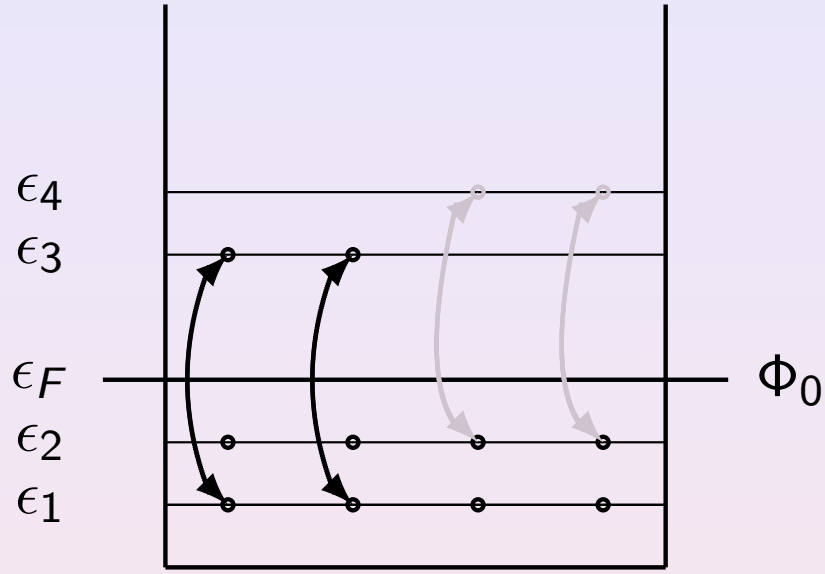
$T_2 \propto a_a^+ a_b^+ a_j a_i$

Excitations in Pictures



From T_1 to T_1^2

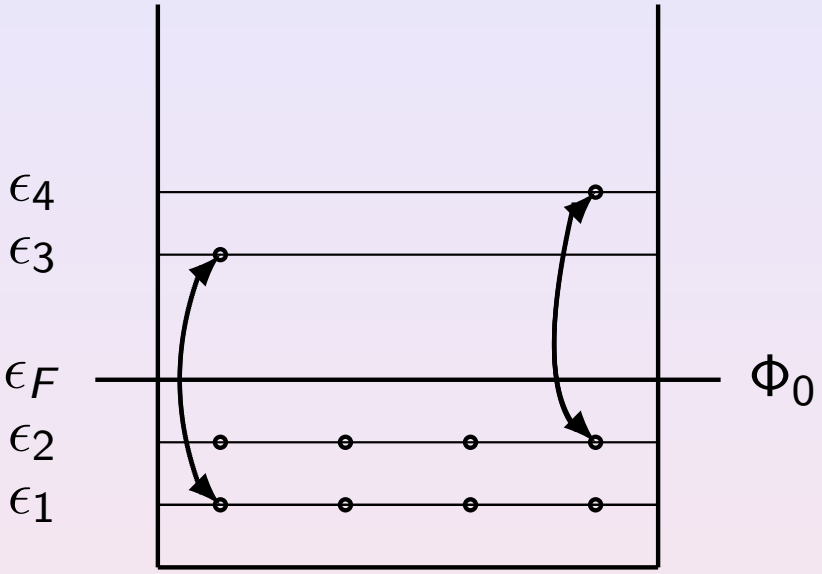
$T_1 \propto a_a^+ a_i$



From T_2 to T_2^2

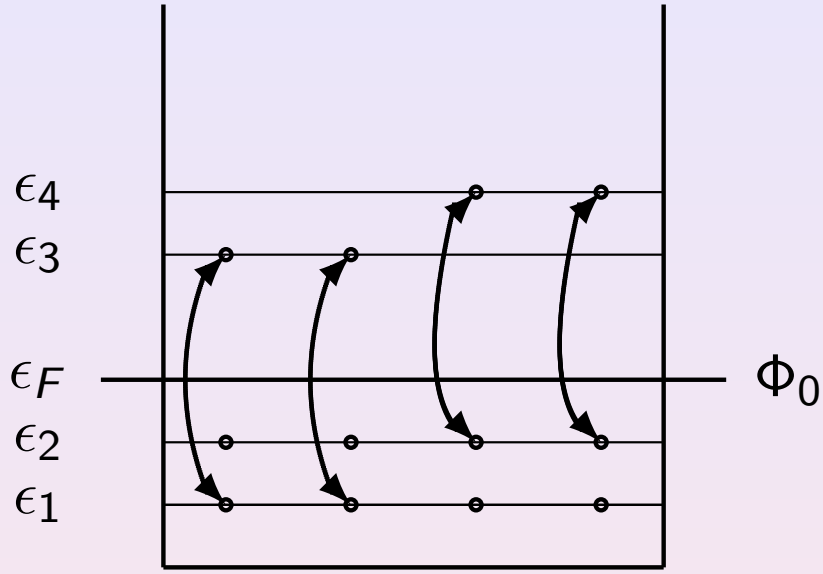
$T_2 \propto a_a^+ a_b^+ a_j a_i$

Excitations in Pictures



From T_1 to T_1^2

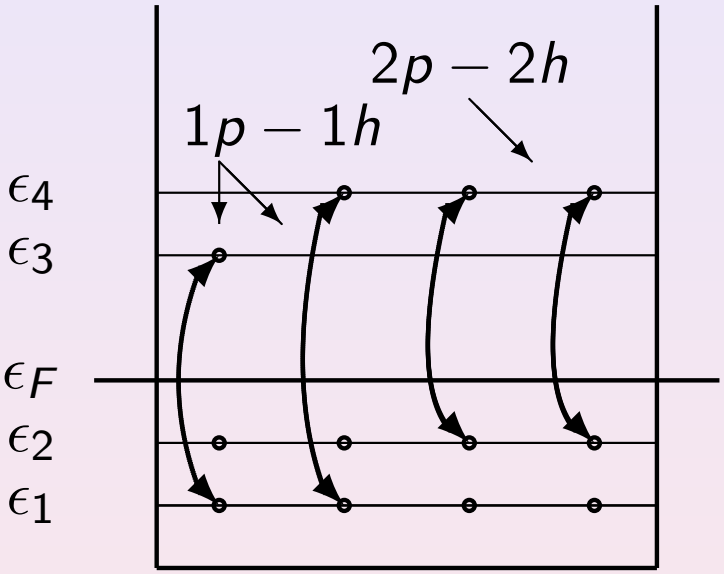
$T_1 \propto a_a^+ a_i$



From T_2 to T_2^2

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

Excitations



Shell-Model Truncations

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

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

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

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

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

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

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

and T is constructed so that $QH'P = PH'Q = 0$ (decoupling condition). 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

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

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

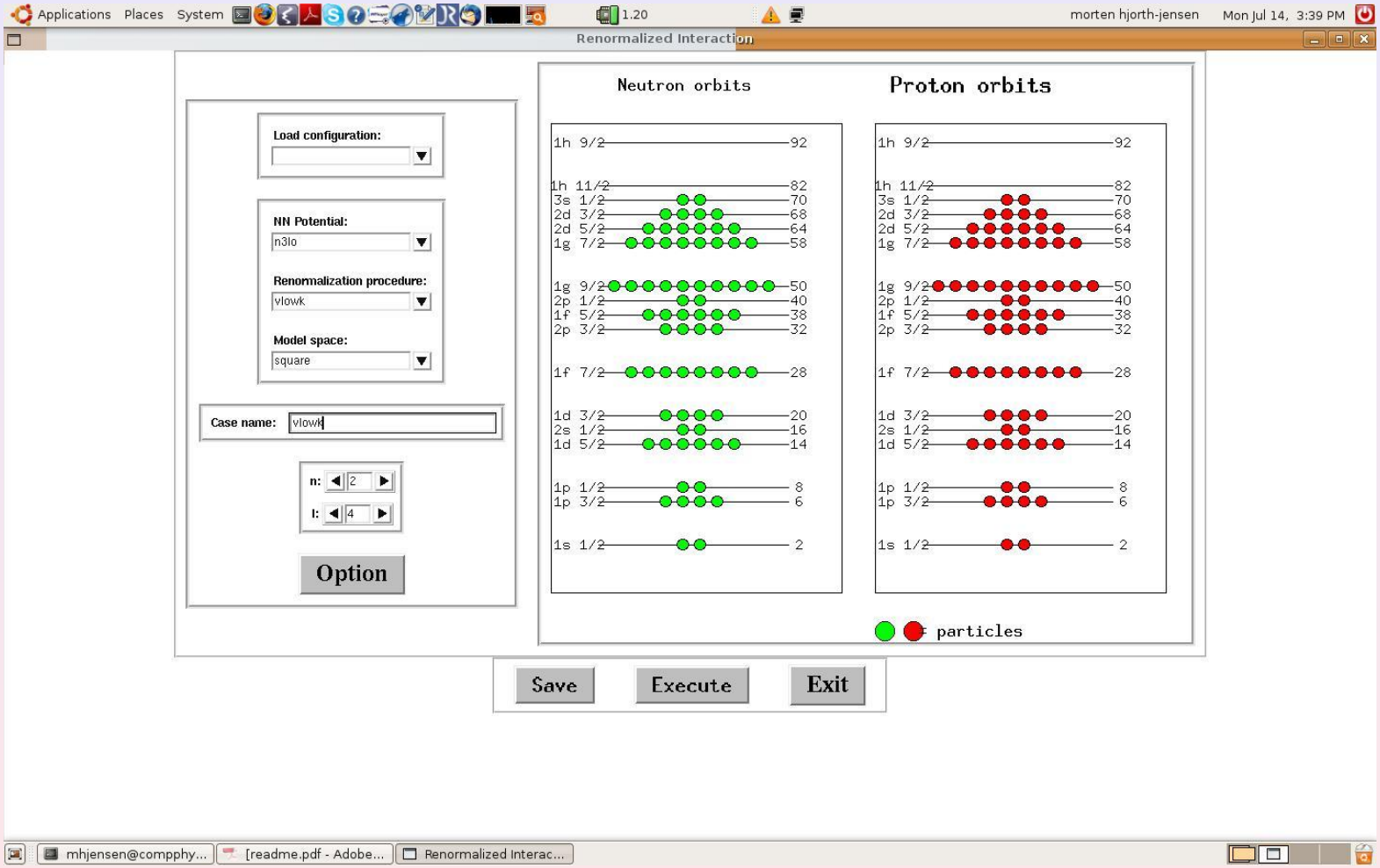
while $k = 1$ changes the diagonal elements

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

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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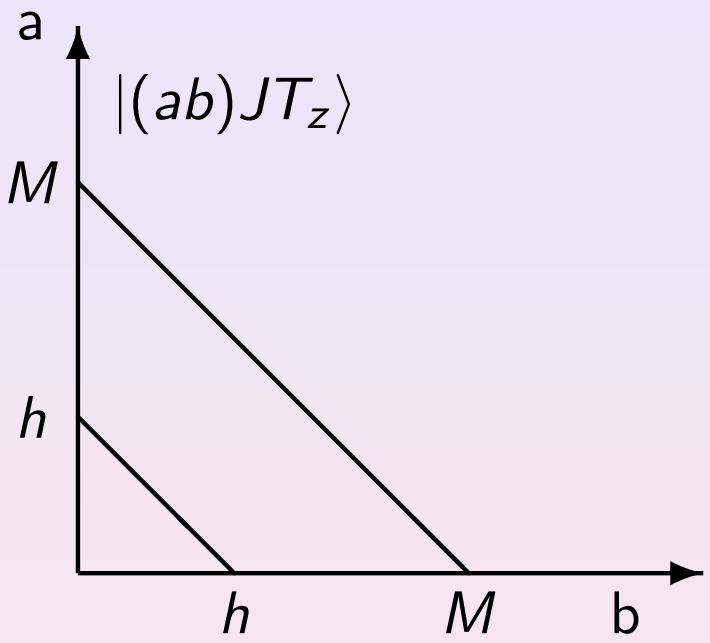
Effective Hamiltonian for Large Spaces, no-core calculations



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

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

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

with

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

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

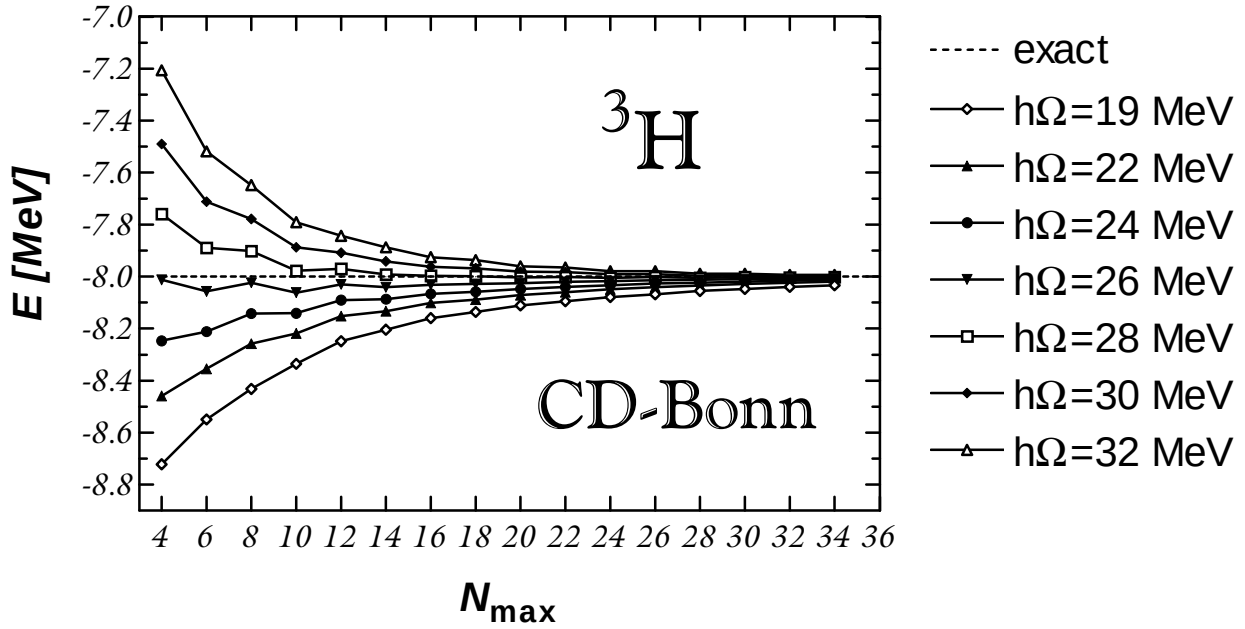
$$H_2^{\Omega} \equiv H_{02}^{\Omega} + V_2^{\Omega} = \frac{\vec{p}_1^{\,2} + \vec{p}_2^{\,2}}{2m} + \frac{1}{2} m\Omega^2 (\vec{r}_1^{\,2} + \vec{r}_2^{\,2}) + V(\vec{r}_1 - \vec{r}_2) - \frac{m\Omega^2}{2A} (\vec{r}_1 - \vec{r}_2)^2 \ .$$

- 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 $2n + l \sim 4 - 20$

See Simen Kvaal, PRC **78**, 044330 (2008) for algo or the appendix of these lecture notes. Codes for this are included in the package.

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
-7.6
-7.8
-8.0
-8.2
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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
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CD-Bonn
exact
hΩ=19 MeV
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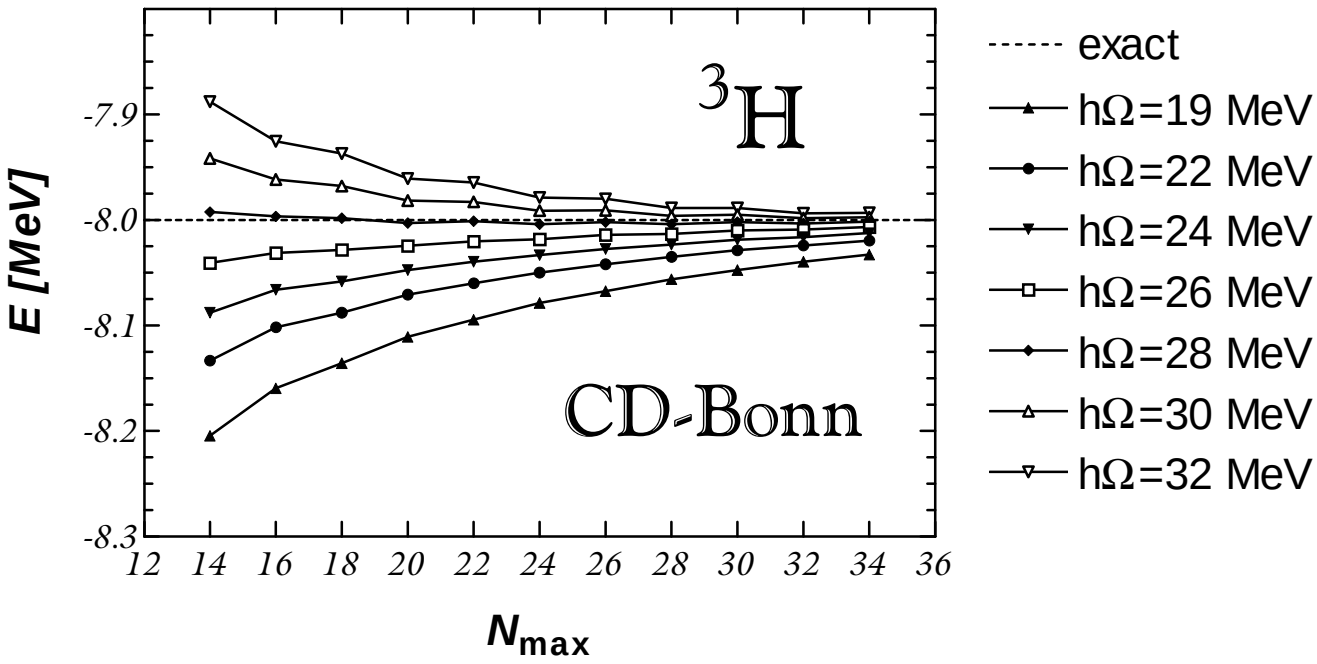
hΩ=32 MeV


^{3}H
CD-Bonn
E [MeV]
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-8.0
-8.1
-8.2
-8.3
12 14 16 18 20 22 24 26 28 30 32 34 36
N_{max}
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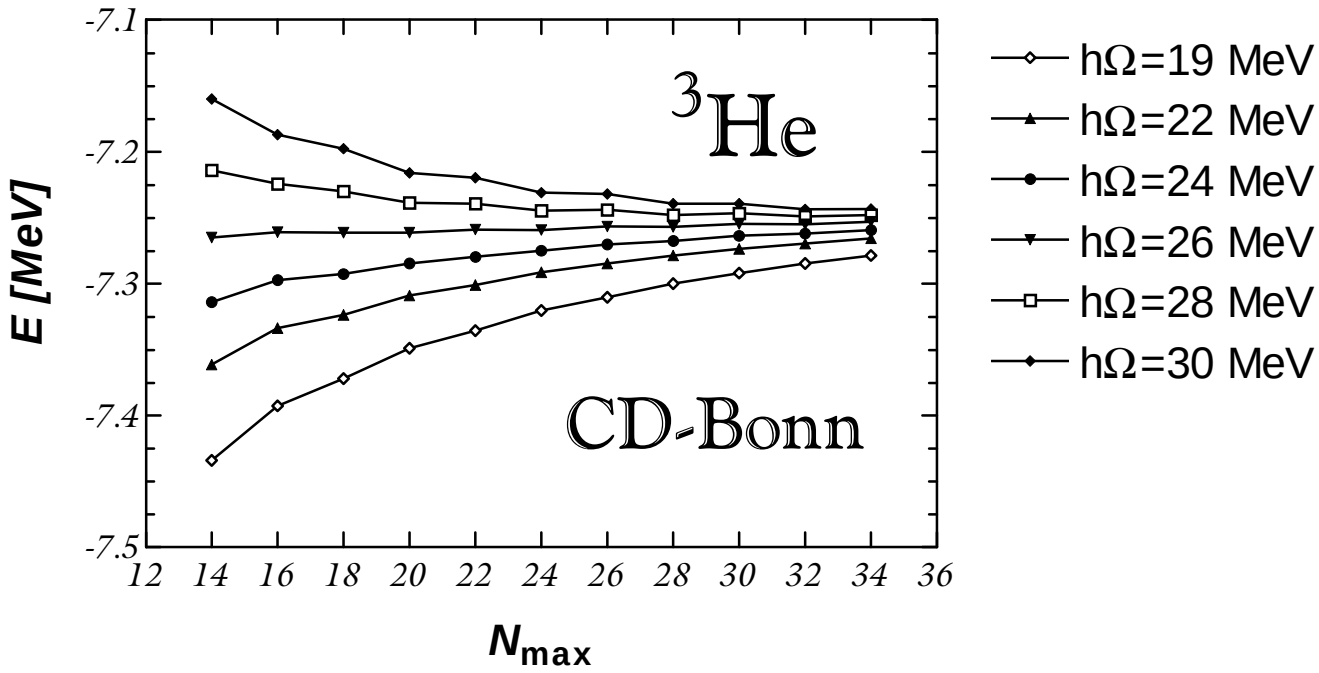
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-7.2
-7.3
-7.4
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E [MeV]
12 14 16 18 20 22 24 26 28 30 32 34 36
N_max
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hΩ=28 MeV
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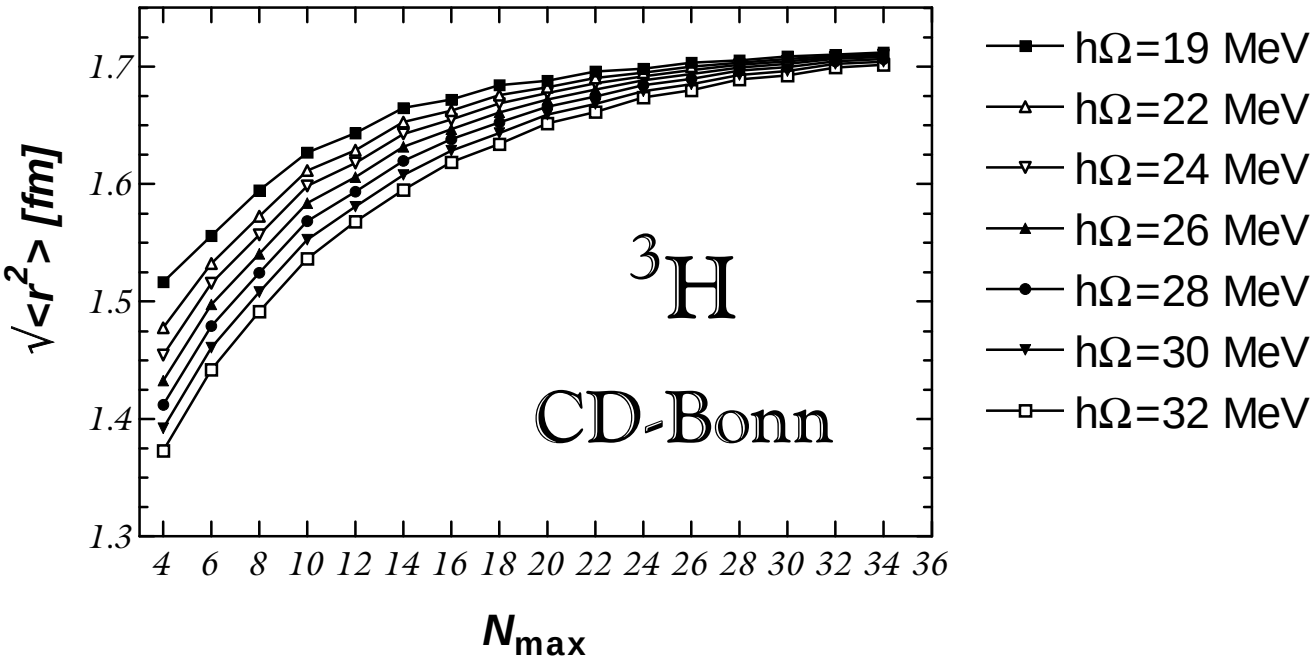
$\sqrt{<r^2>}$ [fm]
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N_{max}
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hΩ=19 MeV
hΩ=22 MeV
hΩ=24 MeV
hΩ=26 MeV
hΩ=28 MeV
hΩ=30 MeV
hΩ=32 MeV

How large a model space do we need?

Estimate for model spaces and Hamiltonian matrix dimension

1. Assume we want to compute the binding energy of a nucleus with mass number A in a wave function based approach. Assume that the interaction has a momentum cutoff Λ
2. What are the minimum requirements for the model space?

How large a model space do we need?

Possible Answer

To make our scheme more explicit, assume that we are planning a calculation of the oxygen isotopes with an effective field theory interaction that employs a cutoff $\Lambda = 600$ MeV. Assume also that our favourite single-particle basis is the harmonic oscillator, with single-particle energies $\varepsilon_{nl} = \hbar\omega(2n + l + 3/2)$, with ω the oscillator frequency, $n = 0, 1, 2, \ldots$ being the number of nodes and l the single-particle orbital momentum. The oscillator length b is defined as

$$b = \sqrt{\frac{\hbar}{m\omega}}.$$

How large a model space do we need?

Possible Answer

We define $p = 0, 1, 2, \ldots, P$ with $P = 2n + l$ as the quantum number p of the highest filled level. The level labelled p can accomodate $(p+1)(p+2)$ fermions, with a spin degeneracy of two for every single-particle state taken into account. For a given maximum value of $P = 2n_{\max} + l_{\max}$ we have a total of

$$N = \sum_{p=0}^{P} (p+1)(p+2) = \frac{(P+1)(P+2)(P+3)}{3},$$

single-particle states.

How large a model space do we need?

Possible Answer

The cutoff Λ defines the maximum excitation energy a system of A nucleons can have. The largest single-particle excitation energy (corresponding to possible one-particle-one-hole correlations) is then

$$\Lambda = \hbar\omega P = \hbar\omega(2n_{\max} + l_{\max}).$$

How large a model space do we need?

Possible Answer

The value of $\hbar\omega$ can be extracted from the mean squared radius of a given nucleus. One can show that this results in [**?**]

$$\hbar\omega \approx \left(\frac{3}{2}\right)^{4/3} \frac{\hbar^2}{2m_N r_0^2} A^{-1/3},$$

with $r_0 \approx 1$ fm. Setting $A = 16$ and $\Lambda = 600$ MeV, results in $P \approx 42$. The largest possible value for n is then $n_{\max} \approx 21$, or 22 major shells. With $P = 42$, the total number of single-particle states in this model space is 28380!

How large a model space do we need?

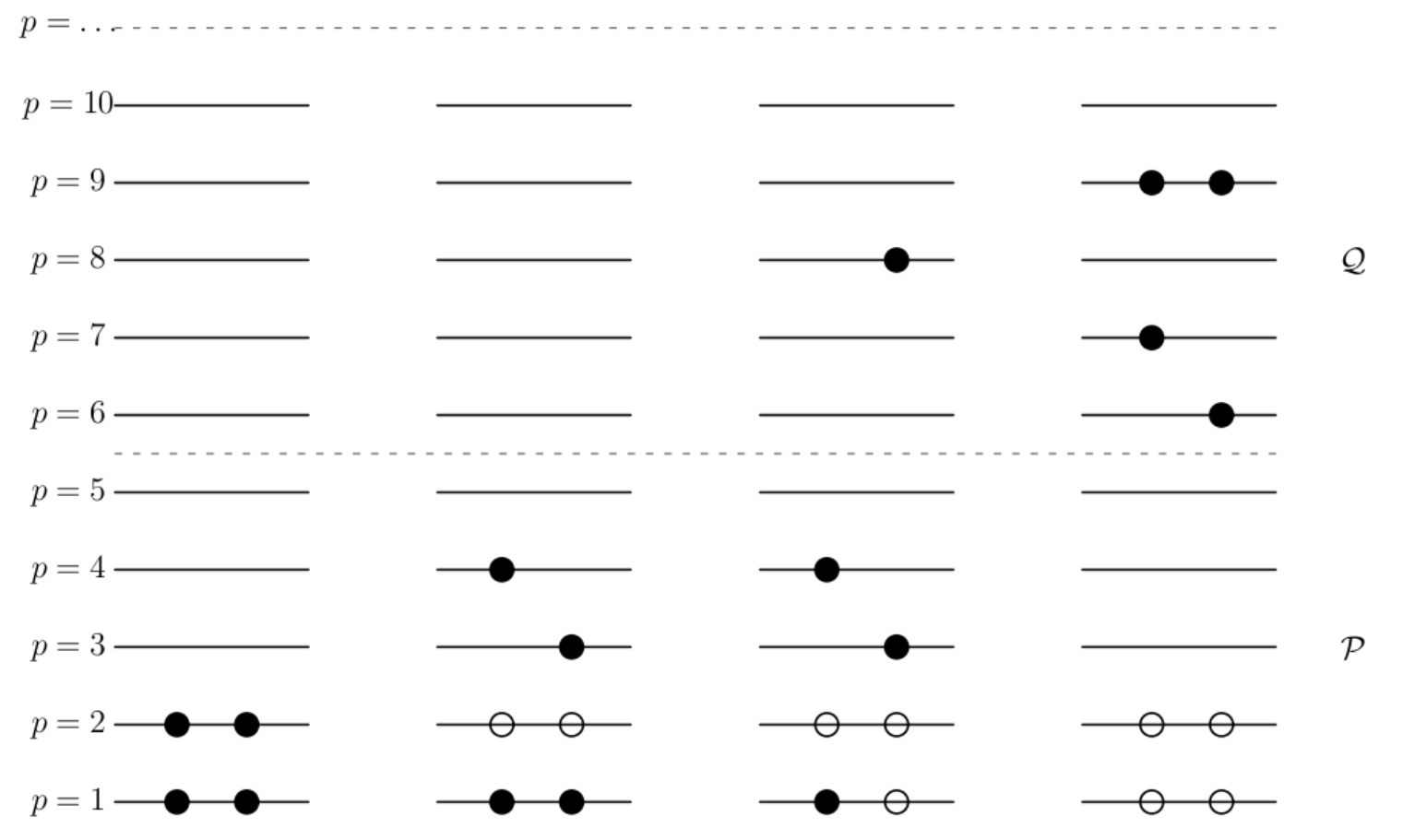
Possible Answer

For ^{16}O this means that we to have distribute eight protons and eight neutrons in 28380 single-particle states, respectively. The total number of Slater determinants, with no restrictions on energy excitations, is

$$\left(\begin{array}{c} 28380 \\ 8 \end{array} \right) \times \left(\begin{array}{c} 28380 \\ 8 \end{array} \right) \approx 10^{62}.$$

Any direct diagonalization method in such a huge basis is simply impossible. Need smaller spaces and/or smarter methods/approximations.

Missing many-body physics? Simple model, see JPG **37**, 064035



Simple model, see JPG **37**, 064035

Our specific model consists of N doubly-degenerate and equally spaced single-particle levels labelled by $p = 1, 2, \ldots$ and spin $\sigma = \pm 1$.
We write the Hamiltonian as

$$\hat{H} = \hat{H}_0 + \hat{V},$$

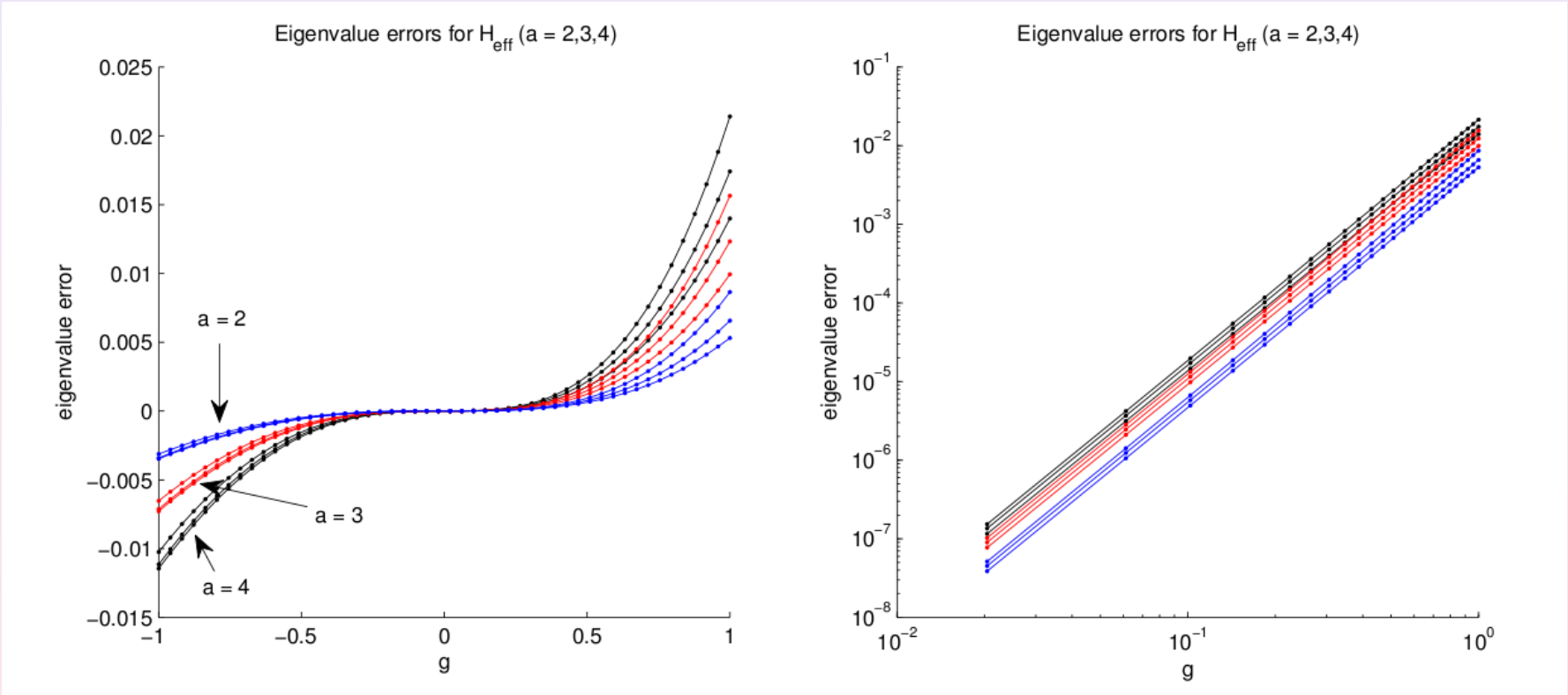
where

$$\hat{H}_0 = \xi \sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma}$$

and

$$\hat{V} = -\frac{1}{2} g \sum_{pq} a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{p+} - \frac{1}{2} f \sum_{pqr} \left(a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{r+} + \text{h.c.} \right)$$

Simple model, pairing only, five fermion case, see JPG **37**, 064035



Recipe for Vlowk

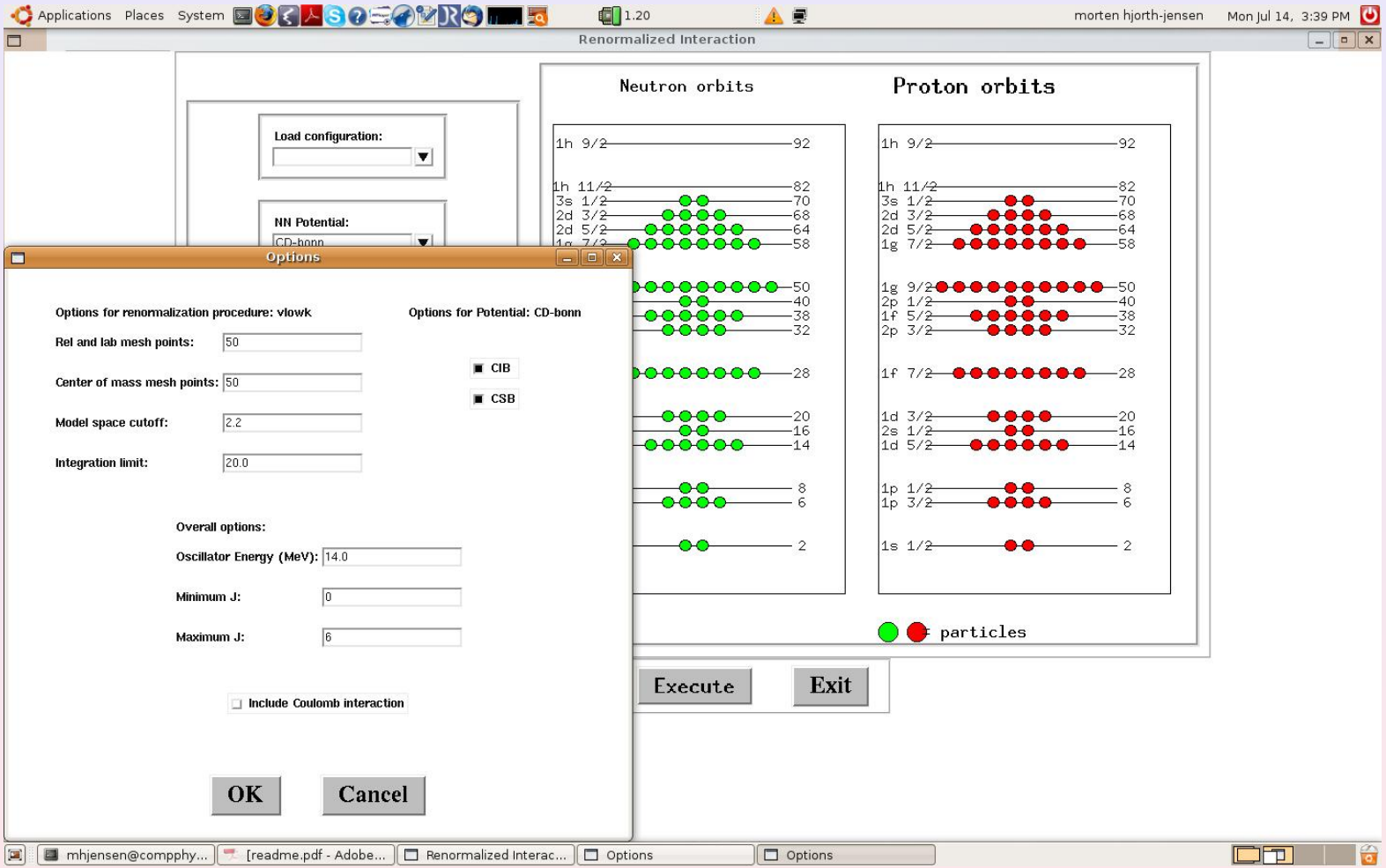
- Diagonalize the two-body Schrödinger equation in momentum space for all momenta
- Choose a cutoff which defines the model space in terms of relative momenta
- Use exact eigenvalues and momenta to perform a similarity transformation
- Obtain effective interaction in relative momenta
- Integrate to get 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
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
50
40
38
32
28
20
16
14
8
6
2
1g 9/2
2p 1/2
1f 5/2
2p 3/2
1f 7/2
1d 3/2
2s 1/2
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1p 1/2
1p 3/2
1s 1/2
particles
Execute
Exit
Options
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Options for Potential: CD-bonn
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Center of mass mesh points: 50
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Integration limit: 20.0
CIB
CSB
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Maximum J: 6
Include Coulomb interaction
OK
Cancel
mhjensen@compphy...
[readme.pdf - Adobe...
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Options
Options

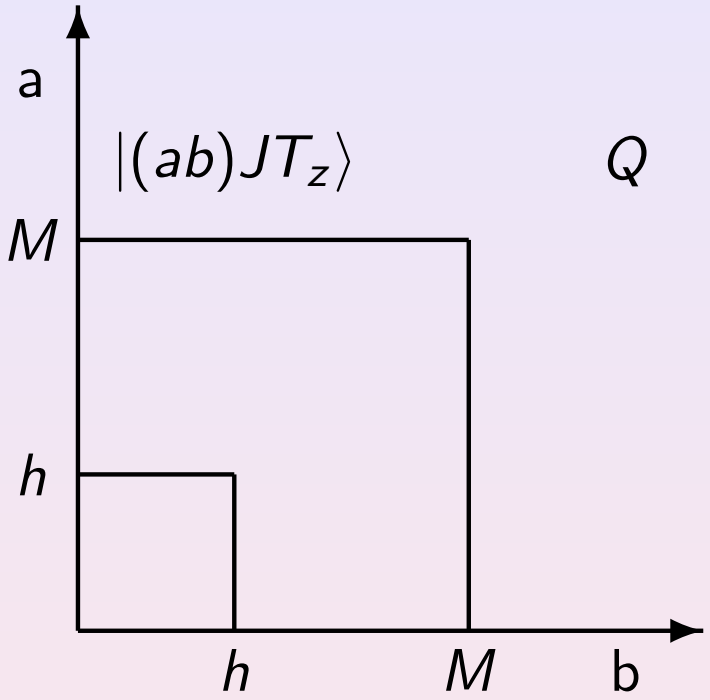
G-matrix: Resummation of a Class of Diagrams

- 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



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

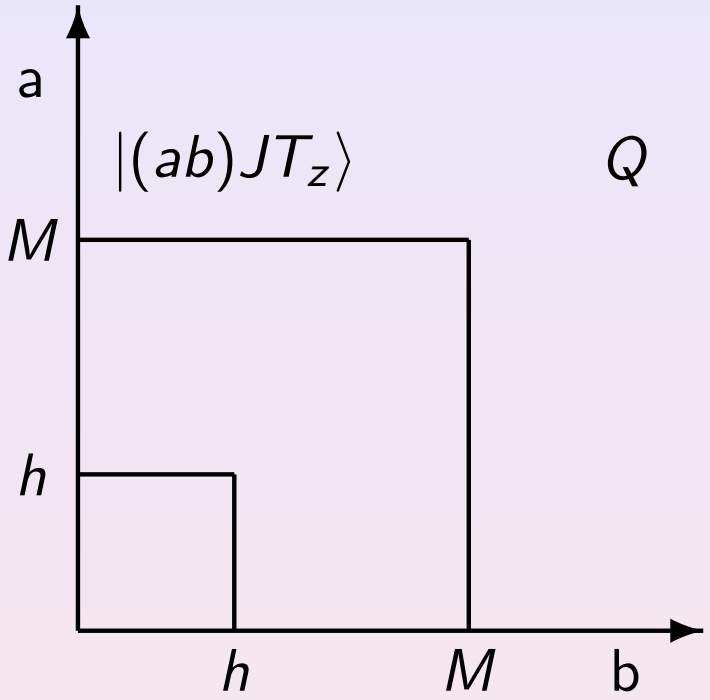
Two-Body Effective Hamiltonian for Large Space

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.

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

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

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

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

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

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

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

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

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

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.

Exercise Lecture 2: CENS tasks

1. Construct a renormalized nucleon-nucleon interaction using the Vlowk prescription with cutoff $\lambda = 2.1$ fm^{-1} and model space consisting of the first eight major shells.
2. Use an oscillator energy of $\hbar\omega = 8.8$ MeV suitable around ^{88}Sr. Use the N^{3}LO interaction with Coulomb and both charge and isospin breaking. Include partial waves up to $J \leq 6$

Exercise Lecture 2: Simple 2×2 system

Exercise: Find the similarity transformed expression for H'_{11} for a simple pairing 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!