Lecture set III and IV: Many-body methods

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Lectures at Universitad Complutense Madrid

Outline

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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?

Homework for next time:

- Define an observable and make a list of observables
- We will look at nuclei in the mass regions between $A = 40$ and $A = 90$. Examples are ^{64}Fe, ^{80}Zn etc.
- Find candidates for closed shell cores
- Find possible single-particle states and argue why
- Define possible shell-model spaces

Monday 7/2 and Tuesday 8/2 we will then run the software in order to perform shell-model studies for these systems. Make sure you have the programs set up.

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.
- Shell-model in smaller spaces, lecture set 5.

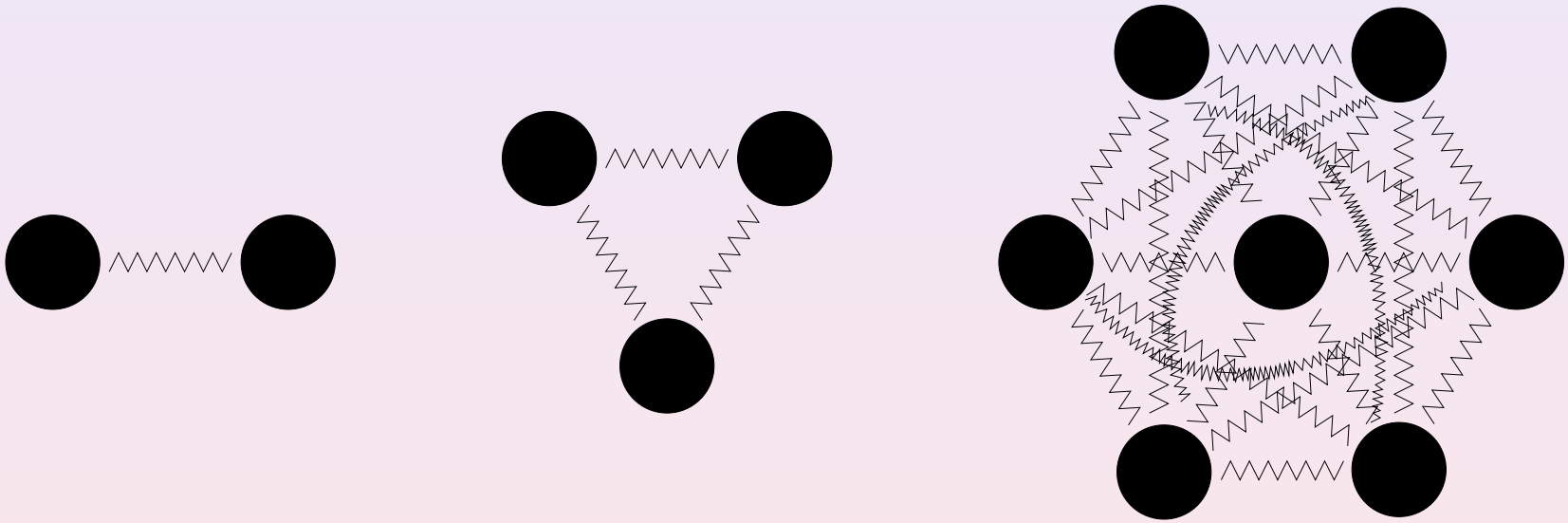
Selected Many-body Methods and mathematics

1. Shell model and No-core shell model (configuration interaction): eigenvalue problem
2. Monte Carlo methods: Stochastic approaches
3. Coupled-Cluster theory: non-linear equations
4. Green's function approach: matrix inversion
5. Similarity Renormalization group: Coupled differential equations
6. Many-body perturbation theory: Taylor expansion

Problem statement

Many-body systems

- We study a bound system of A interacting particles ...



and it quickly becomes unmanageable . . .

Problem statement

We are looking at non-relativistic particles, so the solutions of the A-body system, is given by the A-body Schrödinger equation.

$$\widehat{H}_A|\Psi_A\rangle = E_A|\Psi_A\rangle$$

Manybody wavefunction

The wavefunction of the manybody system can be decomposed into a suitable manybody basis

$$|\Psi_A\rangle = \sum_i c_i |\Phi_i\rangle.$$

For fermions, these are Slater-determinants

$$\begin{aligned} |\Phi_i\rangle &= |\alpha_{i_1}\alpha_{i_2}\ldots\alpha_{i_A}\rangle \\ &= \left(\prod_{j=1}^{A} a_{i_j}^\dagger\right)|0\rangle, \end{aligned}$$

Where $a^\dagger$ is a second quantized operator satisfying

$$a_p^\dagger|0\rangle = |\alpha_p\rangle \qquad a_p|\alpha_q\rangle = \left(a_p^\dagger\right)^\dagger|\alpha_q\rangle = \delta_{pq}|0\rangle$$

$$\left\{a_p, a_q^\dagger\right\} = \delta_{pq} \qquad \{a_p, a_q\} = \left\{a_p^\dagger, a_q^\dagger\right\} = 0$$

Manybody wavefunction

In the **x**-representation the Slater-determinant is written

$$\langle \mathbf{x} | \, \Phi_i = \frac{1}{\sqrt{A}} \sum_{n=1}^{A!} (-1)^{P_n} \prod_{j=1}^{A} \phi_{i,n_j}(\mathbf{x}_j),$$

where

$$\phi_{i,k}(\mathbf{x}_j) = \left\langle \mathbf{x}_j \right| \alpha_{i_k}$$

are the solutions to a selected single particle problem

$$\widehat{h}\phi_k(\mathbf{x}) = \epsilon_k \phi_k(\mathbf{x}).$$

Manybody wavefunction

In the particle-hole formalism all quantities are expressed in relation to the reference state

$$|\Phi_0\rangle = |\alpha_1 \dots \alpha_A\rangle, \quad \alpha_1, \dots, \alpha_A \leq \alpha_F$$

The indices are partitioned according to their relation to the Fermi level

$$i, j, \dots \leq \alpha_F \qquad a, b, \dots > \alpha_F \qquad p, q, \dots : \text{any},$$

and the second quantized operators now satisfy

$$\left\{a_i, a_j^\dagger\right\} = \delta_{ij} \qquad \left\{a_a, a_b^\dagger\right\} = \delta_{ab}$$

$$a_i|\Phi_0\rangle = |\Phi_i\rangle \qquad a_a^\dagger|\Phi_0\rangle = |\Phi^a\rangle$$

$$a_i^\dagger|\Phi_0\rangle = 0 \qquad a_a|\Phi_0\rangle = 0$$

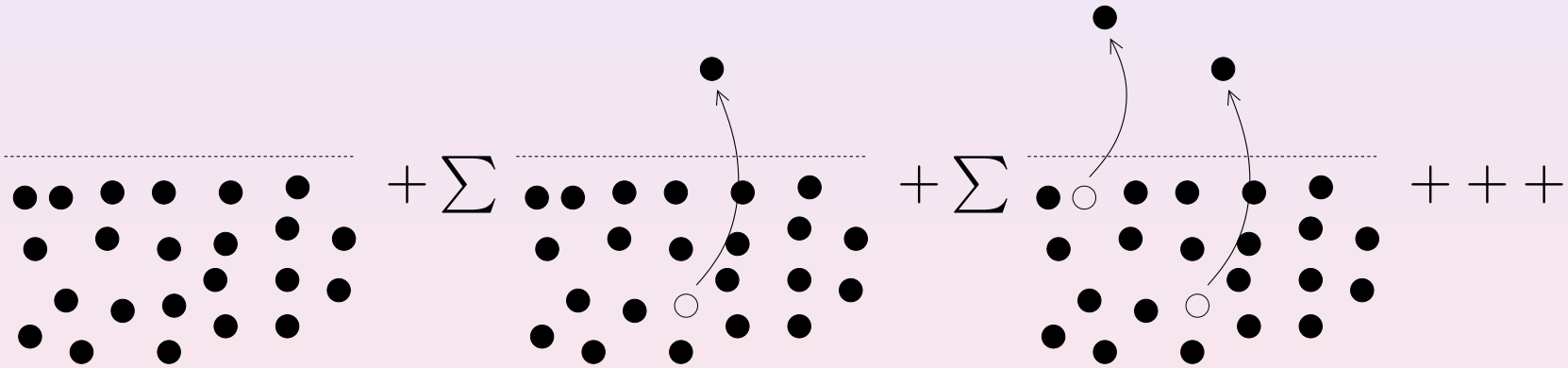
Manybody wavefunction

For use with Wicks theorem, we define the contractions between operators in the particle-hole formalism

$$\overbrace{a_p^\dagger a_q} = \langle \Phi_0 | a_p^\dagger a_q | \Phi_0 \rangle = \delta_{pq \in i}$$
$$\overbrace{a_q a_p^\dagger} = \langle \Phi_0 | a_q a_p^\dagger | \Phi_0 \rangle = \delta_{pq \in a}$$

Manybody wavefunction

The particle-hole expansion of a manybody wavefunction is a linear combination of all possible excitations of the reference wavefuncton.



Manybody wavefunction

The manybody wavefunction can be expanded in a linear combination of particle-hole excitations, which is complete in agiven basis set

$$|\Psi\rangle = \sum_{ia} |\Phi_i^a\rangle + \frac{1}{4}\sum_{ijab} |\Phi_{ij}^{ab}\rangle + \ldots + \frac{1}{(A!)^2}\sum_{\substack{i_1\ldots i_A \\ a_1\ldots a_A}} |\Phi_{i_1\ldots i_A}^{a_1\ldots a_A}\rangle$$

$$= \sum_{ia} c_i^a a_a^\dagger a_i |\Phi_0\rangle + \frac{1}{4}\sum_{ijab} c_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i |\Phi_0\rangle + \ldots +$$

$$\frac{1}{(A!)^2}\sum_{\substack{i_1\ldots i_A \\ a_1\ldots a_A}} c_{i_1\ldots i_A}^{a_1\ldots a_A} a_{a_1}^\dagger \ldots a_{a_A}^\dagger a_{i_A} \ldots a_{i_1} |\Phi_0\rangle$$

Manybody Hamiltonian

A general Hamiltonian contains up to A-body interactions

$$\begin{aligned}\widehat{H}_A &= \sum_{i=1}^{A}\left(\widehat{t}_i + \widehat{u}_i\right) + \sum_{i<j=1}^{A}\widehat{v}_{ij} + + + \sum_{i_1<\cdots<i_A=1}^{A}\widehat{v}_{i_1,\ldots,i_A} \\ &= \widehat{T}_{\rm kin} + \widehat{U} + \sum_{n=2}^{A}\widehat{V}_n,\end{aligned}$$

where $\widehat{T}_{\rm kin}$ is the kinetic energy operator, $\widehat{U}$ is a generic onebody potential and $\widehat{V}_n$ is an n-body potential.

Manybody Hamiltonian

In second quantized form, a general n-body operator is written

$$\widehat{V}_n = \frac{1}{(n!)^2} \sum_{\substack{\alpha_1 \ldots \alpha_n \\ \gamma_1 \ldots \gamma_n}} \langle \alpha_1 \ldots \alpha_n | \widehat{v}_n | \gamma_1 \ldots \gamma_n \rangle a^\dagger_{\alpha_1} \ldots a^\dagger_{\alpha_n} a_{\gamma_n} \ldots a_{\gamma_1},$$

where the matrix elements $\langle \alpha_1 \ldots \alpha_n | \widehat{V}_n | \gamma_1 \ldots \gamma_n \rangle$ are fully anti-symmetric with respect to the interchange of indices and the sum over α_i and γ_i runs over all possible single particle states.

Manybody Hamiltonian

We will truncate the Hamiltonian at the $n = 3$ level at the most and skip the onebody potential, so the Hamiltonian will be written

$$\widehat{H} = \sum_{pq} \langle p|\widehat{t}|q\rangle a_p^\dagger a_q + \frac{1}{4}\sum_{pqrs} \langle pq|\widehat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$
$$\frac{1}{36}\sum_{pqrstu} \langle pqr|\widehat{v}_3|stu\rangle a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

Manybody Hamiltonian

We define the normal ordered operator

$$\left\{a_a a_b \dots a_c^\dagger a_d^\dagger\right\} = (-1)^P a_c^\dagger a_d^\dagger \dots a_a a_b$$

All creation operators to the left and all annihilation operators to the right times a factor determined by how many operators have been switched.
This object has the highly desired property that the expectation value is always zero

$$\langle \Phi_0 | \left\{a_a a_b \dots a_c^\dagger a_d^\dagger\right\} | \Phi_0 \rangle = 0$$

Manybody Hamiltonian

Derivation of the normal ordered Hamiltonian

$$\widehat{T}_{\text{kin}} = \sum_{pq} \langle p|\widehat{t}|q\rangle a_p^\dagger a_q$$

$$a_p^\dagger a_q = \left\{ a_p^\dagger a_q \right\} + \left\{ \overbrace{a_p^\dagger a_q} \right\}$$
$$= \left\{ a_p^\dagger a_q \right\} + \delta_{pq\in i}$$

$$\widehat{T}_{\text{kin}} = \sum_{pq} \langle p|\widehat{t}|q\rangle a_p^\dagger a_q$$
$$= \sum_{pq} \langle p|\widehat{t}|q\rangle \left\{ a_p^\dagger a_q \right\} + \delta_{pq\in i} \sum_{pq} \langle p|\widehat{t}|q\rangle$$
$$= \sum_{pq} \langle p|\widehat{t}|q\rangle \left\{ a_p^\dagger a_q \right\} + \sum_{i} \langle i|\widehat{t}|i\rangle$$

Manybody Hamiltonian

Derivation of the normal ordered Hamiltonian

$$\hat{H}_2 = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$a_p^\dagger a_q^\dagger a_s a_r = \left\{a_p^\dagger a_q^\dagger a_s a_r\right\}$$

$$+\left\{a_p^\dagger \overbrace{a_q^\dagger a_s} a_r\right\} + \left\{a_p^\dagger \overbrace{a_q^\dagger a_s a_r}\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger} a_s a_r\right\}$$

$$+\left\{\overbrace{a_p^\dagger a_q^\dagger} a_s a_r\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger a_s} a_r\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger a_s a_r}\right\}$$

$$= \left\{a_p^\dagger a_q^\dagger a_s a_r\right\}$$

$$+\delta_{qs\in i}\left\{a_p^\dagger a_r\right\} - \delta_{qr\in i}\left\{a_p^\dagger a_s\right\} - \delta_{ps\in i}\left\{a_q^\dagger a_r\right\}$$

$$+\delta_{pr\in i}\left\{a_q^\dagger a_s\right\} + \delta_{pr\in i}\delta_{qs\in i} - \delta_{ps\in i}\delta_{qr\in i}$$

Manybody Hamiltonian

Derivation of the normal ordered Hamiltonian

$$\hat{H}_2 = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$\begin{aligned} a_p^\dagger a_q^\dagger a_s a_r = &\left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\ &+ \left\{a_p^\dagger \overbrace{a_q^\dagger a_s} a_r\right\} + \left\{a_p^\dagger \overbrace{a_q^\dagger a_s a_r}\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger} a_s a_r\right\} \\ &+ \left\{\overbrace{a_p^\dagger a_q^\dagger a_s} a_r\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger} a_s a_r\right\} + \left\{\overbrace{a_p^\dagger \overbrace{a_q^\dagger a_s} a_r}\right\} \\ = &\left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\ &+ \delta_{qs\in i}\left\{a_p^\dagger a_r\right\} - \delta_{qr\in i}\left\{a_p^\dagger a_s\right\} - \delta_{ps\in i}\left\{a_q^\dagger a_r\right\} \\ &+ \delta_{pr\in i}\left\{a_q^\dagger a_s\right\} + \delta_{pr\in i}\delta_{qs\in i} - \delta_{ps\in i}\delta_{qr\in i} \end{aligned}$$

Manybody Hamiltonian

Derivation of the normal ordered Hamiltonian

$$\hat{H}_2 = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$\begin{aligned}
a_p^\dagger a_q^\dagger a_s a_r = &\left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&+ \left\{a_p^\dagger \overbrace{a_q^\dagger a_s} a_r\right\} + \left\{a_p^\dagger \overbrace{a_q^\dagger a_s a_r}\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger} a_s a_r\right\} \\
&+ \left\{\overbrace{a_p^\dagger a_q^\dagger a_s} a_r\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger} a_s a_r\right\} + \left\{\overbrace{a_p^\dagger \overbrace{a_q^\dagger a_s} a_r}\right\} \\
= &\left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&+ \delta_{qs\in i}\left\{a_p^\dagger a_r\right\} - \delta_{qr\in i}\left\{a_p^\dagger a_s\right\} - \delta_{ps\in i}\left\{a_q^\dagger a_r\right\} \\
&+ \delta_{pr\in i}\left\{a_q^\dagger a_s\right\} + \delta_{pr\in i}\delta_{qs\in i} - \delta_{ps\in i}\delta_{qr\in i}
\end{aligned}$$

Manybody Hamiltonian

Derivation of the normal ordered Hamiltonian

$$\hat{H}_2 = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$\begin{aligned}
a_p^\dagger a_q^\dagger a_s a_r &= \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&\quad + \left\{a_p^\dagger \overbrace{a_q^\dagger a_s} a_r\right\} + \left\{a_p^\dagger \overbrace{a_q^\dagger a_s a_r}\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger} a_s a_r\right\} \\
&\quad + \left\{\overbrace{a_p^\dagger a_q^\dagger a_s} a_r\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger a_s a_r}\right\} + \left\{\overbrace{a_p^\dagger \overbrace{a_q^\dagger} a_s} a_r\right\} \\
&= \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&\quad + \delta_{qs\in i}\left\{a_p^\dagger a_r\right\} - \delta_{qr\in i}\left\{a_p^\dagger a_s\right\} - \delta_{ps\in i}\left\{a_q^\dagger a_r\right\} \\
&\quad + \delta_{pr\in i}\left\{a_q^\dagger a_s\right\} + \delta_{pr\in i}\delta_{qs\in i} - \delta_{ps\in i}\delta_{qr\in i}
\end{aligned}$$

Manybody Hamiltonian

Derivation of the normal ordered Hamiltonian

$$\hat{H}_2 = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$\begin{aligned}
a_p^\dagger a_q^\dagger a_s a_r &= \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&\quad + \left\{a_p^\dagger \overbrace{a_q^\dagger a_s} a_r\right\} + \left\{a_p^\dagger \overbrace{a_q^\dagger a_s a_r}\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger} a_s a_r\right\} \\
&\quad + \left\{\overbrace{a_p^\dagger a_q^\dagger a_s} a_r\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger a_s a_r}\right\} + \left\{\overbrace{a_p^\dagger \overbrace{a_q^\dagger} a_s} a_r\right\} \\
&= \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&\quad + \delta_{qs\in i}\left\{a_p^\dagger a_r\right\} - \delta_{qr\in i}\left\{a_p^\dagger a_s\right\} - \delta_{ps\in i}\left\{a_q^\dagger a_r\right\} \\
&\quad + \delta_{pr\in i}\left\{a_q^\dagger a_s\right\} + \delta_{pr\in i}\delta_{qs\in i} - \delta_{ps\in i}\delta_{qr\in i}
\end{aligned}$$

Manybody Hamiltonian

Derivation of the normal ordered Hamiltonian

$$\hat{H}_2 = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$\begin{aligned}
a_p^\dagger a_q^\dagger a_s a_r &= \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&\quad + \left\{a_p^\dagger \overbrace{a_q^\dagger a_s} a_r\right\} + \left\{a_p^\dagger \overbrace{a_q^\dagger a_s a_r}\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger} a_s a_r\right\} \\
&\quad + \left\{\overbrace{a_p^\dagger a_q^\dagger a_s} a_r\right\} + \left\{\overbrace{a_p^\dagger a_q^\dagger a_s a_r}\right\} + \left\{\overbrace{a_p^\dagger \overbrace{a_q^\dagger} a_s} a_r\right\} \\
&= \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&\quad + \delta_{qs\in i}\left\{a_p^\dagger a_r\right\} - \delta_{qr\in i}\left\{a_p^\dagger a_s\right\} - \delta_{ps\in i}\left\{a_q^\dagger a_r\right\} \\
&\quad + \delta_{pr\in i}\left\{a_q^\dagger a_s\right\} + \delta_{pr\in i}\delta_{qs\in i} - \delta_{ps\in i}\delta_{qr\in i}
\end{aligned}$$

Manybody Hamiltonian

Derivation of the normal ordered Hamiltonian

$$\hat{H}_2 = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

$$= \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \frac{1}{4}\sum_{pqrs}\Big(\delta_{qs\in i}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_r\right\}$$

$$- \delta_{qr\in i}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_s\right\} - \delta_{ps\in i}\langle pq|\hat{v}|rs\rangle \left\{a_q^\dagger a_r\right\}$$

$$+ \delta_{pr\in i}\langle pq|\hat{v}|rs\rangle \left\{a_q^\dagger a_s\right\} + \delta_{pr\in i}\delta_{qs\in i} - \delta_{ps\in i}\delta_{qr\in i}\Big)$$

Manybody Hamiltonian

Derivation of the normal ordered Hamiltonian

$$
\begin{aligned}
&= \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&\quad + \frac{1}{4}\sum_{pqi}\Big(\langle pi|\hat{v}|qi\rangle - \langle pi|\hat{v}|iq\rangle - \langle ip|\hat{v}|qi\rangle + \langle ip|\hat{v}|iq\rangle\Big)\left\{a_p^\dagger a_q\right\} \\
&\quad + \frac{1}{4}\sum_{ij}\Big(\langle ij|\hat{v}|ij\rangle - \langle ij|\hat{v}|ji\rangle\Big) \\
&= \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \sum_{pqi}\langle pi|\hat{v}|qi\rangle \left\{a_p^\dagger a_q\right\} + \frac{1}{2}\sum_{ij}\langle ij|\hat{v}|ij\rangle
\end{aligned}
$$

Manybody Hamiltonian

Derivation of the normal ordered Hamiltonian

$$\widehat{G}_N = \frac{1}{36}\sum_{\substack{pqr\\stu}}\langle pqr|\widehat{v}_3|stu\rangle \left\{a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s\right\}$$

$$\widehat{V}_N = \frac{1}{4}\sum_{pqrs}\left(\langle pq|\widehat{v}|rs\rangle + \sum_i \langle ipq|\widehat{v}_3|irs\rangle\right)\left\{a_p^\dagger a_q^\dagger a_s a_r\right\}$$

$$\widehat{F}_N = \sum_{pq}\left(\langle p|\widehat{t}|q\rangle + \sum_i \langle pi|\widehat{v}|qi\rangle + \frac{1}{2}\sum_{ij}\langle ijp|\widehat{v}_3|ijq\rangle\right)\left\{a_p^\dagger a_q\right\}$$

$$E_0 = \sum_i \langle i|\widehat{t}|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|\widehat{v}|ij\rangle + \frac{1}{6}\sum_{ijk}\langle ijk|\widehat{v}_3|ijk\rangle$$

$$\widehat{H} = \widehat{G}_N + \widehat{V}_N + \widehat{F}_N + E_0 \qquad (2.0.1)$$

Perturbation theory (time-independent)

The projection operators defining the model and excluded spaces are defined by

$$P = \sum_{i=1}^{D} |\psi_i\rangle\langle\psi_i|, \tag{3.0.2}$$

and

$$Q = \sum_{i=D+1}^{\infty} |\psi_i\rangle\langle\psi_i|, \tag{3.0.3}$$

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.).

Perturbation theory (time-independent)

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

$$H|\Psi_\alpha\rangle = E_\alpha|\Psi_\alpha\rangle, \tag{3.0.4}$$

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

Perturbation theory (time-independent)

We will now assume that the wave operator Ω has an inverse and consider a similarity transformation of the Hamiltonian H such that Eq. (48) can be rewritten as

$$\Omega^{-1} H \Omega \Omega^{-1} |\Psi_\alpha\rangle = E_\alpha \Omega^{-1} |\Psi_\alpha\rangle. \tag{3.0.5}$$

Recall also that $|\Psi_\alpha\rangle = \Omega |\Psi_\alpha^M\rangle$, which means that $\Omega^{-1}|\Psi_\alpha\rangle = |\Psi_\alpha^M\rangle$ insofar as the inverse of Ω exists.

Perturbation theory (time-independent)

Let us define the transformed hamiltonian $\mathcal{H} = \Omega^{-1} H \Omega$, which can be rewritten in terms of the operators P and Q ($P + Q = I$) as

$$\mathcal{H} = P\mathcal{H}P + P\mathcal{H}Q + Q\mathcal{H}P + Q\mathcal{H}Q. \tag{3.0.6}$$

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

Perturbation theory (time-independent)

If we now operate on Eq. (48), which in terms of the model space wave function reads

$$\mathcal{H}|\Psi_\alpha^M\rangle = E_\alpha|\Psi_\alpha^M\rangle, \tag{3.0.7}$$

with the operator Q, we readily see that

$$Q\mathcal{H}P = 0. \tag{3.0.8}$$

Perturbation theory (time-independent)

Eq. (49) is an important relation which states that the eigenfunction $P|\Psi_\alpha\rangle$ is a *pure model space eigenfunction*. This implies that we can define an *effective model space hamiltonian*

$$H_{\text{eff}} = P\mathcal{H}P = P\Omega^{-1}H\Omega P, \tag{3.0.9}$$

or equivalently

$$H\Omega P = \Omega P H_{\text{eff}} P, \tag{3.0.10}$$

which is the Bloch equation. This equation can be used to determine the wave operator Ω.

Perturbation theory (time-independent)

We assume here that we are only interested in the ground state of the system and expand the exact wave function in term of a series of Slater determinants

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{m=1}^{\infty} C_m |\Phi_m\rangle,$$

where we have assumed that the true ground state is dominated by the solution of the unperturbed problem, that is

$$\hat{H}_0|\Phi_0\rangle = W_0|\Phi_0\rangle.$$

The state $|\Psi_0\rangle$ is not normalized, rather we have used an intermediate normalization $\langle\Phi_0|\Psi_0\rangle = 1$ since we have $\langle\Phi_0|\Phi_0\rangle = 1$.

Perturbation theory (time-independent)

The Schrödinger equation is

$$\hat{H}|\Psi_0\rangle = E_0|\Psi_0\rangle,$$

and multiplying the latter from the left with $\langle\Phi_0|$ gives

$$\langle\Phi_0|\hat{H}|\Psi_0\rangle = E_0\langle\Phi_0|\Psi_0\rangle = E_0,$$

and subtracting from this equation

$$\langle\Psi_0|\hat{H}_0|\Phi_0\rangle = W_0\langle\Psi_0|\Phi_0\rangle = W_0,$$

and using the fact that the both operators $\hat{H}$ and $\hat{H}_0$ are hermitian results in

$$\Delta E_0 = E_0 - W_0 = \langle\Phi_0|\hat{H}_I|\Psi_0\rangle,$$

which is an exact result.

Perturbation theory (time-independent)

This equation forms the starting point for all perturbative derivations. However, as it stands it represents nothing but a mere formal rewriting of Schrödinger's equation and is not of much practical use. The exact wave function $|\Psi_0\rangle$ is unknown. In order to obtain a perturbative expansion, we need to expand the exact wave function in terms of the interaction $\hat{H}_I$.
Here we have assumed that our model space defined by the operator $\hat{P}$ is one-dimensional, meaning that

$$\hat{P} = |\Phi_0\rangle\langle\Phi_0|,$$

and

$$\hat{Q} = \sum_{m=1}^{\infty} |\Phi_m\rangle\langle\Phi_m|.$$

Perturbation theory (time-independent)

We can thus rewrite the exact wave function as

$$|\Psi_0\rangle = (\hat{P} + \hat{Q})|\Psi_0\rangle = |\Phi_0\rangle + \hat{Q}|\Psi_0\rangle.$$

Going back to the Schrödinger equation, we can rewrite it as, adding and a subtractiing a term $\omega|\Psi_0\rangle$ as

$$\left(\omega - \hat{H}_0\right)|\Psi_0\rangle = \left(\omega - E_0 - \hat{H}_I\right)|\Psi_0\rangle,$$

where ω is an energy variable to be specified later.

Perturbation theory (time-independent)

We assume also that the resolvent of $\left(\omega - \hat{H}_0\right)$ exits, that is it has an inverse which defined the unperturbed Green's function as

$$\left(\omega - \hat{H}_0\right)^{-1} = \frac{1}{\left(\omega - \hat{H}_0\right)}.$$

Perturbation theory (time-independent)

We can rewrite Schrödinger's equation as

$$|\Psi_0\rangle = \frac{1}{\omega - \hat{H}_0}\left(\omega - E_0 - \hat{H}_I\right)|\Psi_0\rangle,$$

and multiplying from the left with $\hat{Q}$ results in

$$\hat{Q}|\Psi_0\rangle = \frac{\hat{Q}}{\omega - \hat{H}_0}\left(\omega - E_0 - \hat{H}_I\right)|\Psi_0\rangle,$$

which is possible since we have defined the operator $\hat{Q}$ in terms of the eigenfunctions of $\hat{H}$.

Perturbation theory (time-independent)

These operators commute meaning that

$$\hat{Q}\frac{1}{\left(\omega-\hat{H}_0\right)}\hat{Q}=\hat{Q}\frac{1}{\left(\omega-\hat{H}_0\right)}=\frac{\hat{Q}}{\left(\omega-\hat{H}_0\right)}.$$

With these definitions we can in turn define the wave function as

$$|\Psi_0\rangle=|\Phi_0\rangle+\frac{\hat{Q}}{\omega-\hat{H}_0}\left(\omega-E_0-\hat{H}_I\right)|\Psi_0\rangle.$$

Perturbation theory (time-independent)

$$|\Psi_0\rangle = |\Phi_0\rangle + \frac{\hat{Q}}{\omega - \hat{H}_0}\left(\omega - E_0 - \hat{H}_I\right)|\Psi_0\rangle.$$

This equation is again nothing but a formal rewrite of Schrödinger's equation and does not represent a practical calculational scheme. It is a non-linear equation in two unknown quantities, the energy E_0 and the exact wave function $|\Psi_0\rangle$. We can however start with a guess for $|\Psi_0\rangle$ on the right hand side of the last equation.

Perturbation theory (time-independent)

The most common choice is to start with the function which is expected to exhibit the largest overlap with the wave function we are searching after, namely $|\Phi_0\rangle$. This can again be inserted in the solution for $|\Psi_0\rangle$ in an iterative fashion and if we continue along these lines we end up with

$$|\Psi_0\rangle = \sum_{i=0}^{\infty} \left\{ \frac{\hat{Q}}{\omega - \hat{H}_0} \left(\omega - E_0 - \hat{H}_I \right) \right\}^i |\Phi_0\rangle,$$

for the wave function and

$$\Delta E_0 = \sum_{i=0}^{\infty} \langle \Phi_0 | \hat{H}_I \left\{ \frac{\hat{Q}}{\omega - \hat{H}_0} \left(\omega - E_0 - \hat{H}_I \right) \right\}^i |\Phi_0\rangle,$$

which is now a perturbative expansion of the exact energy in terms of the interaction $\hat{H}_I$ and the unperturbed wave function $|\Psi_0\rangle$.

Brillouin-Wigner theory

In our equations for $|\Psi_0\rangle$ and ΔE_0 in terms of the unperturbed solutions $|\Phi_i\rangle$ we have still an undetermined parameter ω and a dependecy on the exact energy E_0. Not much has been gained thus from a practical computational point of view.
In Brilluoin-Wigner perturbation theory it is customary to set $\omega = E_0$. This results in the following perturbative expansion for the energy ΔE_0

$$\Delta E_0 = \sum_{i=0}^{\infty} \langle \Phi_0 | \hat{H}_I \left\{ \frac{\hat{Q}}{\omega - \hat{H}_0} \left(\omega - E_0 - \hat{H}_I \right) \right\}^i |\Phi_0\rangle =$$

$$\langle \Phi_0 | \left(\hat{H}_I + \hat{H}_I \frac{\hat{Q}}{E_0 - \hat{H}_0} \hat{H}_I + \hat{H}_I \frac{\hat{Q}}{E_0 - \hat{H}_0} \hat{H}_I \frac{\hat{Q}}{E_0 - \hat{H}_0} \hat{H}_I + \dots \right) |\Phi_0\rangle.$$

Brillouin-Wigner theory

$$\Delta E_0 = \sum_{i=0}^{\infty} \langle \Phi_0 | \hat{H}_I \left\{ \frac{\hat{Q}}{\omega - \hat{H}_0} \left(\omega - E_0 - \hat{H}_I \right) \right\}^i |\Phi_0\rangle =$$

$$\langle \Phi_0 | \left(\hat{H}_I + \hat{H}_I \frac{\hat{Q}}{E_0 - \hat{H}_0} \hat{H}_I + \hat{H}_I \frac{\hat{Q}}{E_0 - \hat{H}_0} \hat{H}_I \frac{\hat{Q}}{E_0 - \hat{H}_0} \hat{H}_I + \ldots \right) |\Phi_0\rangle.$$

This expression depends however on the exact energy E_0 and is again not very convenient from a practical point of view. It can obviously be solved iteratively, by starting with a guess for E_0 and then solve till some kind of self-consistency criterion has been reached.

Actually, the above expression is nothing but a rewrite again of the full Schrödinger equation.

Rayleigh-Schrödinger (RS) perturbation theory

In RS perturbation theory we set $\omega = W_0$ and obtain the following expression for the energy difference

$$\Delta E_0 = \sum_{i=0}^{\infty} \langle \Phi_0 | \hat{H}_I \left\{ \frac{\hat{Q}}{W_0 - \hat{H}_0} \left(\hat{H}_I - \Delta E_0 \right) \right\}^i |\Phi_0\rangle =$$

$$\langle \Phi_0 | \left(\hat{H}_I + \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} (\hat{H}_I - \Delta E_0) + \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} (\hat{H}_I - \Delta E_0) \frac{\hat{Q}}{W_0 - \hat{H}_0} (\hat{H}_I - \Delta E_0) + \dots \right) |\Phi_0$$

Rayleigh-Schrödinger perturbation theory

Recalling that $\hat{Q}$ commutes with $\hat{H}_0$ and since ΔE_0 is a constant we obtain that

$$\hat{Q}\Delta E_0|\Phi_0\rangle = \hat{Q}\Delta E_0|\hat{Q}\Phi_0\rangle = 0.$$

Inserting this results in the expression for the energy results in

$$\Delta E_0 = \langle\Phi_0|\left(\hat{H}_I + \hat{H}_I\frac{\hat{Q}}{W_0-\hat{H}_0}\hat{H}_I + \hat{H}_I\frac{\hat{Q}}{W_0-\hat{H}_0}(\hat{H}_I-\Delta E_0)\frac{\hat{Q}}{W_0-\hat{H}_0}\hat{H}_I + \ldots\right)|\Phi_0\rangle.$$

Rayleigh-Schrödinger perturbation theory

We can now this expression in terms of a perturbative expression in terms of $\hat{H}_I$ where we iterate the last expression in terms of ΔE_0

$$\Delta E_0 = \sum_{i=1}^{\infty} \Delta E_0^{(i)}.$$

We get the following expression for $\Delta E_0^{(i)}$

$$\Delta E_0^{(1)} = \langle \Phi_0 | \hat{H}_I | \Phi_0 \rangle,$$

which is just the contribution to first order in perturbation theory,

$$\Delta E_0^{(2)} = \langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I | \Phi_0 \rangle,$$

which is the contribution to second order.

Rayleigh-Schrödinger perturbation theory

$$\Delta E_0^{(3)} = \langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \Phi_0 \rangle - \langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \langle \Phi_0 | \hat{H}_I | \Phi_0 \rangle \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I | \Phi_0 \rangle,$$

being the third-order contribution. The last term is a so-called unlinked diagram!

Rayleigh-Schrödinger perturbation theory

The fourth order term is

$$\Delta E_0^{(4)} = \langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \Phi_0 \rangle -$$

$$\langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \langle \Phi_0 | \hat{H}_I | \Phi_0 \rangle \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \Phi_0 \rangle$$

$$- \langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \langle \Phi_0 | \hat{H}_I | \Phi_0 \rangle \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \Phi_0 \rangle$$

$$+ \langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \langle \Phi_0 | \hat{H}_I | \Phi_0 \rangle \frac{\hat{Q}}{W_0 - \hat{H}_0} \langle \Phi_0 | \hat{H}_I | \Phi_0 \rangle \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \Phi_0 \rangle -$$

$$\langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \langle \Phi_0 | \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I | \Phi_0 \rangle \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I | \Phi_0 \rangle,$$

Wave Operator I

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

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

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

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

Wave Operator II

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

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

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

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

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

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

Wave Operator III

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

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

or equivalently

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

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

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

where χ is known as the correlation operator.

Wave Operator IV

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

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

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

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

where ε are the unperturbed energies of the P-space

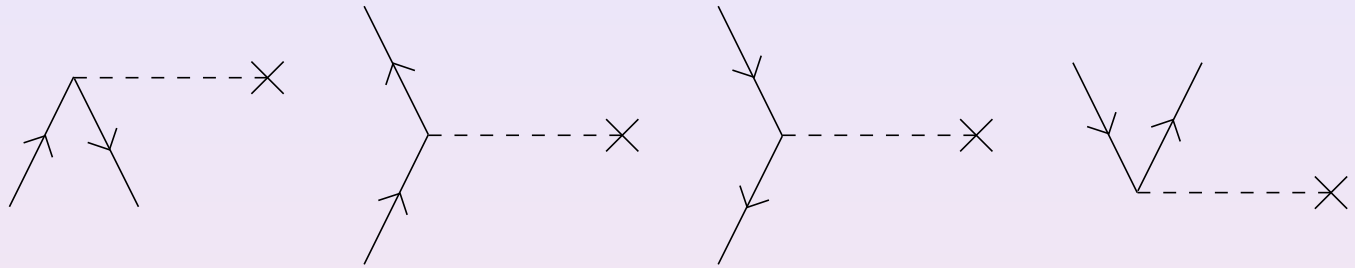
Diagram elements - Directed lines

Figure: Particle line

Figure: Hole line

- Represents a contraction between second quantized operators.
- External lines are connected to one operator vertex and infinity.
- Internal lines are connected to operator vertices in both ends.

Diagram elements - Onebody Hamiltonian



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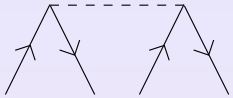
- Horisontal dashed line segment with one vertex.
- Excitation level identify the number of particle/hole pairs created by the operator.

Diagram elements - Twobody Hamiltonian



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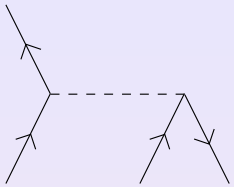

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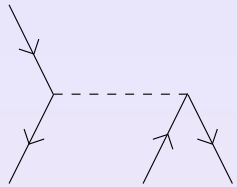

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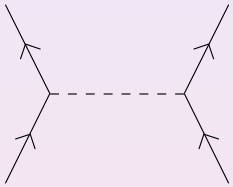

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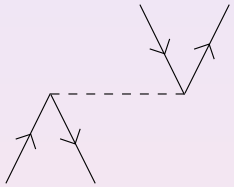

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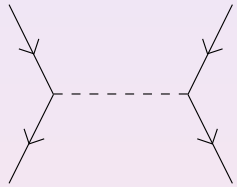

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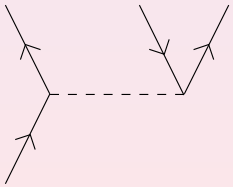

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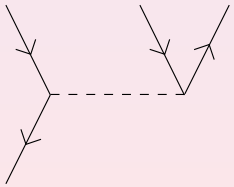

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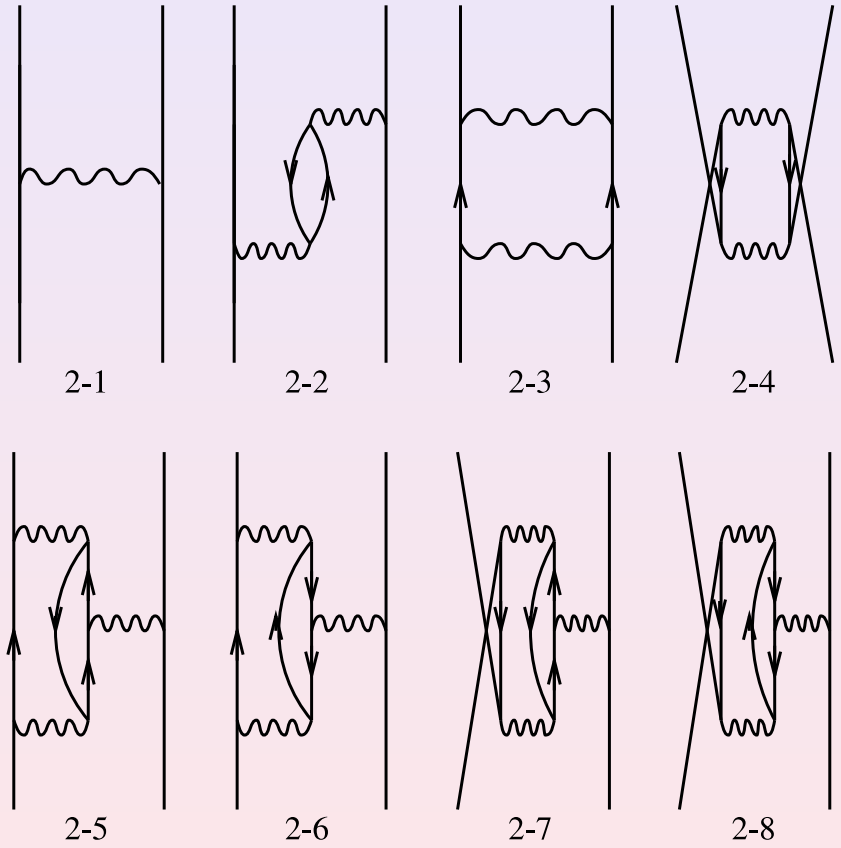
Perturbation Theory

Order by order perturbation theory in terms of the renormalized interaction.



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. Can also study Green's function methods (Parquet class of diagrams).

Reminder of what we typically want to do

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

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

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

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

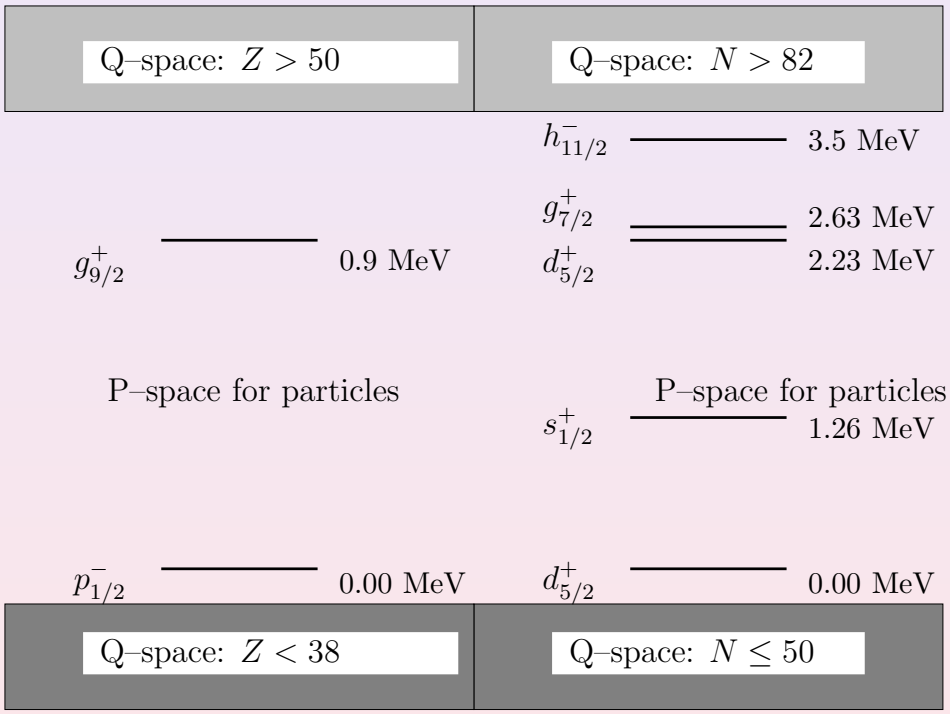
Shell-Model Basics

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

$$\langle \Phi_\lambda | P H_{eff} P | \Phi_{\lambda'} \rangle = E^0_\lambda \delta_{\lambda,\lambda'} + \langle \Phi_\lambda | P (H_I)_{eff} P | \Phi_{\lambda'} \rangle$$

  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 $\Longrightarrow$ 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	$\approx 1.9 \cdot 10^9$

Energy diagonalization of giant matrices: Lanczos iteration
Basic operator

$$\begin{aligned} H &= \text{one-particle} + \text{two–particle} = H_0 + V \\ &= \widetilde{V}(N) \\ &= \sum < j_1 m_1 j_2 m_2 | \widetilde{V}(N) | j_3 m_3 j_4 m_4 > a^{\dagger}_{j_1 m_1} a^{\dagger}_{j_2 m_2} a_{j_4 m_4} a_{j_3 m_3} \end{aligned}$$

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

$$|SD_\nu(N)\rangle = \prod_{(jm)\in\nu} a^\dagger_{jm}|0\rangle, \tag{4.0.11}$$

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

$$|SD\rangle \longrightarrow (\underbrace{00111101010\cdots}_{N1's}), \tag{4.0.12}$$

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 $a^\dagger_\alpha a_\beta$ or $a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta$ 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

$$a^\dagger_\alpha a_\beta,$$

$$a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} a_{\beta_1} a_{\beta_2},$$

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

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

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

for seniority zero,

$$D^\dagger_{JM} = \sum_{j \leq j', m, m'} (1 + \delta_{j,j'})^{-1/2} \beta_{j,j'} \langle jmj'm' \,|JM\rangle \, a^\dagger_{jm} a^\dagger_{j'm'}$$

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

$$\begin{aligned} G(n_1,j_1,n_2,j_2;J,M) &= \left\{D^\dagger_{n_1,j_1}D^\dagger_{n_2,j_2}\right\}_{J.M=0} \\ &= \sum_{\nu_1\ldots\nu_4} g^{JM}_{\nu_1\ldots\nu_4} a^\dagger_{\nu_1}a^\dagger_{\nu_2}a^\dagger_{\nu_3}a^\dagger_{\nu_4} \end{aligned}$$

and a seniority six operator

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

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 $|new_{p+1} >= H|lanc_p >$. 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

$$\langle lanc_p|H|lanc_p\rangle = \langle lanc_p|\ new_{p+1}\rangle\,, \tag{4.0.13}$$

Lanczos Iteration

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

$$|new'_{p+1}\rangle = |new_{p+1}\rangle - |lanc_p\rangle \cdot \langle lanc_p|\ new_{p+1}\rangle - \sum_{q=0}^{p-1} |lanc_q\rangle \cdot \langle lanc_q|\ new_{p+1}\rangle\,, \tag{4.0.14}$$

and finally normalized

$$|lanc_{p+1}\rangle = \frac{1}{\sqrt{\langle new'_{p+1}|\ new'_{p+1}\rangle}} |new'_{p+1}\rangle, \tag{4.0.15}$$

to produce a new Lanczos vector.

Lanczos Iteration

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

$$\langle lanc_{p+1}|H|lanc_p\rangle = \langle new'_{p+1}|\ new'_{p+1}\Big\rangle\,, \tag{4.0.16}$$

and all others are zero.

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

$$\left\{\begin{array}{ccccc} H_{0,0} & H_{0,1} & 0 & \cdots & 0 \\ H_{0,1} & H_{1,1} & H_{1,2} & \cdots & 0 \\ 0 & H_{2,1} & H_{2,2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & H_{p-1,p} \\ 0 & 0 & 0 & H_{p,p-1} & H_{p,p} \end{array}\right\} \tag{4.0.17}$$

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 $|new_{p+1} >= H|lanc_p >$ 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

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

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 ($\geq$ 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 $v = 0$ overlap $|\langle {}^{A}Sn; 0^{+}|(S^{\dagger})^{\frac{n}{2}}|\tilde{0}\rangle|^2$ and the seniority $v = 2$ overlaps $|\langle {}^{A}Sn; J_f|D^{\dagger}_{JM}(S^{\dagger})^{\frac{n}{2}-1}|\tilde{0}\rangle|^2$ for the lowest–lying eigenstates of ${}^{128-120}$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 $^{130-116}$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 $A = 132$, Brown *et al*, PRC 2005

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

Coupled Cluster

The basics

The exponential ansatz

$$|\Psi\rangle \approx |\Psi_{CC}\rangle = e^{\hat{T}}|\Phi_0\rangle = \left(\sum_{i=1}^{\infty} \frac{1}{i!}\hat{T}^i\right)|\Phi_0\rangle$$

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + + + \hat{T}_A$$

$$\hat{T}_1 = \sum_{i,a} t_i^a a_a^\dagger a_i$$

$$\hat{T}_2 = \frac{1}{4}\sum_{i,j,a,b} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$$

$$\hat{T}_n = \left(\frac{1}{n!}\right)^2 \sum_{\substack{i,j,\ldots \\ a,b,\ldots}} t_{ij\ldots}^{ab\ldots} a_a^\dagger a_b^\dagger \ldots a_j a_i$$

CCSD - Coupled Cluster Singles and Doubles

$$\hat{T} = \hat{T}_1 + \hat{T}_2$$

$$|\Psi_{CC}\rangle = e^{\hat{T}_1+\hat{T}_2}|\Phi_0\rangle$$

$$= \left(1 + \hat{T}_1 + \frac{1}{2}\hat{T}_1^2 + \hat{T}_2 + \frac{1}{3!}\hat{T}_1^3 + \hat{T}_1\hat{T}_2 + ++\right)|\Phi_0\rangle$$

CCSD - Coupled Cluster Singles and Doubles

$$\hat{T} = \hat{T}_1 + \hat{T}_2$$
$$|\Psi_{CC}\rangle = e^{\hat{T}_1+\hat{T}_2}|\Phi_0\rangle$$
$$= \left(1 + \hat{T}_1 + \frac{1}{2}\hat{T}_1^2 + \hat{T}_2 + \frac{1}{3!}\hat{T}_1^3 + \hat{T}_1\hat{T}_2 + ++\right)|\Phi_0\rangle$$

CCSDT - Coupled Cluster Singles, Doubles and Triples

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3$$
$$|\Psi_{CC}\rangle = e^{\hat{T}_1+\hat{T}_2+\hat{T}_3}|\Phi_0\rangle$$
$$= \left(1 + \hat{T}_1 + \frac{1}{2}\hat{T}_1^2 + \hat{T}_2 + \frac{1}{3!}\hat{T}_1^3 + \hat{T}_1\hat{T}_2 + \hat{T}_3 + ++\right)|\Phi_0\rangle$$

Coupled Cluster

The basics, Equations

Energy equation

$$\langle \Phi_0 | e^{-\hat{T}} \hat{H} e^{\hat{T}} | \Phi_0 \rangle = E$$

Amplitude equations

$$\langle \Phi_i^a | e^{-\hat{T}} \hat{H} e^{\hat{T}} | \Phi_0 \rangle = 0$$
$$\langle \Phi_{ij}^{ab} | e^{-\hat{T}} \hat{H} e^{\hat{T}} | \Phi_0 \rangle = 0$$
$$\langle \Phi_{ij\ldots}^{ab\ldots} | e^{-\hat{T}} \hat{H} e^{\hat{T}} | \Phi_0 \rangle = 0$$

Note: $\langle \Psi | \neq \langle \Phi_0 | e^{-\hat{T}}$, $e^{-\hat{T}} \neq (e^{\hat{T}})^\dagger$.