

Lecture III: Many-Body Methods for Nuclear Structure

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Outline

- 1 Effective Interactions for the Shell Model
- 2 The Shell Model
- 3 Coupled Cluster equations

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Reminder from Lecture II: $V_{\text{low-k}}$

The A -body Hamiltonian H is defined as

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

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

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

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

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

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

Reminder from Lecture II: G -matrix

The A -body Hamiltonian H is defined as for the $V_{\text{low-}k}$ 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

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

The modified two-body interaction

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

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

Both the G -matrix codes and the $V_{\text{low-}k}$ codes list separately G or $V_{\text{low-}k}$ 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.

Reminder from Lecture II: No-core

The total Hamiltonian is

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

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 explicitly 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 is 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

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

Here H_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 $n_{a\dots d}$ number all bound, resonant and discretized scattering states with orbital and angular momenta $(l_{a\dots d}, j_{a\dots d})$. 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

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

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

$$H_I = \sum_{\alpha \leq \beta} \sum_{\gamma \leq \delta} |\alpha\beta\rangle \langle \alpha\beta| H_I |\gamma\delta\rangle \langle \gamma\delta|,$$

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

$$\langle \alpha\beta | H_I | \gamma\delta \rangle = \left\langle (n_\alpha l_\alpha j_\alpha t_{z_\alpha}) (n_\beta l_\beta j_\beta t_{z_\beta}) J T_z \left| H_I \right| (n_\gamma l_\gamma j_\gamma t_{z_\gamma}) (n_\delta l_\delta j_\delta t_{z_\delta}) J T_z \right\rangle,$$

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

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

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

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

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

$$\langle ab|\alpha\beta\rangle = \langle a|\alpha\rangle\langle b|\beta\rangle$$

for the proton-neutron case.

Exercises Lecture II

- (a) Set up the Hartree-Fock equations in a harmonic oscillator basis and sketch the algorithm for finding the overlaps $\langle a|\alpha\rangle$.
- (b) 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. See the comments to the input file on the next slide.

Simple Toy Model to illustrate Many-Body Perturbation Theory

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

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

A Rayleigh-Schrödinger expansion for the lowest eigenstate

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

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.

Simple Two-Level Model

We can sum diagrams to for example fifth order in the parameter z reads

$$\hat{Q}_5 = zX_P + \frac{z^2X^2}{\epsilon_P - \epsilon_Q} + \frac{z^3X^2X_Q}{(\epsilon_P - \epsilon_Q)^2} + \frac{z^4X^2X_Q^2}{(\epsilon_P - \epsilon_Q)^3} + \frac{z^5X^2X_Q^3}{(\epsilon_P - \epsilon_Q)^4},$$

and it is easy to see that an expansion to order $l + 2$ can be written as

$$\hat{Q}_{l+2} = zX_P + \frac{z^2X^2}{\epsilon_P - \epsilon_Q - zX_Q} \left\{ 1 - \left(\frac{zX_Q}{\epsilon_P - \epsilon_Q} \right)^{l+1} \right\},$$

which in the limit $l \rightarrow \infty$ gives

$$\hat{Q}_{\text{exact}}(\epsilon_P) = zX_P + \frac{z^2X^2}{\epsilon_P - \epsilon_Q - zX_Q},$$

with $|zX_Q/(\epsilon_P - \epsilon_Q)| < 1$.

Simple Two-Level Model

This sum may be used to define the first iteration of an expansion as a function of the starting energy used to generate the exact solution ω as

$$\lambda_1 = \omega + \hat{Q}_{\text{exact}}(\omega)$$

The subsequent steps are

$$\lambda_2 = \lambda_1 + \sum_{m=1}^{\infty} \frac{1}{m!} \frac{d^m \hat{Q}}{d\omega^m} (\lambda_1 - \omega)^m,$$

and

$$\lambda_3 = \lambda_1 + \sum_{m=1}^{\infty} \frac{1}{m!} \frac{d^m \hat{Q}}{d\omega^m} (\lambda_2 - \omega)^m.$$

Simple Two-Level Model

In general we have

$$\lambda_n = \lambda_1 + \sum_{m=1}^{\infty} \frac{1}{m!} \frac{d^m \hat{Q}}{d\omega^m} (\lambda_{n-1} - \omega)^m.$$

If this iteration scheme converges we have, with $\lambda = \lambda_n = \lambda_{n-1}$,

$$\lambda = \omega + zX_P + \frac{z^2 X^2}{\lambda - \epsilon_Q - zX_Q},$$

which is just the exact solution (check it!).

Equation for Effective Two-Body Interaction

The P -space effective hamiltonian can be written as

$$H_{\text{eff}} = PHP + PH\chi = PH_0P + V_{\text{eff}}(\chi),$$

with $V_{\text{eff}}(\chi) = PH_1P + PH_1Q\chi P$ and

$$\chi = \frac{1}{\omega - QHQ}QH_1P - \frac{1}{\omega - QHQ}\chi V_{\text{eff}}(\chi).$$

Introduce the so-called $\hat{Q}$ -box, defined as

$$\hat{Q}(\omega) = PH_1P + PH_1Q \frac{1}{\omega - QHQ}QH_1P.$$

The $\hat{Q}$ -box is made up of non-folded diagrams which are irreducible and valence linked. A diagram is said to be irreducible if between each pair of vertices there is at least one hole state or a particle state outside the model space. In a valence-linked diagram the interactions are linked (via fermion lines) to at least one valence line. Note that a valence-linked diagram can be either connected (consisting of a single piece) or disconnected.

Equation for Effective Two-Body Interaction

Multiplying both sides of the last equation with PH_1 and adding PH_1P to both sides we get

$$PH_1P + PH_1\chi = PH_1P + PH_1Q \frac{1}{\omega - QHQ} QH_1P - PH_1 \frac{1}{\omega - QHQ} \chi V_{\text{eff}}(\chi),$$

which gives

$$V_{\text{eff}}(\chi) = \hat{Q}(\omega) - PH_1 \frac{1}{\omega - QHQ} \chi V_{\text{eff}}(\chi).$$

There are several ways to solve the latter. The idea is to set up an iteration scheme where we determine χ_n and thus $V_{\text{eff}}(\chi_n)$ from χ_{n-1} and $V_{\text{eff}}(\chi_{n-1})$. For the mere sake of simplicity we write $V_{\text{eff}}^{(n)} = V_{\text{eff}}(\chi_n)$.

Folded Diagrams

$$V_{\text{eff}}^{(n)} = \hat{Q}(\omega) - PH_1 \frac{1}{\omega - QHQ} \chi_n V_{\text{eff}}^{(n-1)}.$$

The solution to this equation can be shown to be

$$V_{\text{eff}}^{(n)} = \hat{Q} + \sum_{m=1}^{\infty} \frac{1}{m!} \frac{d^m \hat{Q}}{d\omega^m} \left\{ V_{\text{eff}}^{(n-1)} \right\}^m.$$

Observe also that the effective interaction is $V_{\text{eff}}^{(n)}$ is evaluated at a given model space energy ω . If $V_{\text{eff}}^{(n)} = V_{\text{eff}}^{(n-1)}$, the iteration is said to converge. In the limiting case $n \rightarrow \infty$, the solution $V_{\text{eff}}^{(\infty)}$ agrees with the formal solution of Brandow and Des Cloizeaux

$$V_{\text{eff}}^{(\infty)} = \sum_{m=0}^{\infty} \frac{1}{m!} \frac{d^m \hat{Q}}{d\omega^m} \left\{ V_{\text{eff}}^{(\infty)} \right\}^m.$$

Lee-Suzuki Iteration Scheme

Another iterative solution has been presented by Lee and Suzuki (Prog Theor Phys **64**, 2091 1980). In their approach

$$V_{\text{eff}}^{(n)} = \left\{ 1 + PH_1 \frac{1}{\omega - QHQ} \chi_{n-1} \right\}^{-1} \hat{Q}(\omega),$$

for $n \geq 1$ and with the equation for χ_n given as

$$\chi_n = Q \frac{1}{\omega - QHQ} QH_1 P - Q \frac{1}{\omega - QHQ} \chi_{n-1} V_{\text{eff}}^{(n)}.$$

Lee-Suzuki Iteration Scheme

Since the wave operator Ω is given as $\Omega = P + \chi$, a natural zeroth approximation to χ_0 would be to set $\chi_0 = 0$, resulting in

$$\chi_1 = \frac{1}{\omega - QHQ} QH_1P,$$

and

$$V_{\text{eff}}^{(1)} = \hat{Q}(\omega),$$

The next iterative step yields

$$\chi_2 = Q \frac{1}{\omega - QHQ} QH_1P - Q \frac{1}{\omega - QHQ} \chi_1 V_{\text{eff}}^{(2)},$$

and

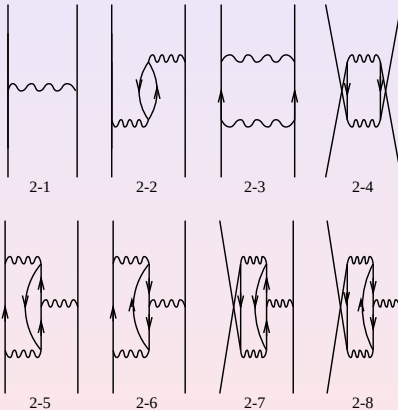
$$V_{\text{eff}}^{(2)} = \left\{ 1 + PH_1 \frac{1}{\omega - QHQ} \chi_1 \right\}^{-1} \hat{Q}(\omega) = \frac{1}{1 - \hat{Q}_1} \hat{Q}(\omega).$$

The solution is

$$V_{\text{eff}}^{(n)} = \left[1 - \hat{Q}_1 - \sum_{m=2}^{n-1} \hat{Q}_m \prod_{k=n-m+1}^{n-1} V_{\text{eff}}^{(k)} \right]^{-1} \hat{Q}.$$

Perturbation Theory

Order by order perturbation theory in terms of G .



Resumming Diagrams

Define the following

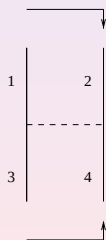
$$V_{1234J}^{[12]} = \langle (12)J | V | (34)J \rangle$$

$$V_{1234J}^{[13]} = \sum_{J'} (-)^{j_1+j_4+J+J'} \hat{j}'^2 \left\{ \begin{matrix} j_3 & j_1 & J \\ j_2 & j_4 & J' \end{matrix} \right\} V_{1234J}^{[12]}$$

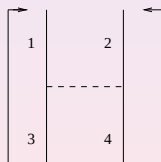
$$V_{1234J}^{[14]} = \sum_{J'} (-)^{j_1+j_4+J+2j_3} \hat{j}'^2 \left\{ \begin{matrix} j_4 & j_1 & J \\ j_2 & j_3 & J' \end{matrix} \right\} V_{1234J}^{[12]}$$

$$V_{1234J}^{[14]} = \sum_{J'} (-)^{2j_1+2j_2+2j_3} \hat{j}'^2 \left\{ \begin{matrix} j_4 & j_1 & J \\ j_3 & j_2 & J' \end{matrix} \right\} V_{1234J}^{[13]}$$

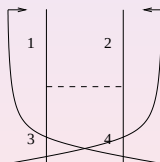
Coupling Order by Pictures



(a)



(b)



(c)

Particle-Particle and Hole-Hole Correlations

Summation of diagrams in the $[12]$ channel

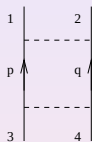
$$\Gamma_{1234J}^{[12]} = \Gamma_{2143J}^{[12]} = -\Gamma_{2134J}^{[12]} = \Gamma_{1243J}^{[12]}$$

$$s = \varepsilon_1 + \varepsilon_2 = \varepsilon_3 + \varepsilon_4$$

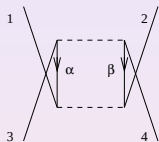
$$\Gamma^{[12]} = V^{[12]} + V^{[12]}(gg)\Gamma^{[12]}$$

$$\hat{\mathcal{G}}^{[12]} = \frac{Q_{pp}^{[12]}}{s - \varepsilon_5 - \varepsilon_6 + \eta} - \frac{Q_{hh}^{[12]}}{s - \varepsilon_5 - \varepsilon_6 - \eta}$$

Examples



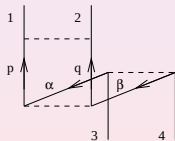
(a)



(b)



(c)



(d)



(e)



(f)

Examples: Analytic Expression

$$(a) = \frac{1}{2} \sum_{pq} V_{12pqJ}^{[12]} \frac{1}{s - \varepsilon_p - \varepsilon_q} V_{pq34J}^{[12]}$$

$$(b) = \frac{1}{2} \sum_{\alpha\beta} V_{12\alpha\beta J}^{[12]} \frac{1}{-s + \varepsilon_\alpha + \varepsilon_\beta} V_{\alpha\beta34J}^{[12]}$$

$$(c) = \frac{1}{4} \sum_{pqrw} V_{12pqJ}^{[12]} \frac{1}{s - \varepsilon_p - \varepsilon_q} V_{pqrwJ}^{[12]} \frac{1}{s - \varepsilon_r - \varepsilon_w} V_{rw34J}^{[12]}$$

Particle-Hole Diagrams

Screening corrections and vertex renormalization, the equations for the [13] and [14] channels

$$\Gamma_{1234J}^{[13]}(t) = V_{1234J}^{[13]} + \sum_{ph} V_{12phJ}^{[13]} \hat{G}^{[13]} \Gamma_{ph34J}^{[13]}(t)$$

$$\Gamma_{1234J}^{[14]}(u) = V_{1234J}^{[14]} - \sum_{ph} V_{12phJ}^{[14]} \hat{G}^{[14]} \Gamma_{ph34J}^{[14]}(u)$$

Particle-Hole Diagrams

Screening corrections and vertex renormalization, the equations for the [13] and [14] channels

$$\Gamma^{[13]} = V^{[13]} + V^{[13]}(gg)\Gamma^{[13]}$$

$$\Gamma^{[14]} = V^{[14]} + V^{[14]}(gg)\Gamma^{[14]}$$

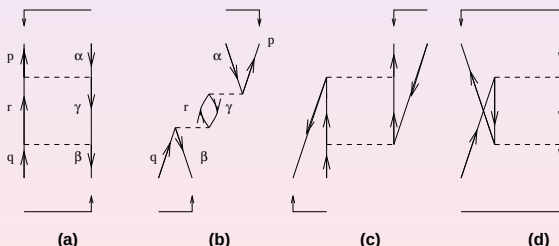
$$t = \varepsilon_3 - \varepsilon_1 = \varepsilon_2 - \varepsilon_4$$

$$u = \varepsilon_1 - \varepsilon_4 = \varepsilon_3 - \varepsilon_2$$

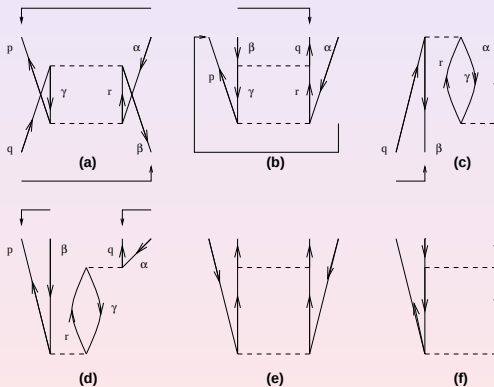
$$\hat{\mathcal{G}}^{[13]} = \frac{Q_{\text{ph}}^{[13]}}{t - \varepsilon_p + \varepsilon_h + \imath\eta} - \frac{Q_{\text{hp}}^{[13]}}{t + \varepsilon_p - \varepsilon_h - \imath\eta}$$

$$\hat{\mathcal{G}}^{[14]} = \frac{Q_{\text{ph}}^{[14]}}{u - \varepsilon_p + \varepsilon_h + \imath\eta} - \frac{Q_{\text{hp}}^{[14]}}{u + \varepsilon_p - \varepsilon_h - \imath\eta}$$

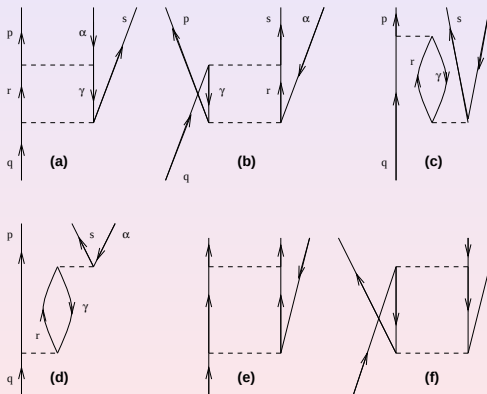
Particle-Hole Examples



Particle-Hole Examples



Particle-Hole Examples



Effective Operators

In Rayleigh-Schrödinger perturbation theory, the effective interaction H_{eff} can be written out order by order in the interaction H_1 as

$$PH_{\text{eff}}P = PH_1P + PH_1\frac{Q}{e}H_1P + PH_1\frac{Q}{e}H_1\frac{Q}{e}H_1P + \dots$$

Here we have defined $e = \omega - H_0$, where ω is the so-called starting energy, defined as the unperturbed energy of the interacting particles. Similarly, the exact wave function $|\Psi_\alpha\rangle$ can now be written in terms of the model space wave function as

$$|\Psi_\alpha\rangle = |\Phi_\alpha\rangle + \frac{Q}{e}H_1|\Phi_\alpha\rangle + \frac{Q}{e}H_1\frac{Q}{e}H_1|\Phi_\alpha\rangle + \dots$$

Effective Operators

In studies of for example nuclear transitions such as beta decay, the quantity of interest is the transition matrix element between an initial state $|\Psi_i\rangle$ and a final state $|\Psi_f\rangle$ of an operator $\mathcal{O}$ defined as

$$\mathcal{O}_{fi} = \frac{\langle \Psi_f | \mathcal{O} | \Psi_i \rangle}{\sqrt{\langle \Psi_f | \Psi_f \rangle \langle \Psi_i | \Psi_i \rangle}}.$$

Since we perform our calculation in a reduced space, the exact wave functions $|\Psi_{f,i}\rangle$ are not known, only their projections onto the model space. We are then confronted with the problem of how to evaluate $\mathcal{O}_{fi}$ when only the model space wave functions are known. In treating this problem, it is usual to introduce an effective operator $\mathcal{O}_{fi}^{\text{eff}}$, defined by requiring

$$\mathcal{O}_{fi} = \langle \Phi_f | \mathcal{O}_{\text{eff}} | \Phi_i \rangle.$$

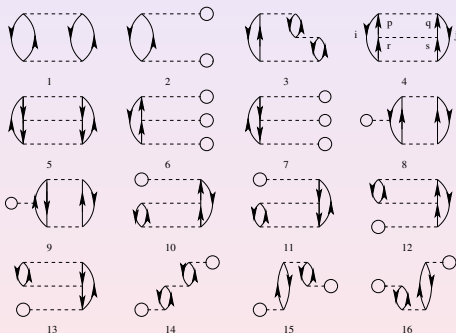
Effective Operators

Observe that $\mathcal{O}_{\text{eff}}$ is different from the original operator $\mathcal{O}_{fi}$. The standard empirical procedure is then to introduce some adjustable parameters in $\mathcal{O}_{fi}^{\text{eff}}$.

The perturbative expansion for the effective operator can then be written as

$$\begin{aligned} \langle \Psi_f | \mathcal{O} | \Psi_i \rangle &= \langle \Phi_f | \mathcal{O} | \Phi_i \rangle + \langle \Phi_f | \mathcal{O} \frac{Q}{e} H_1 | \Phi_i \rangle + \\ &\langle \Phi_f | \frac{Q}{e} H_1 \mathcal{O} | \Phi_i \rangle + \langle \Phi_f | \mathcal{O} \frac{Q}{e} H_1 \frac{Q}{e} H_1 | \Phi_i \rangle + \dots \end{aligned}$$

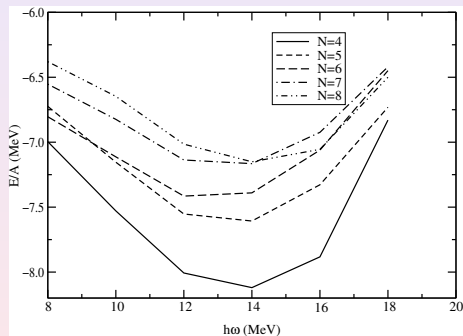
Many-body Perturbation theory, closed-shell systems



Ingredients

- G -matrix computed for various numbers of harmonic oscillator shells
- Function of oscillator energy $\hbar\omega$
- Idaho-A potential and no Coulomb but CoM correction to G -matrix

Closed Shells: Perturbation theory to third-order



To notice

- As the number of shells is increased results stabilize
- Independence of oscillator parameter as number of shells increases
- Need 7 – 8 major shells to get a seemingly converged result

Many-Body Perturbation Theory

Main problems

- 1 Hard to extend beyond third-order. No systematic way of expanding.
- 2 No clear signs of convergence in terms of the interaction. Not even in atomic or molecular physics.
- 3 Difficult to improve upon systematically, e.g., by inclusion of three-body interactions and more complicated correlations.
- 4 However, enjoys considerable success in producing effective interactions for finite nuclei and the shell model. Good agreement with data.
- 5 Need non-perturbative resummation techniques for large classes of diagrams. Coupled cluster is one possibility for $A \leq 100$ at present. No-core for $A \leq 16$. Can also study Green's function methods (Parquet class of diagrams).

Input File bhf.ini for Effective interaction code

```
# Determine what kind of effective interaction you want and the
# of calculation.  If you type shell-model, the code will produ
# an effective interaction taylored to the Oslo shell-model cod
# separated in three files, one for the pp case, one for pn and
# For coupled-cluster calculations you will produce a file con
# the effective interaction, one containing the kinetic energy
# for the total single-particle energies.
# You can also compute the binding energy of various closed cor
# The options are thus 1) open-diagrams for shell-model, 2) co
# and 3) core-diagrams
type_of_interaction = open-diagrams
```

Input File bhf.ini for Effective interaction code

```
# You can also compute results to a given order in
# many-body perturbation
# theory, in this case to third order. Options are 1) first,
# 2) second and
# 3) third. For coupled-cluster you have to stay with first
order_of_interaction = first

# Determine whether you want to do Hartree-Fock or not.
# Options are 1) hf_itations =0 or
# 2) hf_itations = 1 or any
# number larger than 0
hf_itations = 1
```

Input File bhf.ini for Effective interaction code

```
# output_run is prefixed to output file for optional
# printouts, tests etc.
output_run = run1_29march.dat

# input file for the renormalized NN interaction
renorminteraction_file = gint31n3lo_15hbar.dat

# input file for the set of single-particle orbits,
# this file can be
# further manipulated by the effective interaction part
spdata_file = spdata31n3lo_15hbar.dat
```

Input File bhf.ini for Effective interaction code

```
# The new single-particle in case you do a HF calculation
HFspdata_file = HFspdat52n3lo_10hbar.dat

# if you do Hartree-Fock, the new interaction is given
# by this file
HFrenorminteraction_file = HFint52n3lo_10hbar.dat

# If you wan to compute an effective interaction for the
# Oslo shell-model codes,
# you need to define the names of three files, one for the
# proton-proton case
# one for the proton-neutron case and finally one for the
# neutron-neutron case
veff_pp = sdshell_pp.dat
veff_pn = sdshell_pn.dat
veff_nn = sdshell_nn.dat
```

Input File bhf.ini for Effective interaction code

```
# If you do want to compute an effective interaction for
# coupled-cluster calculations
# you need to specify three files, one for the interaction itself
# one for the kinetic energies of all sp orbits
# and one for sp data declarations.
# These files are in turn used as input to coupled-cluster calculations
CCkinetic_file =   kinint31n3lo_15hbar.dat
CCinteraction_file = ccint31n3lo_15hbar.dat
CCspdata_file = spint31n3lo_15hbar.dat
```

Input File bhf.ini for Effective interaction code

```
# You can compute the various diagrams for a given starting ene
# then sum folded diagrams to infinite order. Typical starting
# for calculation should correspond to roughly the two-body ener
# the valence nucleons. It should be negative since you are deal
# bound systems.
# If you choose just one starting energy, then no folded diagra
# are summed up.
n_startenergy_veff = 11
starting_energy = -20.0
```

Reminder of what we typically want to do

Find the lowest (≈ 10 – 50) solution of the eigenvalue problem

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

and compute other properties with obtained wave functions. Use a valence shell effective Hamiltonian H_{eff} defined within a valence P-space with a pertaining excluded Q-space:

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

The model space Hamiltonian reads

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

Shell-Model Basics

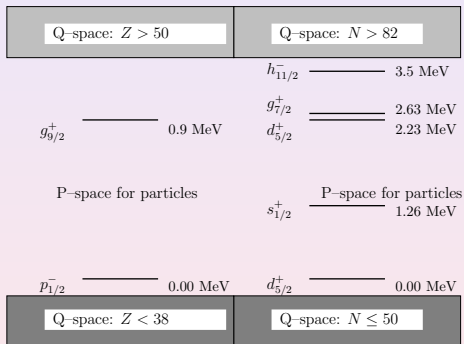
- The choice of basis and the calculation of the matrix elements.

$$\langle \Phi_\lambda | PH_{eff}P | \Phi_{\lambda'} \rangle = E_\lambda^0 \delta_{\lambda,\lambda'} + \langle \Phi_\lambda | P(H_1)_{eff}P | \Phi_{\lambda'} \rangle$$

Here we need to have defined the model space and its effective interaction.

- The treatment of giant matrices – diagonalization (Lanczos).
Based on the single-particle degrees of freedom which define a model space, we can in turn set up an A -body Slater determinant and try to diagonalize.

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



Dimensionalities

Solution of the Schrödinger eq. for N nucleons in a valence P-space $\implies$ 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
${}^4\text{He}$	4E4	9E6
${}^8\text{B}$	4E8	5E13
${}^{12}\text{C}$	6E11	4E19
${}^{16}\text{O}$	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 the Shell Model

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

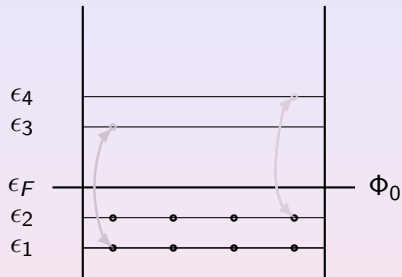
$$\Phi_0 = \frac{1}{\sqrt{4!}} \begin{pmatrix} \phi_1(\mathbf{x}_1) & \phi_1(\mathbf{x}_2) & \phi_1(\mathbf{x}_3) & \phi_1(\mathbf{x}_4) \\ \phi_2(\mathbf{x}_1) & \phi_2(\mathbf{x}_2) & \phi_2(\mathbf{x}_3) & \phi_2(\mathbf{x}_4) \\ \phi_3(\mathbf{x}_1) & \phi_3(\mathbf{x}_2) & \phi_3(\mathbf{x}_3) & \phi_3(\mathbf{x}_4) \\ \phi_4(\mathbf{x}_1) & \phi_4(\mathbf{x}_2) & \phi_4(\mathbf{x}_3) & \phi_4(\mathbf{x}_4) \end{pmatrix}$$

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

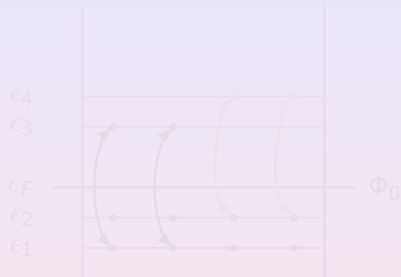
$$\Psi_{2p-2h} = (1 + T_1 + T_2)\Phi_0$$

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

Excitations in Pictures

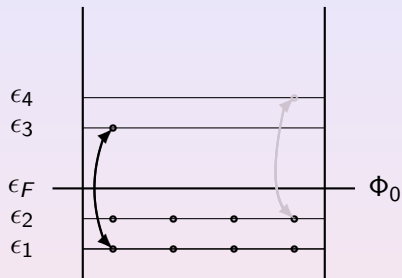


From T_1 to T_1^2
 $T_1 \propto a_a^\dagger a_i$



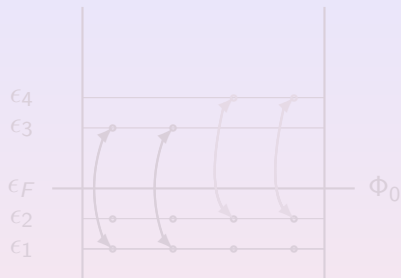
From T_2 to T_2^2
 $T_2 \propto a_a^\dagger a_b^\dagger a_j a_i$

Excitations in Pictures



From T_1 to T_1^2

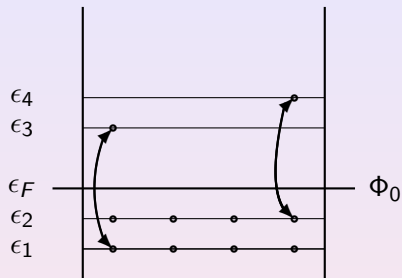
$$T_1 \propto a_a^\dagger a_i$$



From T_2 to T_2^2

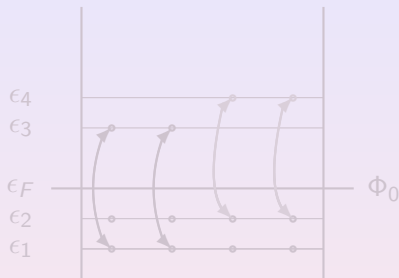
$$T_2 \propto a_a^\dagger a_b^\dagger a_j a_i$$

Excitations in Pictures



From T_1 to T_1^2

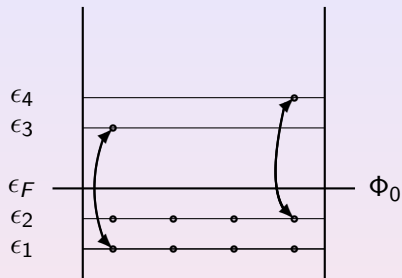
$$T_1 \propto a_a^\dagger a_i$$



From T_2 to T_2^2

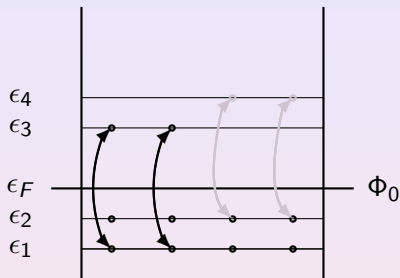
$$T_2 \propto a_a^\dagger a_b^\dagger a_j a_i$$

Excitations in Pictures



From T_1 to T_1^2

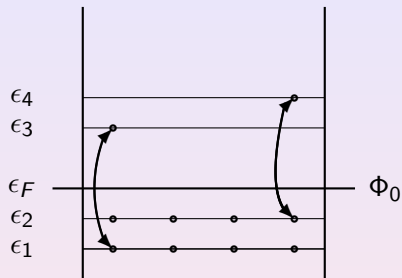
$$T_1 \propto a_a^+ a_i$$



From T_2 to T_2^2

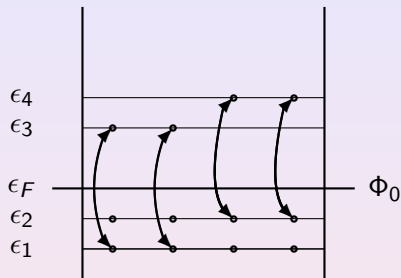
$$T_2 \propto a_a^+ a_b^+ a_j a_i$$

Excitations in Pictures



From T_1 to T_1^2

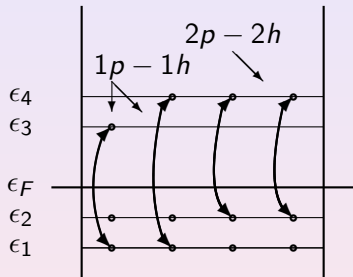
$$T_1 \propto a_a^+ a_i$$



From T_2 to T_2^2

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

Shell-Model Excitations



Shell-Model Truncations

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

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

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

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

Energy diagonalization of giant matrices: Lanczos iteration

Basic operator

$$\begin{aligned}
 H &= \text{one-particle} + \text{two-particle} = H_0 + V \\
 &= \tilde{V}(N) \\
 &= \sum \langle j_1 m_1 j_2 m_2 | \tilde{V}(N) | j_3 m_3 j_4 m_4 \rangle a_{j_1 m_1}^\dagger a_{j_2 m_2}^\dagger a_{j_4 m_4} a_{j_3 m_3}
 \end{aligned}$$

Example of effective m-scheme two-particle matrix elements outside the

$Z = 50$ $N = 50$ core

Type	Spherical	m-scheme
pp or nn	160	5274
pn	542	30105

Shell Model and m -Scheme

In a second quantization representation a Slater determinant (SD) is given by

$$|SD_{\nu}(N)\rangle = \prod_{(jm) \in \nu} a_{jm}^{\dagger} |0\rangle ,$$

and the complete set is generated by distributing the N particles in all possible ways throughout the basic one-particle states constituting the P-space. This is a very efficient representation. A single $|SD\rangle$ requires only one computer word (32 or 64 bits) and in memory a $|SD\rangle$ with N particles is given by

$$|SD\rangle \longrightarrow (\underbrace{00111101010\dots}_{N1's}),$$

where each 0 and 1 corresponds to an m -orbit in the valence P-space. Occupied orbits have a 1 and empty orbits a 0.

Shell Model and *m*-Scheme

Furthermore, all important calculations can be handled in Boolean algebra which is very efficient on modern computers. The action of operators of the form $a_{\alpha}^{\dagger} a_{\beta}$ or $a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta}$ acting on an $|SD\rangle$ is easy to perform.

The *m*-scheme allows also for a straightforward definition of many-body operators such as one-, two- and three-particle operators

$$a_{\alpha}^{\dagger} a_{\beta},$$

$$a_{\alpha_1}^{\dagger} a_{\alpha_2}^{\dagger} a_{\beta_1} a_{\beta_2},$$

$$a_{\alpha_1}^{\dagger} a_{\alpha_2}^{\dagger} a_{\alpha_3}^{\dagger} a_{\beta_1} a_{\beta_2} a_{\beta_3},$$

respectively, or generalized seniority operators. The seniority operators can be very useful in preparing a starting vector for the Lanczos iteration process. This option is not included in the program package.

Shell Model and m -Scheme

The generalized seniority operators can then be written as

$$S^\dagger = \sum_j \frac{1}{\sqrt{2j+1}} C_j \sum_{m \geq 0} (-1)^{j-m} a_{jm}^\dagger a_{j-m}^\dagger$$

for seniority zero,

$$D_{JM}^\dagger = \sum_{j \leq j', m, m'} (1 + \delta_{j,j'})^{-1/2} \beta_{j,j'} \langle j m j' m' | J M \rangle a_{jm}^\dagger a_{j'm'}^\dagger$$

for seniority two. The coefficients C_j and $\beta_{jj'}$ can be obtained from the a chosen two-particle system such as the ^{130}Sn ground state and the excited states, respectively.

Shell Model and m -Scheme

We can also define a seniority four operator

$$\begin{aligned} G(n_1, j_1, n_2, j_2; J, M) &= \left\{ D_{n_1, j_1}^\dagger D_{n_2, j_2}^\dagger \right\}_{J, M=0} \\ &= \sum_{\nu_1 \dots \nu_4} g_{\nu_1 \dots \nu_4}^{JM} a_{\nu_1}^\dagger a_{\nu_2}^\dagger a_{\nu_3}^\dagger a_{\nu_4}^\dagger \end{aligned}$$

and a seniority six operator

$$\begin{aligned} I(n_1, j_1, (n_2, j_2, n_3, j_3) j_{23}; J, M) &= \left\{ D_{n_1, j_1} G(n_2, j_2, n_3, j_3; j_{23}) \right\}_{J, M=0} \\ &= \sum_{\nu_1 \dots \nu_6} g_{\nu_1 \dots \nu_6}^{JM} a_{\nu_1}^\dagger a_{\nu_2}^\dagger a_{\nu_3}^\dagger a_{\nu_4}^\dagger a_{\nu_5}^\dagger a_{\nu_6}^\dagger \end{aligned}$$

Finally, our shell-model code allows also for the inclusion of effective and real three-body interactions. This version is not included in the program package.

Lanczos Iteration

Outline of the algorithm:

- We choose an initial Lanczos vector $|lanc_0\rangle$ as the zeroth order approximation to the lowest eigenvector. Our experience is that any reasonable choice is acceptable as long as the vector does not have special properties such as good angular momentum. That would usually terminate the iteration process at too early a stage.
- The next step involves generating a new vector through the process $|new_{p+1}\rangle = H|lanc_p\rangle$. Throughout this process we construct the energy matrix elements of H in this Lanczos basis. First, the diagonal matrix elements of H are then obtained by

$$\langle lanc_p | H | lanc_p \rangle = \langle lanc_p | new_{p+1} \rangle ,$$

Lanczos Iteration

- The new vector $|new_{p+1}\rangle$ is then orthogonalized to all previously calculated Lanczos vectors

$$|new'_{p+1}\rangle = |new_{p+1}\rangle - |lanc_p\rangle \cdot \langle lanc_p | new_{p+1}\rangle - \sum_{q=0}^{p-1} |lanc_q\rangle \cdot \langle lanc_q | new_{p+1}\rangle,$$

and finally normalized

$$|lanc_{p+1}\rangle = \frac{1}{\sqrt{\langle new'_{p+1} | new'_{p+1}\rangle}} |new'_{p+1}\rangle,$$

to produce a new Lanczos vector.

Lanczos Iteration

- The off-diagonal matrix elements of H are calculated by

$$\langle \text{lanc}_{p+1} | H | \text{lanc}_p \rangle = \langle \text{new}'_{p+1} | \text{new}'_{p+1} \rangle,$$

and all others are zero.

- After n iterations we have an energy matrix of the form

$$\begin{pmatrix} H_{0,0} & H_{0,1} & 0 & \cdots & 0 \\ H_{0,1} & H_{1,1} & H_{1,2} & \cdots & 0 \\ 0 & H_{2,1} & H_{2,2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & H_{p-1,p} \\ 0 & 0 & 0 & H_{p,p-1} & H_{p,p} \end{pmatrix}$$

as the p 'th approximation to the eigenvalue problem.

Lanczos Iteration

The number p is a reasonably small number and we can diagonalize the matrix by standard methods to obtain eigenvalues and eigenvectors which are linear combinations of the Lanczos vectors.

- This process is repeated until a suitable convergence criterium has been reached.

In this method each Lanczos vector is a linear combination of the basic $|SD\rangle$ with dimension n . For $n \approx 10^6 - 10^9$, as in our case of interest. Here is one of the important difficulties associated with the Lanczos method. Large disk storage is needed when the number of Lanczos vector exceeds ≈ 100 . Another difficulty is found in the calculation of $|new_{p+1}\rangle = H|lanc_p\rangle$ when $n > 10^6$.

Problems – Lanczos iteration

- The main cpu time-consuming process

$$H |q_i\rangle = |p\rangle$$

due to the large number of non-diagonal matrix elements

$$H |q_i\rangle = \sum_{\nu, \mu} C_{\nu}^i \langle SD_{\mu} | H | SD_{\nu} \rangle$$

However, each individual matrix element is easy to calculate

- Examples:**

Type	^{122}Sn	^{116}Sn
Dimension	$\approx 2 \cdot 10^6$	$\approx 16 \cdot 10^6$
non-diag. elem	$\approx 4.3 \cdot 10^8$	$\approx 1.2 \cdot 10^9$

Problems – Lanczos iteration

- The matrix elements are needed at every Lanczos iterations Too many non-diagonal two-particle matrix elements to be calculated and saved. Must be recalculated at each iteration
- Numerical roundoff errors requires orthogonalization of all Lanczos vectors. All Lanczos vectors may be kept during the process Slow convergence requires large number of Lanczos vectors (≥ 100)
- Due to numerical roundoff errors symmetry properties like angular momentum J are destroyed through the process. However, The final converged eigenvectors have the symmetry properties given by the total Hamiltonian H .

Selected Results

^{130}Sn				^{128}Sn			
J^π	Exp.	J^π	Theory	J^π	Exp.	J^π	Theory
(2^+)	1.22	2^+	1.46	(2^+)	1.17	2^+	1.28
(4^+)	2.00	4^+	2.39	(4^+)	2.00	4^+	2.18
(6^+)	2.26	6^+	2.64	(6^+)	2.38	6^+	2.53
^{126}Sn				^{124}Sn			
J^π	Exp.	J^π	Theory	J^π	Exp.	J^π	Theory
2^+	1.14	2^+	1.21	2^+	1.13	2^+	1.17
4^+	2.05	4^+	2.21	4^+	2.10	4^+	2.26
		6^+	2.61			6^+	2.70
^{122}Sn				^{120}Sn			
J^π	Exp.	J^π	Theory	J^π	Exp.	J^π	Theory
2^+	1.14	2^+	1.15	2^+	1.17	2^+	1.14
4^+	2.14	4^+	2.30	4^+	2.19	4^+	2.30
6^+	2.56	6^+	2.78			6^+	2.86
^{118}Sn				^{116}Sn			
J^π	Exp.	J^π	Theory	J^π	Exp.	J^π	Theory
2^+	1.22	2^+	1.15	2^+	1.30	2^+	1.17

Seniority Analysis

Seniority $\nu = 0$ overlap $|\langle {}^A\text{Sn}; 0^+ | (S^\dagger)^{\frac{n}{2}} | \tilde{0} \rangle|^2$ and the seniority $\nu = 2$ overlaps $|\langle {}^A\text{Sn}; J_f | D_{JM}^\dagger (S^\dagger)^{\frac{n}{2}-1} | \tilde{0} \rangle|^2$ for the lowest-lying eigenstates of ${}^{128-120}\text{Sn}$.

	A=128	A=126	A=124	A=122	A=120
0_1^+	0.96	0.92	0.87	0.83	0.79
2_1^+	0.92	0.89	0.84	0.79	0.74
4_1^+	0.73	0.66	0.44	0.13	0.00
4_2^+	0.13	0.18	0.39	0.66	0.74
6_1^+	0.81	0.85	0.83	0.79	0.64

Partial Waves and Spectra

$2_1^+ - 0_1^+$ excitation energy for the even tin isotopes $^{130-116}\text{Sn}$ for various approaches to the effective interaction.

	^{116}Sn	^{118}Sn	^{120}Sn	^{122}Sn	^{124}Sn	^{126}Sn	^{128}Sn	^{130}Sn
Expt	1.29	1.23	1.17	1.14	1.13	1.14	1.17	1.23
V_{eff}	1.17	1.15	1.14	1.15	1.14	1.21	1.28	1.46
G-matrix	1.14	1.12	1.07	0.99	0.99	0.98	0.98	0.97
$^1S_0$ G-matrix	1.38	1.36	1.34	1.30	1.25	1.21	1.19	1.18
No $^1S_0$ & $^3P_2$ in G					0.15	-0.32	0.02	-0.21

Shell-Model Studies of Nuclei around $A = 132$

Third-order effective interaction with G -matrix for ^{132}Sn and effective interaction consisting of a model space with

- ① $(0g_{7/2}, 1d_{5/2}, 1d_{3/2}, 2s_{1/2}, 0h_{11/2})^{Z-50}$ for proton particles
- ② $(0g_{7/2}, 1d_{5/2}, 1d_{3/2}, 2s_{1/2}, 0h_{11/2})^{N-82}$ for neutron holes.
- ③ The wave functions for $N \geq 82$ were obtained with the same model space for protons as above and with a model space for neutrons of $(0h_{9/2}, 1f_{7/2}, 1f_{5/2}, 2p_{3/2}, 2p_{1/2}, 0i_{13/2})^{N-82}$

Spectra

Results: ^{132}Te

J^π	Experiment	CD-Bonn
0_1^+	0.0	0.0
2_1^+	0.97	0.95
$(2)_2^+$	1.66	1.64
4_1^+	1.67	1.54
6_1^+	1.77	1.68
0_2^+		1.70
$(2)_3^+$	1.79	1.93
$(7)_1^-$	1.92	1.88
$(5)_1^-$	2.05	2.01
4_1^-		2.12

Results: ^{134}Te

J^π	Experiment	CD-Bonn
0_1^+	0.0	0.0
2_1^+	1.28	1.21
4_1^+	1.57	1.48
6_1^+	1.69	1.61
6_2^+	2.40	2.17
2_2^+	2.46	2.45
4_2^+	2.55	2.45
1_1^+	2.63	2.41
3_1^+	2.68	2.54
5_1^+	2.73	2.54

Results: Magnetic Moments

Nuclide	J^π	Experiment	Effective	Free	proton	neutron
^{134}Sn	2^+		-0.469	-0.745	0	-0.469
^{130}Sn	2^+		-0.275	-0.385	0	-0.275
^{128}Sn	2^+		-0.253	-0.343	0	-0.253
^{126}Sn	2^+		-0.262	-0.355	0	-0.262
^{124}Sn	2^+	-0.3(2)	-0.270	-0.364	0	-0.270
^{136}Te	2^+		0.695	0.544	0.846	-0.151
^{134}Te	2^+		1.724	1.035	1.724	0
^{132}Te	2^+	0.70(10)	0.975	0.575	1.027	-0.052
^{130}Te	2^+	0.59(7)	0.693	0.360	0.806	-0.113
^{134}Xe	2^+	0.708(14)	0.825	0.541	0.886	-0.061
^{136}Xe	2^+	1.53(9)	1.823	1.165	1.823	0
^{138}Xe	2^+		0.775	0.623	0.912	-0.137
^{138}Ba	2^+	1.44(22)	2.00	1.52	2.00	0

Exercises Lecture III

- (a) Compute an effective interaction based on the N3LO interaction using the Vlowk method for six major shells. Use then this interaction to compute an effective interaction for the *sd*-shell using second-order perturbation theory.
- (b) Compute thereafter the low-lying spectrum of ^{20}Ne .
- (c) Compute the $B(E2)$ transition from the first 2_1^+ state to the ground state 0_1^+ . You need to load down the last codes, the effective interaction part and the shell-model part. Note that we have separated the shell-model codes in two different codes, one which runs for identical particles only and one for the pn case only.

Why Coupled-Cluster theory?

Advantages

- Fully microscopic. Only linked diagrams enter, size extensive
- Can be improved upon systematically, e.g., by inclusion of three-body interactions and more complicated correlations. To be contrasted to many-body perturbation theory.
- Allows for description of both closed-shell systems and valence systems
- Derivation of effective two and three-body interactions for the shell model
- Amenable to parallel computing
- Huge development in Quantum Chemistry. Exploit this for the nuclear many-body problem.

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- Fully microscopic. Only linked diagrams enter, size extensive
- Can be improved upon systematically, e.g., by inclusion of three-body interactions and more complicated correlations. To be contrasted to many-body perturbation theory.
- Allows for description of both closed-shell systems and valence systems
- Derivation of effective two and three-body interactions for the shell model
- Amenable to parallel computing
- Huge development in Quantum Chemistry. Exploit this for the nuclear many-body problem.

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More on Coupled Cluster

More advantages

- Can be used to generate excited spectra for nuclei like ^{16}O or ^{40}Ca with many shells. Hard for the shell model to go beyond one major shell. Huge dimensionalities in shell-model calcs

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

Shell-model codes can today reach dimensionalities of $d \sim 10^{10}$ basis states.

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Coupled Cluster, Basics

The single-reference coupled-cluster theory is based on the exponential ansatz for the ground-state wave function of the A -body system,

$$|\Psi_0^{(A)}\rangle = e^{T^{(A)}}|\Phi\rangle, \quad (1)$$

where $T^{(A)}$ is the cluster operator (a p - h excitation operator) and $|\Phi\rangle$ is the corresponding reference determinant (defining the Fermi vacuum) obtained by performing some mean-field calculation or by simply filling A lowest-energy single-particle states. Superscripts, such as (A) , indicate the number of particles in a system under consideration, at the relevant operators and energies.

Formally, this equation is a direct consequence of the connected-cluster theorem, first clearly stated by Hubbard, which is, in turn, related to the linked cluster theorem of many-body perturbation theory. According to the connected-cluster theorem, the cluster operator $T^{(A)}$ generates connected wave function diagrams summed through infinite order. Operationally, $T^{(A)}$ is a simple many-body excitation operator, which in all standard coupled-cluster approximations is truncated at a given (usually low) p - h excitation level $M < A$.

Coupled Cluster, Basics

The general form of the truncated cluster operator, defining a standard single-reference coupled-cluster approximation characterized by the excitation level M , is

$$T^{(A)}(M) = \sum_{n=1}^M T_n, \quad (2)$$

where

$$T_n = \left(\frac{1}{n!} \right)^2 t_{a_1 \dots a_n}^{i_1 \dots i_n} a^{a_1} \dots a^{a_n} a_{i_n} \dots a_{i_1} \quad (3)$$

are the many-body components of $T^{(A)}(M)$, and $t_{a_1 \dots a_n}^{i_1 \dots i_n}$ are the corresponding cluster amplitudes.

Coupled Cluster, Basics

The cluster amplitudes $t_{a_1 \dots a_n}^{i_1 \dots i_n}$ are determined by solving a coupled system of nonlinear and energy-independent algebraic equations of the form:

$$\langle \Phi_{i_1 \dots i_n}^{a_1 \dots a_n} | \bar{H}_N(M) | \Phi \rangle = 0, \quad i_1 < \dots < i_n, \quad a_1 < \dots < a_n, \quad (4)$$

where $n = 1, \dots, M$. Here,

$$\bar{H}_N(M) = e^{-T^{(A)}(M)} H_N e^{T^{(A)}(M)} = (H_N e^{T^{(A)}(M)})_C \quad (5)$$

is the similarity-transformed Hamiltonian of the coupled-cluster theory truncated at Mp - Mh excitations, subscript C designates the connected part of the corresponding operator expression, and $|\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}\rangle \equiv a^{a_1} \dots a^{a_n} a_{i_n} \dots a_{i_1} |\Phi\rangle$ are the np - nh or n -tuply excited determinants relative to $|\Phi\rangle$.

Coupled Cluster, Basics

The basic CCSD (coupled-cluster singles and doubles) method corresponds to $M = 2$ and the cluster operator $T^{(A)}$ is approximated by

$$T^{(A)}(\text{CCSD}) \equiv T^{(A)}(2) = T_1 + T_2, \quad (6)$$

where

$$T_1 = t_a^i a^a a_i \quad (7)$$

and

$$T_2 = \frac{1}{4} t_{ab}^{ij} a^a a^b a_j a_i \quad (8)$$

are $1p$ - $1h$ or singly excited and $2p$ - $2h$ or doubly excited cluster components, t_a^i and t_{ab}^{ij} are the corresponding singly and doubly excited cluster amplitudes, and $i, j, \dots$ ($a, b, \dots$) are the single-particle states occupied (unoccupied) in the reference determinant $|\Phi\rangle$.

Coupled Cluster, Basics

The standard CCSD equations for the singly and doubly excited cluster amplitudes t_a^i and t_{ab}^{ij} , defining T_1 and T_2 , respectively, can be written as

$$\langle \Phi_i^a | \bar{H}_N(\text{CCSD}) | \Phi \rangle = 0, \quad (9)$$

$$\langle \Phi_{ij}^{ab} | \bar{H}_N(\text{CCSD}) | \Phi \rangle = 0, \quad i < j, \quad a < b, \quad (10)$$

where

$$\begin{aligned} \bar{H}_N(\text{CCSD}) &\equiv \bar{H}_N(2) = e^{-T^{(A)}(\text{CCSD})} H_N e^{T^{(A)}(\text{CCSD})} \\ &= (H_N e^{T^{(A)}(\text{CCSD})})_C \end{aligned} \quad (11)$$

is the similarity-transformed Hamiltonian of the CCSD approach.

Coupled Cluster, Basics

The system of coupled-cluster equations, is obtained in the following way.

We first insert the coupled-cluster wave function $|\Psi_0^{(A)}\rangle$ into the A -body Schrödinger equation,

$$H_N |\Psi_0^{(A)}\rangle = \Delta E_0^{(A)} |\Psi_0^{(A)}\rangle, \quad (12)$$

where

$$\Delta E_0^{(A)} = E_0^{(A)} - \langle \Phi | H | \Phi \rangle$$

is the corresponding energy relative to the reference energy $\langle \Phi | H | \Phi \rangle$, and premultiply both sides on the left by $e^{-T^{(A)}}$ to obtain the connected-cluster form of the Schrödinger equation

$$\bar{H}_N |\Phi\rangle = \Delta E_0^{(A)} |\Phi\rangle, \quad (13)$$

where

$$\bar{H}_N = e^{-T^{(A)}} H_N e^{T^{(A)}} = (H_N e^{T^{(A)}})_C \quad (14)$$

is the similarity-transformed Hamiltonian.

Coupled Cluster, Basics

Next, we project Eq. (13), in which $T^{(A)}$ is replaced by its approximate form $T^{(A)}(M)$, Eq. (2), onto the excited determinants $|\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}\rangle$, corresponding to the p - h excitations included in $T^{(A)}(M)$. The excited determinants $|\Phi_{i_1 \dots i_n}^{a_1 \dots a_n}\rangle$ are orthogonal to the reference determinant $|\Phi\rangle$, so that we end up with nonlinear and energy-independent algebraic equations of the form of Eq. (4).

Coupled Cluster, Basics

Once the system of equations, Eq. (4), is solved for $T^{(A)}(M)$ or $t_{a_1 \dots a_n}^{i_1 \dots i_n}$ (or Eqs. (9) and (10) are solved for T_1 and T_2 or t_a^i and t_{ab}^{ij}), the ground-state coupled-cluster energy is calculated using the equation

$$\begin{aligned}
 E_0^{(A)}(M) &= \langle \Phi | H | \Phi \rangle + \Delta E_0^{(A)}(M) \\
 &= \langle \Phi | H | \Phi \rangle + \langle \Phi | \bar{H}_N(M) | \Phi \rangle \\
 &= \langle \Phi | H | \Phi \rangle + \langle \Phi | \bar{H}_{N,\text{close}}(M) | \Phi \rangle,
 \end{aligned} \tag{15}$$

where $\bar{H}_{N,\text{close}}(M)$ is the closed part of $\bar{H}_N(M)$ which is represented by those diagrams contributing to $\bar{H}_N^{(M)}$ that have no external (uncontracted) Fermion lines.

Coupled Cluster, Basics

It can easily be shown that if H contains only up to two-body interactions and $2 \leq M \leq A$, we can write

$$E_0^{(A)}(M) = \langle \Phi | H | \Phi \rangle + \langle \Phi | [H_N(T_1 + T_2 + \frac{1}{2}T_1^2)]_C | \Phi \rangle. \quad (16)$$

In other words, we only need T_1 and T_2 clusters to calculate the ground-state energy $E_0^{(A)}(M)$ of the A -body ($A \geq 2$) system even if we solve for other cluster components T_n with $n > 2$. As long as the Hamiltonian contains up to two-body interactions, the above energy expression is correct even in the exact case, when the cluster operator T is not truncated.

Coupled Cluster, Equations

To see this we compute the expectation of the energy from

$$E = \langle \Psi_0 | \exp(-T) H \exp(T) | \Psi_0 \rangle .$$

In addition, if we stop at the Singles and Doubles level we have the equations for the amplitudes are found by left projection of excited Slater determinants so that

$$0 = \langle \Psi_i^a | \exp(-T) H \exp(T) | \Psi_0 \rangle ,$$

$$0 = \langle \Psi_{ij}^{ab} | \exp(-T) H \exp(T) | \Psi_0 \rangle .$$

The Baker-Campbell-Hausdorf relation

$$\begin{aligned} \exp(-T) H \exp(T) &= H + [H, T_1] + [H, T_2] \\ &+ \frac{1}{2} [[H, T_1], T_1] + \frac{1}{2} [[H, T_2], T_2] \\ &+ [[H, T_1], T_2] + \dots . \end{aligned}$$

can be used to terminate exactly at quadruply nested commutators when the Hamiltonian contains at most two-body terms.

Coupled Cluster, Basics

The nonlinear character of the system of coupled-cluster equations of the form of Eq. (4) does not mean that the resulting equations contain very high powers of $T^{(A)}(M)$. For example, if the Hamiltonian H does not contain higher-than-pairwise interactions, the CCSD equations for the T_1 and T_2 clusters, or for the amplitudes t_a^i and t_{ab}^{ij} that represent these clusters, become

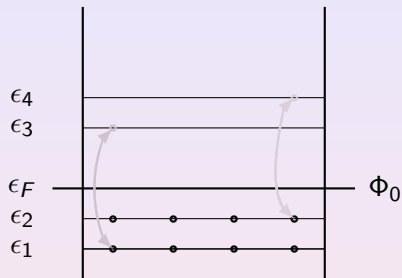
$$\langle \Phi_i^a | [H_N(1 + T_1 + T_2 + \frac{1}{2} T_1^2 + T_1 T_2 + \frac{1}{6} T_1^3)]_C | \Phi \rangle = 0, \quad (17)$$

$$\begin{aligned} \langle \Phi_{ij}^{ab} | [H_N(1 + T_1 + T_2 + \frac{1}{2} T_1^2 + T_1 T_2 + \frac{1}{6} T_1^3 \\ + \frac{1}{2} T_2^2 + \frac{1}{2} T_1^2 T_2 + \frac{1}{24} T_1^4)]_C | \Phi \rangle = 0. \end{aligned} \quad (18)$$

Coupled Cluster, Basics

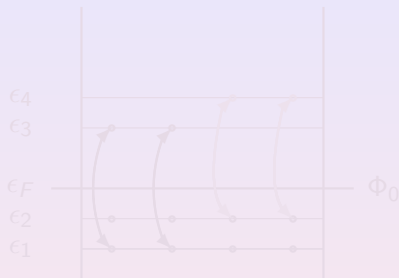
The explicitly connected form of the coupled-cluster equations, such as Eqs. (4) or (17) and (18), guarantees that the process of solving these equations leads to connected terms in cluster components T_n and connected terms in the energy $E_0^{(A)}(M)$, independent of the truncation scheme M used to define $T^{(A)}(M)$. The absence of disconnected terms in $T^{(A)}(M)$ and $E_0^{(A)}(M)$ is essential to obtain the rigorously size-extensive results.

Coupled Cluster in Pictures



From T_1 to T_1^2

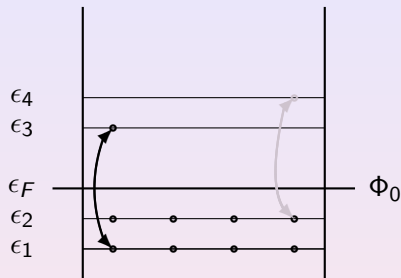
$$T_1 = \sum_{i < \epsilon_f, a > \epsilon_f} t_i^a a_a^+ a_i$$



From T_2 to T_2^2

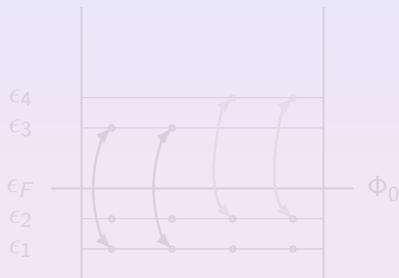
$$T_2 = \sum_{i,j < \epsilon_f; ab > \epsilon_f} t_{ij}^{ab} a_a^+ a_b^+ a_j a_i$$

Coupled Cluster in Pictures



From T_1 to T_1^2

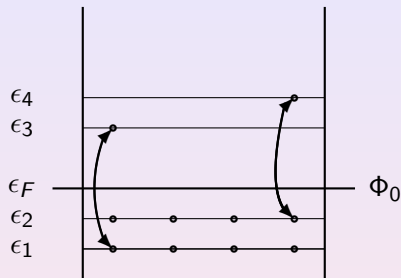
$$T_1 = \sum_{i < \epsilon_f, a > \epsilon_f} t_i^a a_a^+ a_i$$



From T_2 to T_2^2

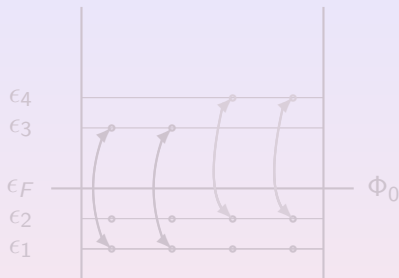
$$T_2 = \sum_{i,j < \epsilon_f; ab > \epsilon_f} t_{ij}^{ab} a_a^+ a_b^+ a_j a_i$$

Coupled Cluster in Pictures



From T_1 to T_1^2

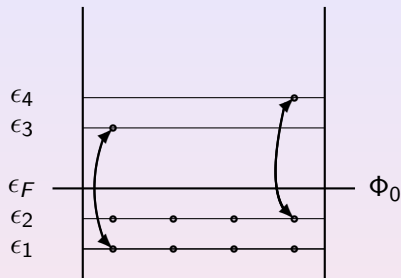
$$T_1 = \sum_{i < \epsilon_f, a > \epsilon_f} t_i^a a_a^+ a_i$$



From T_2 to T_2^2

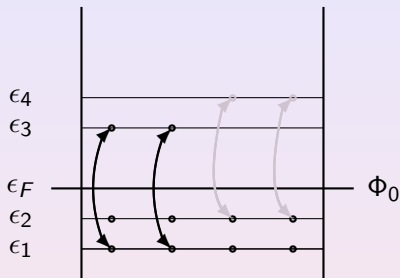
$$T_2 = \sum_{i,j < \epsilon_f; ab > \epsilon_f} t_{ij}^{ab} a_a^+ a_b^+ a_j a_i$$

Coupled Cluster in Pictures



From T_1 to T_1^2

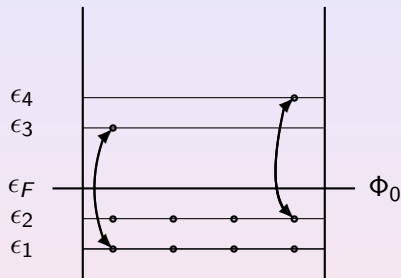
$$T_1 = \sum_{i < \epsilon_f, a > \epsilon_f} t_i^a a_a^+ a_i$$



From T_2 to T_2^2

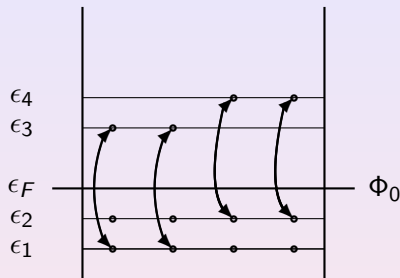
$$T_2 = \sum_{i,j < \epsilon_f; ab > \epsilon_f} t_{ij}^{ab} a_a^+ a_b^+ a_j a_i$$

Coupled Cluster in Pictures



From T_1 to T_1^2

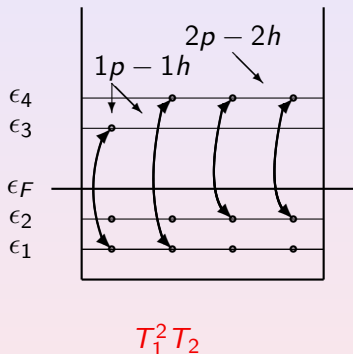
$$T_1 = \sum_{i < \epsilon_f, a > \epsilon_f} t_i^a a_a^+ a_i$$



From T_2 to T_2^2

$$T_2 = \sum_{i,j < \epsilon_f; ab > \epsilon_f} t_{ij}^{ab} a_a^+ a_b^+ a_j a_i$$

More Coupled Cluster in Pictures



CCSD and Shell-Model Truncations

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

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

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

- But CCSD has also $T_1^2 T_2$. Not in truncated shell model. Crucial.

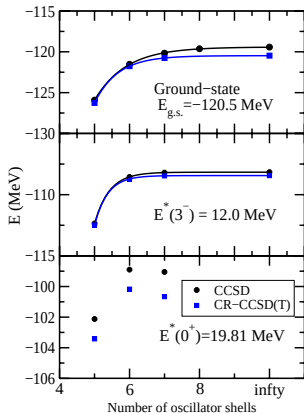
Triples and ^{16}O

4 Major Shells, $0s0p1s0d1p0f$

The ground-state energy of ^{16}O calculated using various coupled cluster methods and oscillator basis states. CISD is shell-model with $2p - 2h$, CISDT is shell-model with $3p - 3h$ and CISDTQ is shell-model with $4p - 4h$ truncations. Cannot go longer for shell model. Total shell-model dimension $d \sim 10^{14}$. Idaho-A interaction.

Method	Energy
CCSD	-139.310
CR-CCSD(T)	-139.621
CISD	-131.887
CISDT	-135.489
CISDTQ	-138.387

More on Excited ^{16}O States



Idaho-A results

- GS: Stable at 7 – 8 major shells. Agrees with no-core shell model.
- Expt for 3_1^- is 6.12 MeV, 1p-1h structure. Three-body force?
- Expt for 0_2^+ is 6.05, 4p-4h state. No convergence for triples.

Coupled Cluster, Results with N³LO

Nucleus	$N = 5$	$N = 6$	$N = 7$	$N = 8$	Expt
¹⁵ O	113.904 (7.594)	101.150 (6.743)	99.869 (6.658)	99.646 (6.643)	111.955 (7.464)
¹⁵ N	116.983 (7.799)	103.810 (6.921)	102.341 (6.823)	102.360 (6.824)	115.492 (7.699)
¹⁶ O	131.800 (8.787)	120.720 (7.545)	119.101 (7.444)	118.491 (7.406)	127.619 (7.976)
¹⁷ O	132.075 (8.805)	122.910 (7.230)	121.980 (7.175)	121.547 (7.150)	131.762 (7.751)
¹⁷ F	128.954 (8.597)	120.250 (7.074)	119.430 (7.026)	118.780 (6.987)	128.220 (7.542)
$\hbar\Omega$	13	11	10	11	
β_{CoM}	1.50	0.15	0.05	0.0	

Coupled Cluster, Results with $N^3\text{LO}$

Nucleus	$N = 6$	$N = 6$	$N = 6$	$N = 7$	$N = 7$
^{15}O	101.15	100.731	99.708	99.869	95.328
^{15}N	103.81	103.731	103.034	102.335	98.686
^{16}O	120.72	119.781	118.171	119.10	113.864
^{17}O	122.91	121.952	120.082	121.977	116.409
^{17}F	120.25	118.977	116.792	119.432	113.230
$\hbar\Omega$	11	12.5	14	10	14
β_{CoM}	0.15	0.3	0.5	0.05	0.3

We see from this Table that for six major shells and $\hbar\Omega = 14$ MeV we have a binding energy difference $\text{BE}(^{15}\text{N}) - \text{BE}(^{15}\text{O}) = 3.326$ MeV and $\text{BE}(^{17}\text{O}) - \text{BE}(^{17}\text{F}) = 3.290$ MeV, to be compared with the experimental values $\text{BE}(^{15}\text{N}) - \text{BE}(^{15}\text{O}) = 3.537$ MeV and $\text{BE}(^{17}\text{O}) - \text{BE}(^{17}\text{F}) = 3.542$ MeV.

Coupled Cluster, Results with N³LO

The charge radius for the ground state of ^{16}O , which is our reference system, also does not change much. The charge radius for six major shells changes from 2.647 fm to 2.572 fm for $\hbar\Omega = 11$ and 14 MeV, respectively. For seven major shells, the result for $\hbar\Omega = 14$ MeV is 2.595 fm, indicating a good convergence of the underlying CCSD calculations for ^{16}O .

Coupled Cluster, Results with N³LO

Excited state	$N = 5$	$N = 6$	$N = 7$	$N = 8$	Expt
$^{15}\text{O} (3/2)_1^-$	6.515	6.602	6.166	6.264	6.176
$^{15}\text{N} (3/2)_1^-$	6.354	6.680	6.256	6.318	6.323
$^{17}\text{O} (3/2)_1^+$	6.298	6.031	5.489	5.675	5.084
$^{17}\text{O} (1/2)_1^+$	0.328	0.130	-0.349	-0.025	0.870
$^{17}\text{F} (3/2)_1^+$	6.460	6.207	5.686	5.891	5.000
$^{17}\text{F} (1/2)_1^+$	0.748	0.544	0.088	0.428	0.495

Coupled Cluster, Results with $N^3\text{LO}$

Dependence on $\hbar\Omega$ of the excited state spectrum for the $N = 6$ model space, computed with $N^3\text{LO}$ at the optimal values of β_{CoM} , which are $\beta_{\text{CoM}} = 0.05, 0.3,$ and 0.5 , for $\hbar\Omega = 10, 12.5$, and 14 MeV, respectively.

Excited state	$\hbar\Omega = 11$	$\hbar\Omega = 12.5$	$\hbar\Omega = 14$	Expt
$^{15}\text{O} (3/2)_1^-$	6.602	6.841	6.990	6.176
$^{15}\text{N} (3/2)_1^-$	6.680	6.889	7.034	6.323
$^{17}\text{O} (3/2)_1^+$	6.031	6.536	7.129	5.084
$^{17}\text{O} (1/2)_1^+$	0.130	0.440	1.219	0.870
$^{17}\text{F} (3/2)_1^+$	6.207	6.740	7.199	5.000
$^{17}\text{F} (1/2)_1^+$	0.544	0.884	1.219	0.495

Coupled Cluster, Results with $N^3\text{LO}$

Dependence on $\hbar\Omega$ of the excited state spectrum for the $N = 7$ model space, computed with $N^3\text{LO}$ at the optimal values of β_{CoM} , which are $\beta_{\text{CoM}} = 0.05$ for $\hbar\Omega = 11$ MeV and $\beta_{\text{CoM}} = 0.3$ for $\hbar\Omega = 14$ MeV.

Excited state	$\hbar\Omega = 11$	$\hbar\Omega = 14$	Expt
$^{15}\text{O} (3/2)_1^-$	6.166	6.668	6.176
$^{15}\text{N} (3/2)_1^-$	6.256	6.703	6.323
$^{17}\text{O} (3/2)_1^+$	5.489	6.419	5.084
$^{17}\text{O} (1/2)_1^+$	-0.349	0.481	0.870
$^{17}\text{F} (3/2)_1^+$	5.686	6.672	5.000
$^{17}\text{F} (1/2)_1^+$	0.088	1.002	0.495

Coupled Cluster, Results with N³LO

The low-lying excited states of ^{16}O and, in general, states which involve cross-shell excitations, have always eluded a proper microscopic description. Let us concentrate on the lowest-energy 3_1^- state of ^{16}O . In a zero-order approximation, this state may be regarded as a state that arises from the single $i \rightarrow a$ excitation from the $i = 0p_{1/2}$ hole state to the $a = 0d_{5/2}$ particle state. Relative to the ^{16}O ground state, the energy required to produce such an excitation equals

$$\begin{aligned}\Delta\epsilon_\pi &= \epsilon_\pi(0d_{5/2}) - \epsilon_\pi(0p_{1/2}) \\ &= [\text{BE}(^{16}\text{O}) - \text{BE}(^{17}\text{F})] + [\text{BE}(^{16}\text{O}) - \text{BE}(^{15}\text{N})] \\ &= 11.526 \text{ MeV},\end{aligned}$$

for the proton case.

Coupled Cluster, Results with N³LO

$$\begin{aligned}\Delta\epsilon_\nu &= \epsilon_\nu(0d_{5/2}) - \epsilon_\nu(0p_{1/2}) \\ &= [\text{BE}(^{16}\text{O}) - \text{BE}(^{17}\text{O})] + [\text{BE}(^{16}\text{O}) - \text{BE}(^{15}\text{O})] \\ &= 11.521 \text{ MeV},\end{aligned}$$

for the neutron case, where the acronym BE in the above equations represents the relevant total binding energies.

Coupled Cluster, Results with N^3LO

In calculating the above values of the $1p$ - $1h$ excitation energies $\Delta\epsilon_\pi$ and $\Delta\epsilon_\nu$ that provide us with the zero-order estimates of the excitation energy of the lowest 3_1^- state of ^{16}O , we used the experimental binding energies.

The proton and neutron excitation energies are nearly identical. This reflects a well-known feature of spin-isospin saturated systems. Without interactions among nucleons and with the above single-particle orbits used as the only active degrees of freedom, all negative parity states with quantum numbers $J^\pi = 2^-, 3^-$ would be at the above energies of approximately 11.5 MeV. The interactions among nucleons lower the energy of the first excited 3^- state by $11.5 - 6.1 = 5.4$ MeV.

Coupled Cluster, Results with N³LO

Let us now compare the approximate energy spacing defining the lowest 3^- state of ^{16}O , resulting from the use of experimental binding energies, as shown above (11.5 MeV), with the values of $\Delta\epsilon_\pi$ and $\Delta\epsilon_\nu$ based on the results of coupled-cluster calculations for the binding energies of ^{16}O and valence systems around ^{16}O obtained with the N³LO interaction and eight major oscillator shells. These results are $\Delta\epsilon_\pi = 15.846$ MeV and $\Delta\epsilon_\nu = 15.789$ MeV, for proton and neutron excitations, respectively, with almost the same difference between the proton and neutron cases as observed in experiment. Fijii *et al* obtained 14.72 MeV and 14.64 MeV for protons and neutrons, respectively, using the same N³LO interaction as used here.

Coupled Cluster, Results with N^3LO

Using the above elementary picture of the $1p$ - $1h$ excitation defining the lowest 3^- state of ^{16}O , which involves only two orbits in the definition of the relevant model space, we can see that we are off by approximately $15.8 - 11.5 = 4.3$ MeV, when we compare the $\Delta\epsilon_\pi$ and $\Delta\epsilon_\nu$ energy spacings resulting from coupled-cluster calculations with the experimental estimates of these spacings. This difference is obviously an interaction and method dependent result. It is, however, converged as a function of the number of oscillator shells in a basis set, showing that the discrepancy of 4.3 MeV between theory and experiment for the energy gap between the $0p$ and $1s0d$ shells accounts for a large fraction of the missing 6 MeV needed to reproduce the first 3^- state of ^{16}O . This is, perhaps, the most likely candidate for a consistent explanation of the large difference between converged coupled-cluster result for the lowest 3^- state of ^{16}O and experiment. This conclusion is not substantially altered by the slight $\hbar\Omega$ dependence within the calculations.

Coupled Cluster, Results with N^3LO

The above analysis indicates that a large fraction of the difference between theory and experiment can be traced in this case to errors in reproducing the experimental binding energies of ^{16}O and valence systems around ^{16}O by coupled-cluster methods employing pairwise interactions only. This allows us to conclude that a 6 MeV difference between coupled-cluster result and experiment for the lowest 3^- state of ^{16}O is primarily caused by the lack of three-body interactions in our calculations, and much less by the approximate treatment of particle correlations by the coupled-cluster methods used in our studies. The above analysis also implies that with an adjusted gap between the $0p$ and $1s0d$ shells, one should be able to get a better reproduction of the excited states of ^{16}O which have a well-defined $1p-1h$ structure, such as the lowest 3^- state discussed here. One possible strategy for describing excited states of closed-shell nuclei dominated by $1p-1h$ excitations might be to keep the original two-body Hamiltonian and add additional three-body terms via corrections to the single-particle energies.

Coupled Cluster Summary

Challenges

- CCSD in 8 major shells in ^{16}O seems to yield stable results for the binding energy. Quick calculations compared to no-core shell-model.
- Can now do valence systems: first test for $^{15,17}\text{O}$.
- Can now do all closed core nuclei up to ^{100}Sn , 10 major shells.
- Triples give nearly exact shell-model results. Good agreement with No-Core shell-model and UMOA calculations.
- Problem: harmonic oscillator basis. Even if we can do many shells, wave function not correct for many states. Now complex coupled cluster, Hagen *et al* nucl-th/0610072, Lecture V.
- Three-body forces implemented, Hagen *et al*