Nuclear ab initio methods

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December 16, 2021

Overview

Ab initio Many-Body Methods in Nuclear Physics

(personal statement)

- describe the atomic nucleus from the bottom up with (systematically improvable) bare nuclear forces compatible with the symmetries of QCD
- solve the quantum mechanical many-body problem for all constituent nucleons either exactly for very light nuclei or by employing certain well-controlled approximations for heavier nuclei.

Nuclear forces

- Short-range repulsion (hard core)
- Strong coupling of high- and low-momenta states

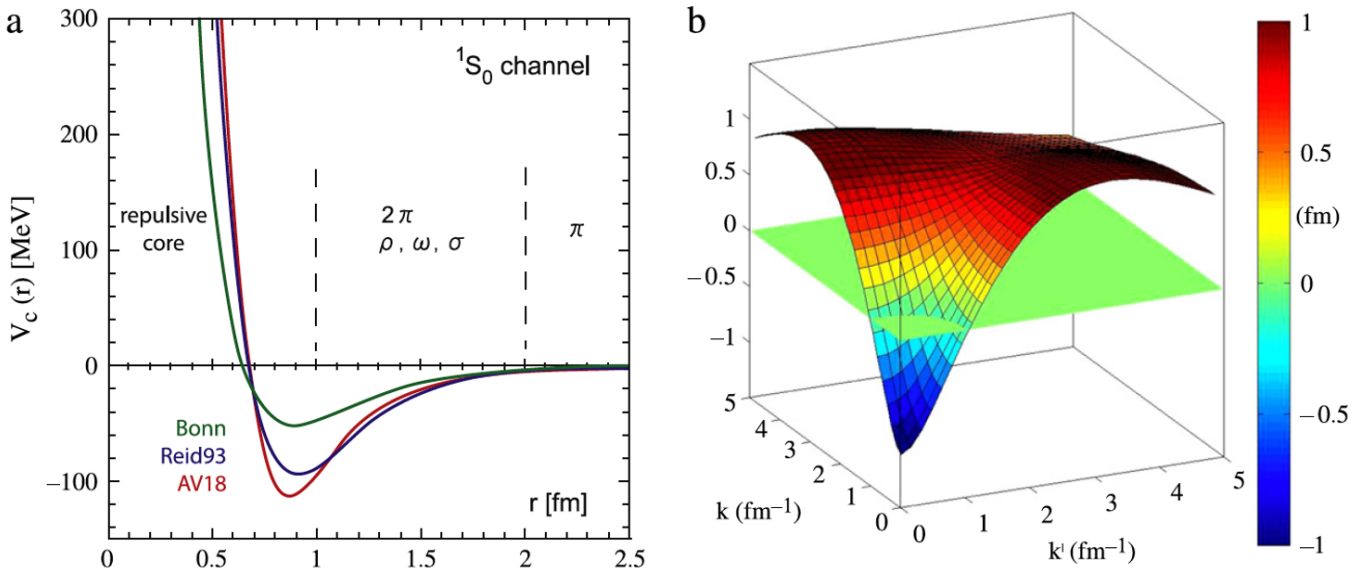


Figure: Several phenomenological NN potentials in the $^1S_0$ channel and momentum space matrix elements of the Argonne v18 (AV18).

S.K. Bogner et al. Prog. Part. Nucl. Phys. 65 (2010) 94.

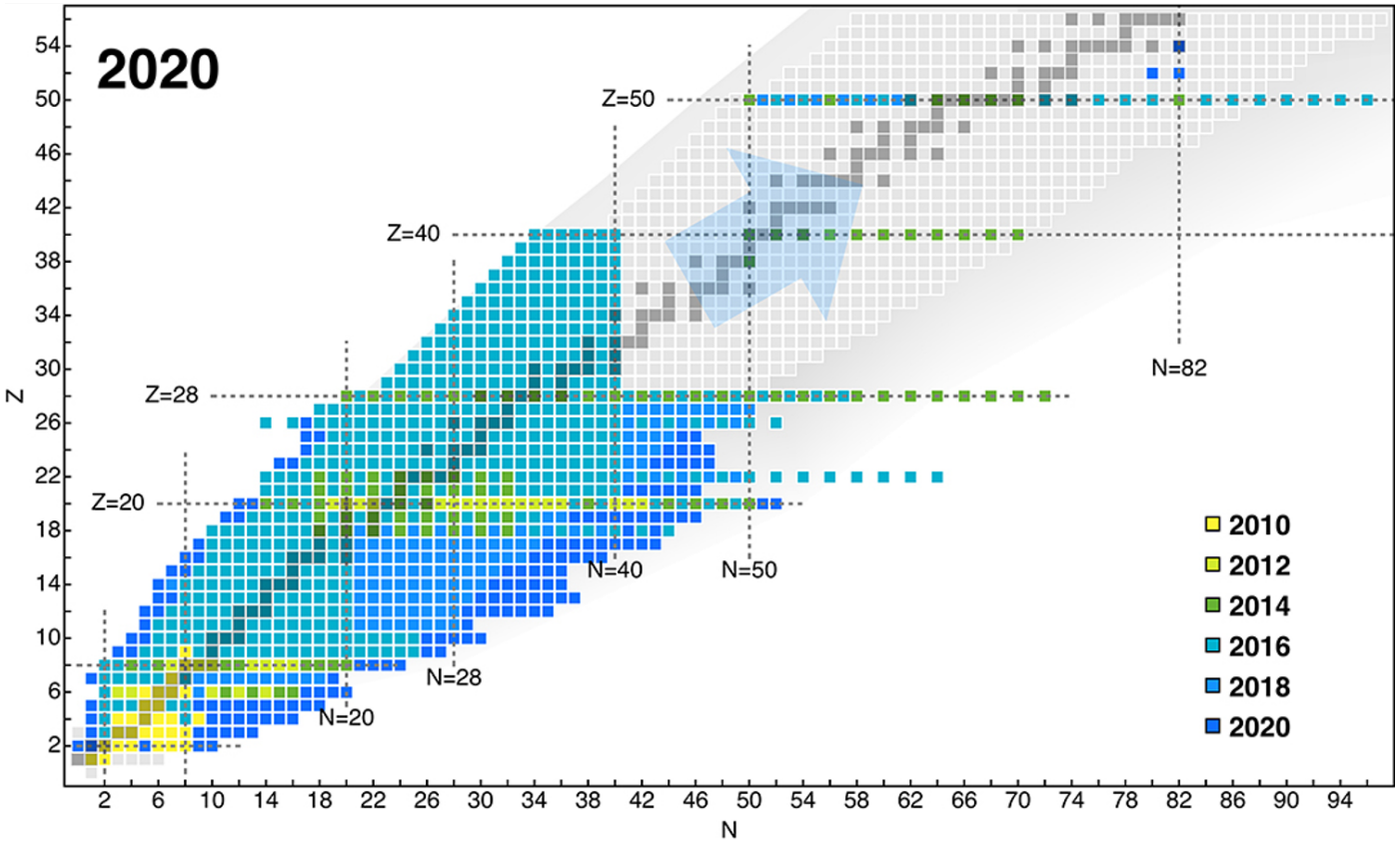
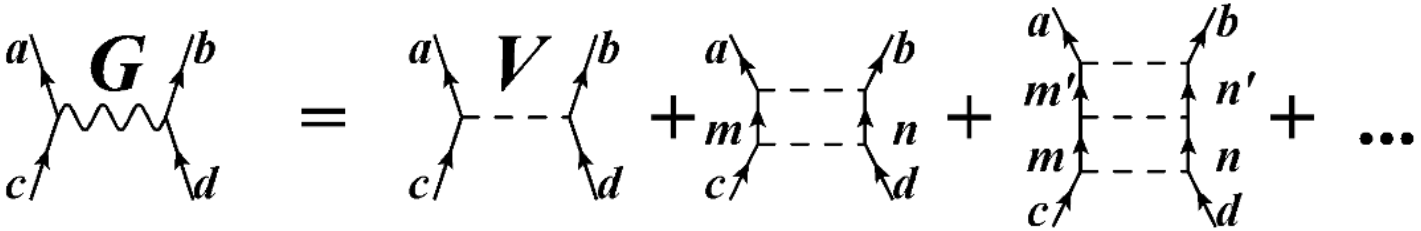


Figure: H. Hergert, Front. Phys. (2020)

The G matrix is given by:

$$\langle ab|G(W)|cd\rangle = \langle ab|V|cd\rangle + \sum_{mn}\langle ab|V|mn\rangle \frac{Q(m,n)}{W-\varepsilon_m-\varepsilon_n}\langle mn|G(W)|cd\rangle$$



- W is the starting energy (parameter). In many cases, one chooses $W = \varepsilon_a + \varepsilon_b$.
- ϵ_m, ϵ_n are the HF single-particle energies.
- Q is the Pauli operator which forbids the states being scattered below Fermi surface.

K. Brueckner, C. Levinson, H. Mahmoud, Phys. Rev. 95, 217 (1954)

- The HF equation is given by:

$$\sum_j (T+U)_{ij} D_{ja} = \varepsilon_a D_{ia},$$

where the one-body mean-field potential is

$$U_{ij} = \sum_{c=1}^{A} \langle ic|\bar{G}(W)|jc\rangle.$$

Rel. BHF: S.H. Shen et al., Prog. Part. Nucl. Phys. 109, 103713 (2019).

Procedure of the (R)BHF calculation

1. Initial single-particle basis $\{|i\rangle\}$ trial for RBHF final solution $\{|a\rangle\}$.

2. Bethe-Goldstone equation $\bar{G}_{aba'b'}(W) = \bar{V}_{aba'b'} + \frac{1}{2}\sum_{cd} \frac{\bar{V}_{abcd}Q(c,d)}{W - \varepsilon_c - \varepsilon_d}\bar{G}_{cda'b'}(W),$
   Solving with matrix inversion method
   M. Haftel and F. Tabakin, *NPA* **158**, 1 (1970)

3. Single-particle potential $U_{ab} = \sum_{c=1}^{A} \langle ac|\bar{G}(W)|bc\rangle.$

4. RHF iteration $\sum_j (T_{ij} + U_{ij})\, D_{ji'} = \varepsilon_{i'} D_{ii'},$

   If converged $\{|i'\rangle\} = \{|i\rangle\} = \{|a\rangle\}$, RBHF iteration finishes.

5. Basis transformation $\bar{V}_{k'l'm'n'} = \sum_{klmn} D^*_{kk'} D^*_{ll'} D_{mm'} D_{nn'} \bar{V}_{klmn}.$
   Go back to step 2.

Stolen from J. Meng's talk.

- All A nucleons are considered active.
- The nuclear wave function in the FCI is expanded in a set of Slater determinant basis functions,

$$|\Psi^{(\mathrm{FCI})}\rangle = \sum_k C_k |\Phi_k\rangle$$

where the many-body basis $|\Phi_k\rangle$ consists of all Slater determinants constructed from the single-particle basis set

$$\left\{ |\Phi_k\rangle = \hat{\mathcal{A}} \left(\phi_{k_1} \dots \phi_{k_A} \right) \right\}.$$

- The expansion coefficients are obtained from a large-scale Hamiltonian matrix diagonalization.

$$\sum_l H_{kl} C_l = E C_k, \quad H_{kl} = \langle \Phi_k | H | \Phi_l \rangle$$

- Starting from a reference state

$$|\Phi_0\rangle = \hat{\mathcal{A}}\left(\phi_{i_1} \dots \phi_{i_A}\right)$$

which is a single Slater determinant build from the set of single-particle orbitals that minimize the energy functional $E_{\mathrm{ref}}[\phi_{i_1}, \dots, \phi_{i_A}]$, such as a HF state.

- The FCI wave function can be parametrized by the linear ansatz

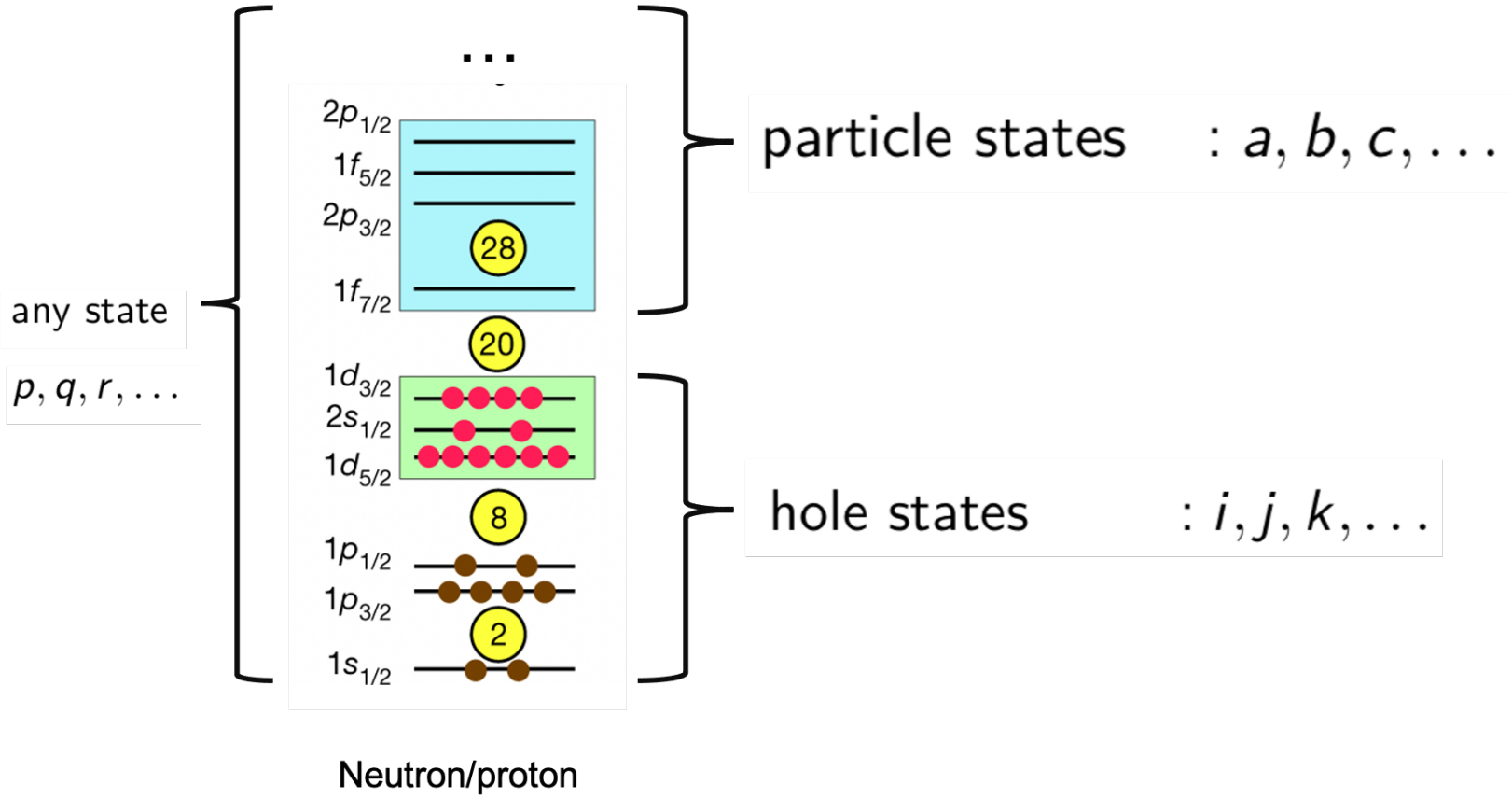
$$|\Psi^{(\mathrm{FCI})}\rangle = \left(1 + \hat{C}^{(\mathrm{FCI})}\right)|\Phi_0\rangle, \quad \hat{C}^{(\mathrm{FCI})} = \sum_{n=1}^{A} \hat{C}_n^{(\mathrm{FCI})}$$

where the $np - nh$ excitation operator generating all possible $np - nh$ excitations reads

$$\hat{C}_n = \frac{1}{(n!)^2} \sum_{\substack{i_1, i_n \\ a_1, \dots, a_n}} c_{i_1, \dots i_n}^{a_1, a_n} \hat{a}_{a_1}^{\dagger} \dots \hat{a}_{a_n}^{\dagger} \hat{a}_{i_n} \dots \hat{a}_{i_1}.$$

The orbitals occupied by the reference state (referred to as hole states) and the unoccupied (particle) states

hole states : $i, j, k, \ldots \in$ occupied in $|\Phi\rangle$
particle states : $a, b, c, \ldots \in$ unoccupied in $|\Phi\rangle$
any state : $p, q, r, \ldots$



Dimension of model space

- N neutrons distributed among n single-particle states

$$\left(\begin{array}{c} n \\ N \end{array} \right) = \frac{n!}{(n-N)!N!}.$$

As an example, for a model space which comprises the first 4 major harmonic oscillator shells only ($0s, 0p, 1s, 0d$ and $1p, 0f$ shells), we have 40 single particle states for neutrons and protons. For ^{16}O,

$$\left(\begin{array}{c} 40 \\ 8 \end{array} \right) = \frac{40!}{(32)!8!} \sim 8 \times 10^7,$$

possible Slater determinants. Multiplying this with the number of proton Slater determinants gives $d \sim 10^{15}$ possible Slater determinants and a Hamiltonian matrix of dimension $10^{15} \times 10^{15}$.

In practical calculation, the wave function is truncated up to the $Mp - Mh$ and the FCI in this case is called CIM

$$\hat{C}^{(\mathrm{FCI})} \simeq \sum_{n=1}^{M} \hat{C}_n^{(\mathrm{CIM})}$$

and

$$\hat{H}\left(1 + \sum_{n=1}^{M} \hat{C}_n^{(\mathrm{CIM})}\right)|\Phi_0\rangle = E^{(\mathrm{CIM})}\left(1 + \sum_{n=1}^{M} \hat{C}_n^{(\mathrm{CIM})}\right)|\Phi_0\rangle$$

A set of coupled equations are obtained for the energy $E^{(\mathrm{CIM})}$ and the amplitudes $c_{i_1,\ldots 1_k}^{a_1\cdots a_k}$ by left-projecting the CIM Schrödinger equation onto the reference $\left|\Phi\right\rangle$ and excited determinants $\left|\Phi_{i_1,\ldots i_k}^{a_1\cdots a_k}\right\rangle$,

$$\begin{aligned}
\left\langle \Phi_0 \left| \hat{H} \left(1 + \sum_{n=1}^{M} \hat{C}_n^{(\mathrm{CIM})} \right) \right| \Phi_0 \right\rangle &= E^{(\mathrm{CIM})} \\
\left\langle \Phi_{i_1}^{a_1} \left| \hat{H} \left(1 + \sum_{n=1}^{M} \hat{C}_n^{(\mathrm{CIM})} \right) \right| \Phi_0 \right\rangle &= E^{(\mathrm{CIM})} c_{i_1}^{a_1} \quad , \forall a_1, i_1 \\
\left\langle \Phi_{i_1\ldots i_M}^{a_1\cdots a_M} \left| \hat{H} \left(1 + \sum_{n=1}^{M} \hat{C}_n^{(\mathrm{CIM})} \right) \right| \Phi_0 \right\rangle &= E^{(\mathrm{CIM})} c_{i_1\ldots i_M}^{a_1\cdots a_M} \quad , \forall a_1, \ldots, i_M
\end{aligned}$$

where $np-nh$ excitation $\left|\Phi_{i_1,\ldots i_n}^{a_1\cdots a_n}\right\rangle$ of the reference determinant is defined as the Slater determinant in which, relative to the reference state $|\Phi\rangle$, n hole states have been replaced by n particle states, i.e.,

$$\begin{aligned}\left|\Phi_{i_1,\ldots i_n}^{a_1,a_n}\right\rangle &= \left(\hat{a}_{a_1}^{\dagger}\hat{a}_{i_1}\right)\left(\hat{a}_{a_2}^{\dagger}\hat{a}_{i_2}\right)\ldots\left(\hat{a}_{a_n}^{\dagger}\hat{a}_{i_n}\right)|\Phi_0\rangle \\ &= \hat{a}_{a_1}^{\dagger}\ldots\hat{a}_{a_n}^{+}\hat{a}_{i_n}\ldots\hat{a}_{i_1}|\Phi_0\rangle\end{aligned}$$

The eigenvalue equation reads,

$$\sum_{I} \left(H_{kI} - E\delta_{kI} \right) C_I = 0$$

If the configurations are truncated up to 2p-2h, one has

- $k = 0$: $\langle \Phi_k | = \langle \Phi_0 |$,

$$\left\langle \Phi_0 | \hat{H} - E | \Phi_0 \right\rangle + \sum_{ai} \left\langle \Phi_0 | \hat{H} - E | \Phi_i^a \right\rangle C_i^a + \sum_{abij} \left\langle \Phi_0 | \hat{H} - E | \Phi_{ij}^{ab} \right\rangle C_{ij}^{ab} = 0$$

or

$$E - E_{\text{Ref}} = \Delta E = \sum_{ai} \left\langle \Phi_0 | \hat{H} | \Phi_i^a \right\rangle C_i^a + \sum_{abij} \left\langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \right\rangle C_{ij}^{ab},$$

where the energy E_{Ref} is the reference energy and ΔE defines the so-called correlation energy.

For the HF reference state we have already computed the matrix $\left\langle \Phi_0 | \hat{H} | \Phi_i^a \right\rangle$ and $\left\langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \right\rangle$.

$$\left\langle \Phi_0 | \hat{H} | \Phi_i^a \right\rangle = 0$$

and we are left with a correlation energy given by

$$E - E_{\mathrm{Ref}} = \Delta E^{HF} = \sum_{abij} \left\langle \Phi_0 | \hat{H} | \Phi_{ij}^{ab} \right\rangle C_{ij}^{ab}$$

Inserting the various matrix elements we can rewrite the previous equation as

$$\Delta E = \sum_{ai} \langle i | \hat{f} | a \rangle C_i^a + \sum_{abij} \langle ij | \hat{v} | ab \rangle C_{ij}^{ab}$$

- $k = 1$: $\langle \Phi_k | = \langle \Phi_i^a |$,

$$\left\langle \Phi_i^a | \hat{H} - E | \Phi_0 \right\rangle + \sum_{bj} \left\langle \Phi_i^a | \hat{H} - E | \Phi_j^b \right\rangle C_j^b + \sum_{bcjk} \left\langle \Phi_i^a | \hat{H} - E | \Phi_{jk}^{bc} \right\rangle C_{jk}^{bc} + \sum_{bcdjkl} \left\langle \Phi_i^a | \hat{H} - E | \Phi_{jkl}^{bcd} \right\rangle C_{jkl}^{bcd} = 0 \quad (1)$$

Substituting the expression of H in normal-ordering form

$$\hat{H} = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle + \sum_{pq} f_q^p \left\{ \hat{a}_p^\dagger \hat{a}_q \right\} + \frac{1}{4} \sum_{pqrs} v_{rs}^{pq} \left\{ \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r \right\} \quad (2)$$

one finds an expression for the coefficients C_i^a through

$$f_i^a + \left\langle \Phi_i^a | \hat{H} | \Phi_i^a \right\rangle C_i^a - E C_i^a + \sum_{bj \neq ai} \left\langle \Phi_i^a | \hat{H} | \Phi_j^b \right\rangle C_j^b + \sum_{bcjk} \left\langle \Phi_i^a | \hat{H} | \Phi_{jk}^{bc} \right\rangle C_{jk}^{bc} + \sum_{bcdjkl} \left\langle \Phi_i^a | \hat{H} | \Phi_{jkl}^{bcd} \right\rangle C_{jkl}^{bcd} = 0 \quad (3)$$

The above equations are normally solved iteratively, that is we start with a guess for the coefficients C_i^a . A common choice is to use perturbation theory as a starting point for the unknown coefficients. Replacing $\left\langle \Phi_i^a | \hat{H} | \Phi_i^a \right\rangle$ with $E + \epsilon_a - \epsilon_i$, and setting the right three terms to be zero, one finds the 1p-1h coefficient

$$C_i^a = \frac{f_i^a}{\epsilon_i - \epsilon_a}, \quad f_i^a = f_a^i \tag{4}$$

Similarly, one obtains an equation for C_{jk}^{bc},

$$\begin{aligned} 0 = & \left\langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_0 \right\rangle + \sum_{kc} \left\langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_k^c \right\rangle C_k^c \\ & + \sum_{cdkl} \left\langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{kl}^{cd} \right\rangle C_{kl}^{cd} + \sum_{cdeklm} \left\langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{klm}^{cde} \right\rangle C_{klm}^{cde} \\ & + \sum_{cdefklmn} \left\langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{klmn}^{cdef} \right\rangle C_{klmn}^{cdef}. \end{aligned}$$

One can isolate the coefficients C_{kl}^{cd} in a similar way as we did for the coefficients C_i^a. A standard choice for the first iteration is to use again perturbation theory to first order in the interaction and set

$$C_{ij}^{ab} = \frac{\langle ij|\hat{v}|ab\rangle}{\epsilon_i + \epsilon_i - \epsilon_a - \epsilon_b} \tag{5}$$

NCSM: truncation not at excitation rank but rather on excitation energy of a Slater determinant relative to the unperturbed reference state is defined by

$$e_{i_1 \ldots i_n}^{a_1 \ldots a_n} \equiv \sum_{k=1}^{n} \left(e_{a_k} - e_{i_k} \right),$$

then the NCSM again uses a linear parametrization of the wave function similar to the FCI parametrization,

$$\left| \Psi^{(\mathrm{NCSM})} \right\rangle = \left(1 + \sum_{n=1}^{A} \hat{C}_n^{(\mathrm{NCSM})} \right) |\Phi\rangle,$$

with excitation operators

$$\hat{C}_n^{(\mathrm{NCSM})} = \frac{1}{(n!)^2} \sum_{\substack{i_1, \ldots, i_n \\ a_1, \ldots, a_n}}{}' c_{i_1, \ldots i_n}^{a_1 \ldots a_n} \hat{a}_{a_1}^{\dagger} \ldots \hat{a}_{a_n}^{\dagger} \hat{a}_{i_n} \ldots \hat{a}_{i_1}$$

where the summations

$$\sum_{\substack{i_1,\ldots,i_n \\ a_1,\ldots,a_n}}{}'$$

are constrained to maximum excitation energies, generated by the operator string $\hat{a}^\dagger_{a_1} \ldots \hat{a}^\dagger_{a_n} \hat{a}_{i_n} \ldots \hat{a}_{i_1}$ acting on the reference state, according to

$$e^{a_1 \ldots a_n}_{i_1 \ldots i_n} \leq N_{\max}.$$

This $N_{\max}$ truncation is of particular significance in NCSM calculations using a harmonic-oscillator basis, since despite of the use of single-particle coordinates this truncation allows for any choice of $N_{\max}$ an exact factorization of the NCSM wavefunction into a center-of-mass and a relative part,

$$\left|\Psi^{(\mathrm{NCSM})}\right\rangle = \left|\Psi_{\mathrm{int}}\right\rangle \otimes \left|\Psi_{\mathrm{CM}}\right\rangle ,$$

The Exponential Ansatz

- The wave function is constructed as

$$|\Psi\rangle = e^{\hat{T}}|\Phi\rangle, \quad \hat{T} = \sum_{n=1}^{A} \hat{T}_n$$

where the cluster operator $\hat{T}$ is defined in close analogy to the CI case.

$$\hat{T}_1 = \quad = \frac{1}{(1!)^2} \sum_{ai} t_i^a \{\hat{a}_a^\dagger \hat{a}_i\}$$

$$\hat{T}_2 = \quad = \frac{1}{(2!)^2} \sum_{abij} t_{ij}^{ab} \{\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i\}$$

$$\vdots$$

$$\hat{T}_n = \quad = \frac{1}{(n!)^2} \sum_{\substack{a_1 \ldots a_n \\ i_1 \ldots i_n}} t_{i_1 \ldots i_n}^{a_1 \ldots a_n} \{\hat{a}_{a_1}^\dagger \ldots \hat{a}_{a_n}^\dagger \hat{a}_{i_n} \ldots \hat{a}_{i_1}\} .$$

By definition, the expectation values of normal-ordered operator products in the reference state, which serves as new vacuum, vanish

$$\left\langle \Phi \left| \left\{ \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i \right\} \right| \Phi \right\rangle = \left\langle \Phi \mid \Phi_{ij}^{ab} \right\rangle = 0.$$

The Hamiltonian operator can be rewritten in normal-ordering form

$$\begin{aligned} \hat{H} &= h_0 + \sum_{pq} \left\langle p \left| \hat{h}_1 \right| q \right\rangle \hat{a}_p^\dagger \hat{a}_q + \frac{1}{4} \sum_{pqrs} \left\langle pq \left| \hat{h}_2 \right| rs \right\rangle \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r \\ &= \langle \Phi | \hat{H} | \Phi \rangle + \sum_{pq} f_q^p \left\{ \hat{a}_p^\dagger \hat{a}_q \right\} + \frac{1}{4} \sum_{pqrs} v_{rs}^{pq} \left\{ \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r \right\} \\ &\equiv \langle \Phi | \hat{H} | \Phi \rangle + \hat{F}_N + \hat{V}_N \end{aligned} \tag{6}$$

The matrix elements are given by

$$\langle \Phi | \hat{H} | \Phi \rangle = h_0 + \sum_i \left\langle i \left| \hat{h}_1 \right| i \right\rangle + \frac{1}{2} \sum_{ij} \left\langle ij \left| \hat{h}_2 \right| ij \right\rangle \tag{7}$$

$$f_q^p \equiv \langle p | \hat{f} | q \rangle = \left\langle p \left| \hat{h}_1 \right| q \right\rangle + \sum_i \left\langle pi \left| \hat{h}_2 \right| qi \right\rangle \tag{8}$$

$$v_{rs}^{pq} \equiv \langle pq | \hat{v} | rs \rangle = \left\langle pq \left| \hat{h}_2 \right| rs \right\rangle \tag{9}$$

Using the normal-ordered Hamiltonian,

$$\hat{H}_N = \hat{H} - \langle\Phi|\hat{H}|\Phi\rangle,$$

and after subtracting the zero-body contribution, the Schrödinger equation can be written in the form

$$\hat{H}_N e^{\hat{T}}|\Phi\rangle = \Delta E e^{\hat{T}}|\Phi\rangle,$$

in which the quantity

$$\Delta E \equiv E - \langle\Phi|\hat{H}|\Phi\rangle$$

is called the correlation energy. Since $\langle\Phi|\hat{H}|\Phi\rangle$ is the expectation value of the Hamiltonian in the reference state, it is also referred to as reference energy E_{ref} ,

$$E_{\text{ref}} \equiv \langle\Phi|\hat{H}|\Phi\rangle.$$

The total energy is a sum of reference and correlation energy. By left-multiplication with $e^{-\hat{T}}$, arriving at

$$\hat{\mathcal{H}}|\Phi\rangle = \Delta E|\Phi\rangle,$$

where the (normal-ordered) Coupled-Cluster effective Hamiltonian $\hat{\mathcal{H}}$ is defined as

$$\hat{\mathcal{H}} \equiv e^{-\hat{T}} \hat{H}_N e^{\hat{T}}.$$

The above form of the Schrödinger equation is of particular importance and will be the starting point for the derivation of the Coupled-Cluster equations.

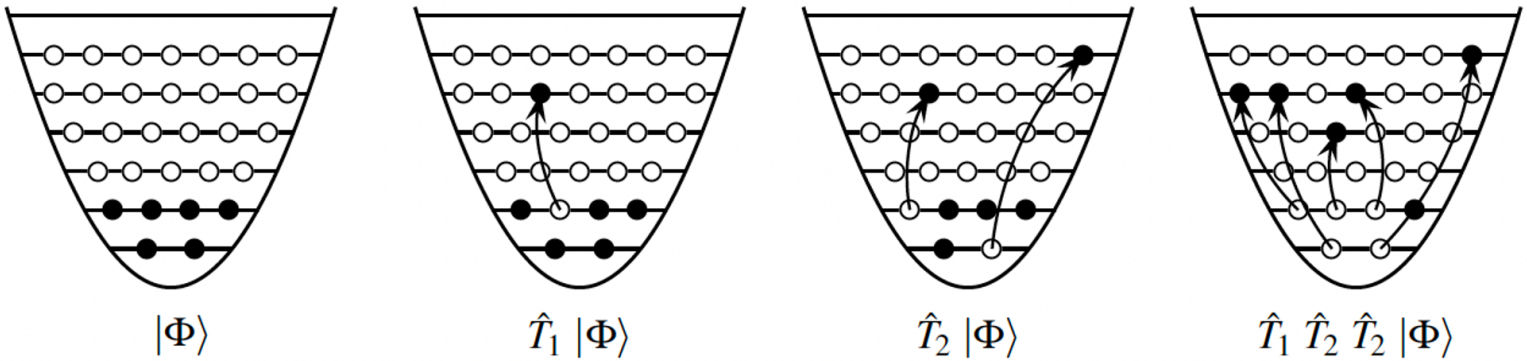
Since $\hat{T}^\dagger \neq -\hat{T}$, the transformation $e^{\hat{T}}$ is not unitary, and thus $\mathcal{H}$ is not Hermitian. The transformation is, however, a similarity transformation (also referred to as similarity transformed Schrödinger equation) and, therefore, the spectrum of the original Hamiltonian is not altered.

Coupled-Cluster method (CCM)

In this method, the cluster operator is truncated to some excitation rank M ,

$$\hat{T}^{(M)} = \sum_{n=1}^{M} \hat{T}_n.$$

For $M = 2$, it is called *CCSD*, and so on. Due to its nonlinear nature, the Coupled-Cluster Ansatz allows to generate higher-order excitations from products of lower-order excitation operators.



For a truncated CCM with the cluster operator

$$\hat{T} \approx \hat{T}^{(\mathrm{M})} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_M$$

the expression for the correlation energy $\Delta E^{(\mathrm{M})} = \Delta E\left(\boldsymbol{t}^{(\mathrm{M})}\right)$ as function of the cluster amplitudes

$$\boldsymbol{t}^{(M)} \equiv \left\{\left\{t_i^a\right\}, \left\{t_{ij}^{ab}\right\}, \ldots, \left\{t_{i_1,\ldots,i_M}^{a_1,a_M}\right\}\right\},$$

can be derived by left-projecting the similarity-transformed Schrödinger equation

$$\hat{\mathcal{H}}^{(\mathrm{M})}|\Phi\rangle = \Delta E^{(\mathrm{M})}|\Phi\rangle$$

with

$$\hat{\mathcal{H}}^{(\mathrm{M})} \equiv e^{-\hat{T}^{(\mathrm{M})}} \hat{H}_N e^{\hat{T}^{(\mathrm{M})}}$$

onto the reference state.

A coupled set of algebraic equations for the determination of the amplitudes $t^{(\mathrm{M})}$ is obtained by left-projecting the similarity-transformed Schrödinger equation onto the excited determinants $\left|\Phi_{i_1,\ldots i_n}^{a_1\cdots a_n}\right\rangle$ with $n \leq M$, i.e.,

$$\left\langle \Phi \left| \hat{\mathcal{H}}^{(\mathrm{M})} \right| \Phi \right\rangle = \Delta E^{(\mathrm{M})} \tag{10}$$

$$\left\langle \Phi_i^a \left| \hat{\mathcal{H}}^{(\mathrm{M})} \right| \Phi \right\rangle = 0, \quad \forall a, i \tag{11}$$

$$\left\langle \Phi_{ij}^{ab} \left| \hat{\mathcal{H}}^{(\mathrm{M})} \right| \Phi \right\rangle = 0, \quad \forall a, b, i, j \tag{12}$$

$$\vdots \tag{13}$$

$$\left\langle \Phi_{i_1,\ldots M}^{a_1,\cdots M} \left| \hat{\mathcal{H}}^{(\mathrm{M})} \right| \Phi \right\rangle = 0, \quad \forall a_1, \ldots, a_M, i_1, \ldots, i_M. \tag{14}$$

In the case of CCSD, for example, the $\hat{T}_1$ and $\hat{T}_2$ amplitudes can be determined by solving the system of the first three equations.

The effective Hamiltonian $\hat{\mathcal{H}}^{(\mathrm{M})}$ in case of two-body Hamiltonians actually terminates at finite expansion order due to $\hat{T}^{(\mathrm{M})}$ being an excitation operator

$$\begin{aligned}\hat{\mathcal{H}}^{(\mathrm{M})} = \hat{H}_N &+ \frac{1}{1!}\left[\hat{H}_N, \hat{T}^{(\mathrm{M})}\right] \\ &+ \frac{1}{2!}\left[\left[\hat{H}_N, \hat{T}^{(\mathrm{M})}\right], \hat{T}^{(\mathrm{M})}\right] \\ &+ \frac{1}{3!}\left[\left[\left[\hat{H}_N, \hat{T}^{(\mathrm{M})}\right], \hat{T}^{(\mathrm{M})}\right], \hat{T}^{(\mathrm{M})}\right] \\ &+ \frac{1}{4!}\left[\left[\left[\left[\hat{H}_N, \hat{T}^{(\mathrm{M})}\right], \hat{T}^{(\mathrm{M})}\right], \hat{T}^{(\mathrm{M})}\right], \hat{T}^{(\mathrm{M})}\right]. \qquad (15)\end{aligned}$$

Let's approximate the cluster operator $\hat{T}$ by including only $2p-2h$ correlations. This leads to the so-called CCD approximation, that is

$$\hat{T} \approx \hat{T}_2 = \frac{1}{4}\sum_{abij} t_{ij}^{ab}\{a_a^\dagger a_b^\dagger a_j a_i\},$$

meaning that we have

$$|\Psi_0\rangle \approx |\Psi_{CCD}\rangle = \exp\left(\hat{T}_2\right)|\Phi_0\rangle\,.$$

Inserting these equations in the expression for the computation of the energy we have, with a Hamiltonian defined with respect to a general reference vacuum

$$\hat{H} = \hat{H}_N + E_{\rm ref},$$

with

$$\hat{H}_N = \sum_{pq}\langle p|\hat{f}|q\rangle\{a_p^\dagger a_q\} + \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle\{a_p^\dagger a_q^\dagger a_s a_r\}.$$

Considering the fact that

$$\left\langle \Phi_0 \left| \hat{T}_2 \hat{H}_N \right| \Phi_0 \right\rangle = 0,$$

and the $\hat{H}_N$ is truncated up to normal-ordered two-body term, so that

$$\left\langle \Phi_0 \left| \hat{H}_N (\hat{T}_2)^2 \right| \Phi_0 \right\rangle = 0,$$

the energy in the CCD can be written as

$$\left\langle \Phi_0 \left| \exp\left(-\hat{T}_2\right) \hat{H}_N \exp\left(\hat{T}_2\right) \right| \Phi_0 \right\rangle = \left\langle \Phi_0 \left| \hat{H}_N \left(1 + \hat{T}_2\right) \right| \Phi_0 \right\rangle = E_{CCD}.$$

This quantity becomes

$$E_{\mathrm{CCD}} = E_{\mathrm{ref}} + \frac{1}{4} \sum_{abij} \langle ij|\hat{v}|ab\rangle t_{ij}^{ab},$$

The unknown amplitudes t_{ij}^{ab} is determined by

$$\left\langle \Phi_{ij}^{ab} \left| \exp\left(-\hat{T}_2\right) \hat{H}_N \exp\left(\hat{T}_2\right) \right| \Phi_0 \right\rangle = 0.$$

These equations can be reduced to (after several applications of Wick's theorem), for all $i > j$ and all $a > b$,

$$\begin{aligned} 0 =& \langle ab|\hat{v}|ij\rangle + \left(\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j\right) t_{ij}^{ab} + \frac{1}{2}\sum_{cd} \langle ab|\hat{v}|cd\rangle t_{ij}^{cd} + \frac{1}{2}\sum_{kl} \langle kl|\hat{v}|ij\rangle t_{kl}^{ab} \\ &+ \hat{P}(ij \mid ab) \sum_{kc} \langle kb|\hat{v}|cj\rangle t_{ik}^{ac} + \frac{1}{4}\sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{ij}^{cd} t_{kl}^{ab} + \hat{P}(ij) \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{ik}^{ac} t_{jl}^{bd} \\ &- \frac{1}{2}\hat{P}(ij) \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{ik}^{dc} t_{lj}^{ab} - \frac{1}{2}\hat{P}(ab) \sum_{klcd} \langle kl|\hat{v}|cd\rangle t_{lk}^{ac} t_{ij}^{db} \end{aligned}$$

where we have defined $\hat{P}(ab) = 1 - \hat{P}_{ab}$, and $\hat{P}_{ab}$ interchanges two particles occupying the quantum numbers a and b. The operator $\hat{P}(ij \mid ab)$ is defined as

$$\hat{P}(ij \mid ab) = \left(1 - \hat{P}_{ij}\right)\left(1 - \hat{P}_{ab}\right).$$

The single-particle energies ϵ_p are normally taken to be Hartree-Fock single-particle energies. Recall also that the unknown amplitudes t_{ij}^{ab} represent anti-symmetrized matrix elements, meaning that they obey the same symmetry relations as the two-body interaction, that is

$$t_{ij}^{ab} = -t_{ji}^{ab} = -t_{ij}^{ba} = t_{ji}^{ba}.$$

The two-body matrix elements are also anti-symmetrized, meaning that

$$\langle ab|\hat{v}|ij\rangle = -\langle ab|\hat{v}|ji\rangle = -\langle ba|\hat{v}|ij\rangle = \langle ba|\hat{v}|ji\rangle.$$

The non-linear equations for the unknown amplitudes t_{ij}^{ab} are solved iteratively. We discuss the implementation of these equations below.

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A simple case: CCD

Iterative solvers need a guess for the amplitudes. A good starting point is to use the correlated wave operator from perturbation theory to first order in the interaction. This means that we define the zeroth approximation to the amplitudes as

$$(t_{ij}^{ab})^{(0)} = \frac{\langle ab|\hat{v}|ij\rangle}{\left(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b\right)},$$

leading to our first approximation for the correlation energy at the CCD level to be equal to second-order perturbation theory without $1p-1h$ excitations, namely

$$\Delta E_{\mathrm{CCD}}^{(0)} = \frac{1}{4}\sum_{abij}\langle ij|\hat{v}|ab\rangle (t_{ij}^{ab})^{(0)} = \frac{1}{4}\sum_{abij}\frac{\langle ij|\hat{v}|ab\rangle\langle ab|\hat{v}|ij\rangle}{\left(\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b\right)}.$$

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Before we attack the full equations, it is however instructive to study a truncated version of the equations.
We will first study the following approximation where we take away all terms except the linear terms that involve the single-particle energies and the two-particle intermediate excitations, that is

$$0 = \langle ab|\hat{v}|ij\rangle + (\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j)\, t_{ij}^{ab} + \frac{1}{2}\sum_{cd}\langle ab|\hat{v}|cd\rangle\, t_{ij}^{cd} \qquad (16)$$

Setting the single-particle energies for the hole states equal to an energy variable $\omega = \epsilon_i + \epsilon_j$, the above equation reduces to the equations for the so-called G-matrix.

Defining an energy-dependent quantity

$$\tau_{ij}^{ab}(\omega) = (\omega - \epsilon_a - \epsilon_b) t_{ij}^{ab},$$

and inserting the identity

$$1 = \frac{\omega - \epsilon_c - \epsilon_d}{\omega - \epsilon_c - \epsilon_d}$$

the previous equation (16) becomes

$$\tau_{ij}^{ab}(\omega) = \langle ab|\hat{v}|ij\rangle + \frac{1}{2}\sum_{cd}\langle ab|\hat{v}|cd\rangle \frac{1}{\omega - \epsilon_c - \epsilon_d}\tau_{ij}^{cd}(\omega)$$

This equation, transforming a two-particle configuration into a single index, can be rewritten as a matrix inversion problem. It can be solved by iteration. Solving the equations for a fixed energy ω allows us to compare directly with results from Green's function theory when only two-particle intermediate states are included.

The next approximation is to include the two-hole term, a term which allows us to make a link with Green's function theory with two-particle and two-hole correlations

$$\begin{aligned} 0 &= \langle ab|\hat{v}|ij\rangle + (\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j)\, t_{ij}^{ab} \\ &\quad + \frac{1}{2}\sum_{cd}\langle ab|\hat{v}|cd\rangle\, t_{ij}^{cd} + \frac{1}{2}\sum_{kl}\langle kl|\hat{v}|ij\rangle\, t_{kl}^{ab}. \end{aligned} \tag{17}$$

This equation can be solved in the same way.

- The exact wave function of non-degenerate ground state of a given system is expanded in terms of a series of Slater determinants

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{m=1}^{\infty} C_m |\Phi_m\rangle \tag{18}$$

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

$$\hat{H}_0 |\Phi_0\rangle = W_0 |\Phi_0\rangle \tag{19}$$

The state $|\Psi_0\rangle$ is normalized as $\langle \Phi_0 \mid \Psi_0 \rangle = 1$.

The Schrödinger equation is given by

$$\hat{H}\left|\Psi_0\right\rangle = E\left|\Psi_0\right\rangle \tag{20}$$

Multiplying from the left with $\langle\Phi_0|$ gives

$$\left\langle \Phi_0|\hat{H}|\Psi_0 \right\rangle = E\left\langle \Phi_0 \mid \Psi_0\right\rangle = E.$$

Substituting $\hat{H} = \hat{H}_0 + \hat{H}_I$ and consdering the fact that the operators $\hat{H}$ and $\hat{H}_0$ are hermitian

$$\left\langle \Phi_0|\hat{H}_0 + \hat{H}_I|\Psi_0 \right\rangle = W_0 + \left\langle \Phi_0|\hat{H}_I|\Psi_0 \right\rangle,$$

and thus

$$\Delta E = E - W_0 = \left\langle \Phi_0 \left| \hat{H}_I \right| \Psi_0 \right\rangle. \tag{21}$$

The ΔE is just the correlation energy except that the reference energy $E_{\mathrm{ref}} = \langle\Phi_0|\hat{H}|\Phi_0\rangle$ is replaced by the unperturbed energy W_0.

Model space

Let's assume our model space is defined by the operator $\hat{P}$

$$\hat{P} = |\Phi_0\rangle \langle\Phi_0| , \tag{22}$$

and the excluded model space Q

$$\hat{Q} = \sum_{m=1}^{\infty} |\Phi_m\rangle \langle\Phi_m| . \tag{23}$$

We can thus rewrite the exact wave function as

$$|\Psi_0\rangle = (\hat{P} + \hat{Q})\,|\Psi_0\rangle = |\Phi_0\rangle + \hat{Q}\,|\Psi_0\rangle \tag{24}$$

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

$$\left(\omega - \hat{H}_0\right)|\Psi_0\rangle = \left(\omega - E + \hat{H}_I\right)|\Psi_0\rangle \tag{25}$$

where ω is an energy variable to be specified later. We assume also that the resolvent of $\left(\omega - \hat{H}_0\right)$ exits, that is it has an inverse which defines the unperturbed Green's function as

$$\left(\omega - \hat{H}_0\right)^{-1} = \frac{1}{\left(\omega - \hat{H}_0\right)} \tag{26}$$

We can rewrite Schrödinger's equation as

$$|\Psi_0\rangle = \frac{1}{\omega - \hat{H}_0}\left(\omega - E + \hat{H}_I\right)|\Psi_0\rangle\,, \tag{27}$$

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

$$\hat{Q}\,|\Psi_0\rangle = \frac{\hat{Q}}{\omega - \hat{H}_0}\left(\omega - E + \hat{H}_I\right)|\Psi_0\rangle\,, \tag{28}$$

which is possible since we have defined the operator $\hat{Q}$ in terms of the eigenfunctions of $\hat{H}_0$. Since these operators commute we have

$$\hat{Q}\frac{1}{\left(\omega - \hat{H}_0\right)}\hat{Q} = \hat{Q}\frac{1}{\left(\omega - \hat{H}_0\right)} = \frac{\hat{Q}}{\left(\omega - \hat{H}_0\right)}. \tag{29}$$

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

$$|\Psi_0\rangle = |\Phi_0\rangle + \frac{\hat{Q}}{\omega - \hat{H}_0}\left(\omega - E + \hat{H}_I\right)|\Psi_0\rangle\,. \tag{30}$$

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 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.

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

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

for the wave function and

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

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

- In Brilluoin-Wigner perturbation theory: it is customary to set $\omega = E$. This results in the following perturbative expansion for the energy ΔE

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

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

This expression depends however on the exact energy E 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 and then solve till some kind of self-consistency criterion has been reached.

Defining $e = E - \hat{H}_0$ and recalling that $\hat{H}_0$ commutes with $\hat{Q}$ by construction and that $\hat{Q}$ is an idempotent operator $\hat{Q}^2 = \hat{Q}$, we can rewrite the denominator in the above expansion for ΔE as

$$\hat{Q}\frac{1}{\hat{e} - \hat{Q}\hat{H}_I\hat{Q}} = \hat{Q}\left[\frac{1}{\hat{e}} + \frac{1}{\hat{e}}\hat{Q}\hat{H}_I\hat{Q}\frac{1}{\hat{e}} + \frac{1}{\hat{e}}\hat{Q}\hat{H}_I\hat{Q}\frac{1}{\hat{e}}\hat{Q}\hat{H}_I\hat{Q}\frac{1}{\hat{e}} + \ldots\right]\hat{Q}$$

Inserted in the expression for ΔE we obtain

$$\Delta E = \left\langle \Phi_0 \left| \hat{H}_I + \hat{H}_I\hat{Q}\frac{1}{E - \hat{H}_0 - \hat{Q}\hat{H}_I\hat{Q}}\hat{Q}\hat{H}_I \right| \Phi_0 \right\rangle$$

- In Rayleigh-Schrödinger (RS) perturbation theory: we set $\omega = W_0$ and obtain the following expression for the energy difference

$$\begin{aligned}\Delta E &= \sum_{i=0}^{\infty} \left\langle \Phi_0 \left| \hat{H}_I \left\{ \frac{\hat{Q}}{W_0 - \hat{H}_0} \left(\hat{H}_I - \Delta E \right) \right\}^i \right| \Phi_0 \right\rangle \\ &= \left\langle \Phi_0 \left| \left(\hat{H}_I + \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \left(\hat{H}_I - \Delta E \right) + \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \left(\hat{H}_I - \Delta E \right) \frac{\hat{Q}}{W_0 - \hat{H}_0} \left(\hat{H}_I - \Delta E \right) + \ldots \right) \right| \Phi_0 \right\rangle \end{aligned} \quad (31)$$

The operator $\hat{Q}$ commutes with $\hat{H}_0$ and since ΔE is a constant we obtain that

$$\hat{Q}\Delta E \left| \Phi_0 \right\rangle = \hat{Q}\Delta E \left| \hat{Q}\Phi_0 \right\rangle = 0$$

Inserting this result in the expression for the energy gives us

$$\Delta E = \left\langle \Phi_0 \left| \left(\hat{H}_I + \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I + \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \left(\hat{H}_I - \Delta E \right) \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I + \ldots \right) \right| \Phi_0 \right\rangle \quad (32)$$

- The first correction:

$$\Delta E^{(1)} = \left\langle \Phi_0 \left| \hat{H}_I \right| \Phi_0 \right\rangle, \tag{33}$$

- The second correction:

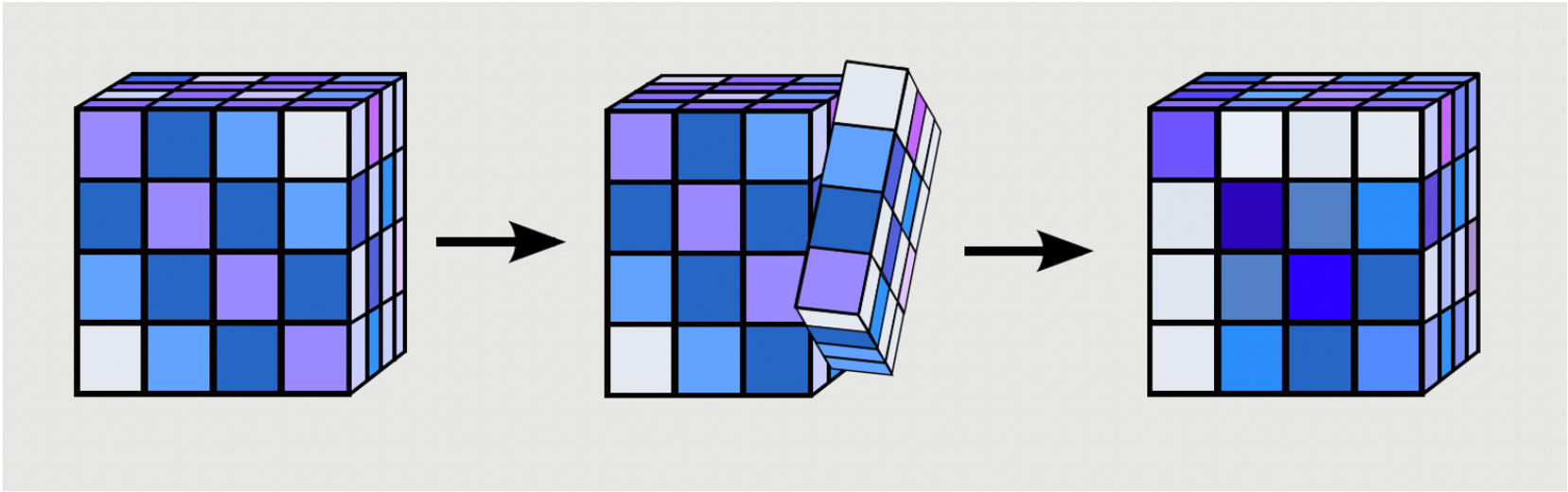
$$\begin{aligned} \Delta E^{(2)} &= \left\langle \Phi_0 \left| \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \right| \Phi_0 \right\rangle \\ &= \frac{1}{4} \sum_{abij} \langle ij|\hat{v}|ab\rangle \frac{\langle ab|\hat{v}|ij\rangle}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}. \end{aligned} \tag{34}$$

The second equivalence is based on the assumption that $|\Phi_0\rangle$ is a HF state, in which case one also has $\Delta E^{(1)} = 0$.

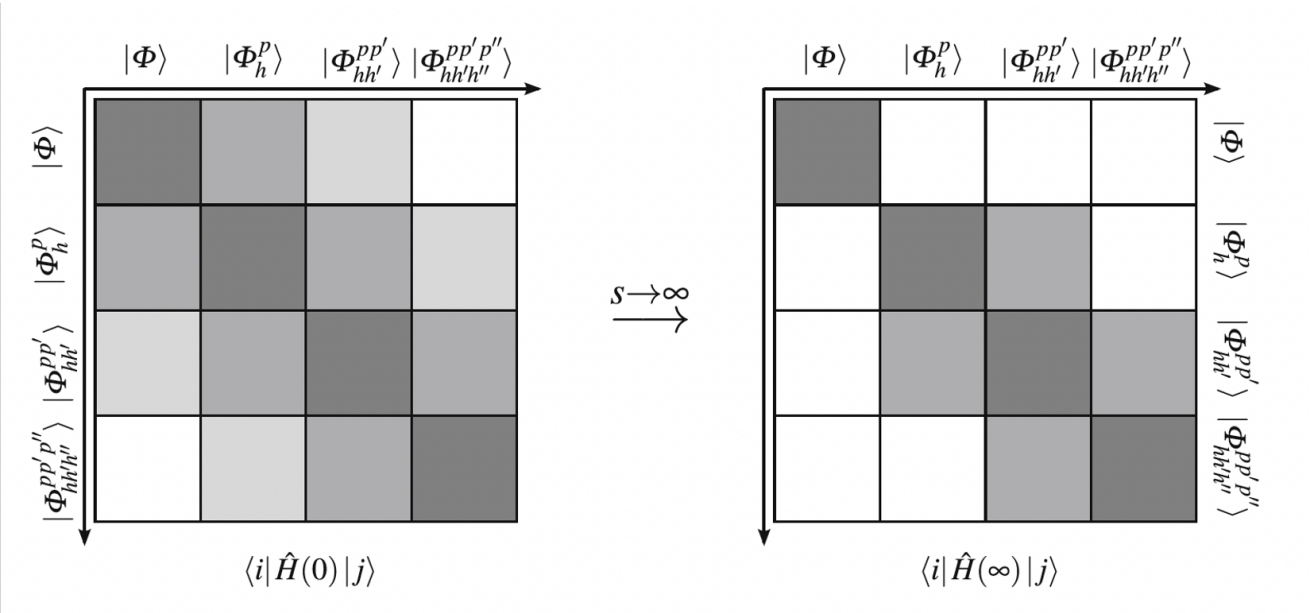
- The third correction:

$$\Delta E^{(3)} = \left\langle \Phi_0 \left| \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \left(\hat{H}_I - \Delta E \right) \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \right| \Phi_0 \right\rangle, \tag{35}$$

The in-medium similarity renormalization group



$$\hat{H}(s) = \hat{U}(s)\hat{H}(0)\hat{U}^{\dagger}(s)$$



Taking the derivative $H(s)$ with respect to the flow parameter s,

$$\frac{d\hat{H}(s)}{ds} = \frac{d\hat{U}(s)}{ds}\hat{H}(0)\hat{U}^\dagger(s) + \hat{U}(s)\hat{H}(0)\frac{d\hat{U}^\dagger(s)}{ds}$$
$$= \frac{d\hat{U}(s)}{ds}\hat{U}^\dagger(s)\hat{H}(s) + \hat{H}(s)\hat{U}(s)\frac{d\hat{U}^\dagger(s)}{ds}$$

Since $\hat{U}(s)$ is unitary, we also have

$$\frac{d}{ds}\left(\hat{U}(s)\hat{U}^{\dagger}(s)\right) = \frac{d}{ds}(\hat{I}) = 0 \quad \Longrightarrow \quad \frac{d\hat{U}(s)}{ds}\hat{U}^{\dagger}(s) = -\hat{U}(s)\frac{d\hat{U}^{\dagger}(s)}{ds}$$

Defining the anti-Hermitian operator

$$\hat{\eta}(s) \equiv \frac{d\hat{U}(s)}{ds}\hat{U}^{\dagger}(s) = -\hat{\eta}^{\dagger}(s)$$

we can write the differential equation for the s-dependent Hamiltonian as

$$\frac{d}{ds}\hat{H}(s) = [\hat{\eta}(s), \hat{H}(s)]$$

This is the SRG flow equation for the Hamiltonian, which describes the evolution of $\hat{H}(s)$ under the action of a dynamical generator $\hat{\eta}(s)$.

The $\hat{H}(s)$ can be obtained by integrating the flow equation numerically, without explicitly constructing the unitary transformation itself. Formally, we can also obtain $\hat{U}(s)$ by

$$\frac{d}{ds}\hat{U}(s) = \hat{\eta}(s)\hat{U}(s).$$

The solution to this differential equation is given by the S-ordered exponential

$$U(s) = \mathcal{S}\exp\int_0^s ds'\eta\left(s'\right),$$

because the generator changes dynamically during the flow. This expression is defined equivalently either as a product of infinitesimal unitary transformations,

$$U(s) = \lim_{N\to\infty}\prod_{i=0}^{N} e^{\eta(s_i)\delta s_i}, \quad s_{i+1} = s_i + \delta s_i, \quad \sum_i \delta s_i = s$$

or through a series expansion:

$$U(s) = \sum_n \frac{1}{n!}\int_0^s ds_1\int_0^s ds_2\ldots\int_0^s ds_n \mathcal{S}\left\{\eta\left(s_1\right)\ldots\eta\left(s_n\right)\right\}.$$

- Wegner proposed the generator

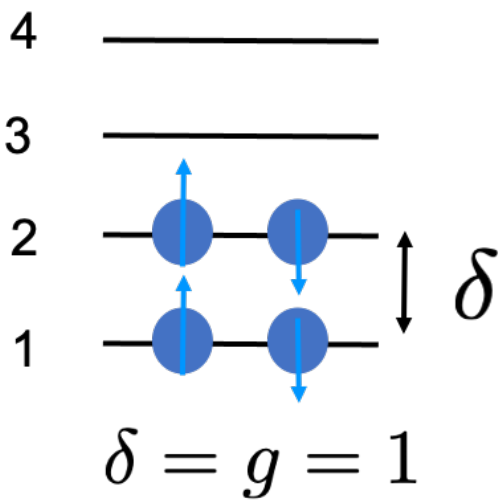
$$\hat{\eta}(s) = [\hat{H}_d(s), \hat{H}_{od}(s)]$$

which will be able to drive the $\hat{H}_{od}(s) \to 0$ as the flow parameter $s \to \infty$.

- The pairing Hamiltonian:

$$\hat{H} = \delta \sum_{p\sigma} (p-1) a^{\dagger}_{p\sigma} a_{p\sigma} - \frac{1}{2} g \sum_{pq} a^{\dagger}_{p+} a^{\dagger}_{p-} a_{q-} a_{q+},$$

where δ controls the spacing of single-particle levels that are indexed by a principal quantum number $p = 1, \ldots, 4$ and their spin projection σ, and g the strength of the pairing interaction.



$\delta = g = 1$

state	p	$2s_z$	ε
0	1	1	0
1	1	−1	0
2	2	1	δ
3	2	−1	δ
4	3	1	2δ
5	3	−1	2δ
6	4	1	3δ
7	4	−1	3δ

- Let's only consider the $S_z = 0$ sub block with two particle pairs. In this block, the Hamiltonian is represented by the six-dimensional matrix

$$H = \begin{pmatrix} 2\delta - g & -g/2 & -g/2 & -g/2 & -g/2 & 0 \\ -g/2 & 4\delta - g & -g/2 & -g/2 & -0 & -g/2 \\ -g/2 & -g/2 & 6\delta - g & 0 & -g/2 & -g/2 \\ -g/2 & -g/2 & 0 & 6\delta - g & -g/2 & -g/2 \\ -g/2 & 0 & -g/2 & -g/2 & 8\delta - g & -g/2 \\ 0 & -g/2 & -g/2 & -g/2 & -g/2 & 10\delta - g \end{pmatrix}.$$

We split the Hamiltonian matrix into diagonal and off-diagonal parts:

$$H_d(s) = \mathrm{diag}\left(E_0(s), \ldots, E_5(s)\right), \quad H_{od}(s) = H(s) - H_d(s)$$

The flow equation in the configuration basis in which one has $\hat{H}_d|i\rangle = E_i|i\rangle$, and

$$\begin{aligned}\frac{d}{ds}\langle i|\hat{H}|j\rangle &= \sum_k \left(\langle i|\hat{\eta}|k\rangle\langle k|\hat{H}|j\rangle - \langle i|\hat{H}|k\rangle\langle k|\hat{\eta}|j\rangle\right) \\ &= -\left(E_i - E_j\right)\langle i|\hat{\eta}|j\rangle + \sum_k \left(\langle i|\hat{\eta}|k\rangle\left\langle k\left|\hat{H}_{od}\right|j\right\rangle - \left\langle i\left|\hat{H}_{od}\right|k\right\rangle\langle k|\hat{\eta}|j\rangle\right)\end{aligned}$$

where $\left\langle i\left|\hat{H}_{od}\right|i\right\rangle = 0$ and block indices as well as the s-dependence have been suppressed for brevity. The Wegner generator is given by

$$\langle i|\hat{\eta}|j\rangle = \left\langle i\left|\left[\hat{H}_d, \hat{H}_{od}\right]\right|j\right\rangle = \left(E_i - E_j\right)\left\langle i\left|\hat{H}_{od}\right|j\right\rangle,$$

and inserting this into the flow equation, we obtain

$$\frac{d}{ds}\langle i|\hat{H}|j\rangle = -\left(E_i - E_j\right)^2\left\langle i\left|\hat{H}_{od}\right|j\right\rangle + \sum_k \left(E_i + E_j - 2E_k\right)\left\langle i\left|\hat{H}_{od}\right|k\right\rangle\left\langle k\left|\hat{H}_{od}\right|j\right\rangle \quad (36)$$

If $\left\|\hat{H}_{od}(s_0)\right\| \ll 1$ in some suitable norm, the second term in the flow equation can be neglected compared to the first one. For the diagonal and off-diagonal matrix elements, this implies

$$\frac{dE_i}{ds} = \frac{d}{ds}\left\langle i\left|\hat{H}_d\right|i\right\rangle = 2\sum_k (E_i - E_k)\left\langle i\left|\hat{H}_{od}\right|k\right\rangle\left\langle k\left|\hat{H}_{od}\right|i\right\rangle \approx 0$$

and

$$\frac{d}{ds}\langle i|\hat{H}|j\rangle \approx -(E_i - E_j)^2\left\langle i\left|\hat{H}_{od}\right|j\right\rangle$$

respectively. Thus, the diagonal matrix elements will be (approximately) constant in the asymptotic region,

$$E_i(s) \approx E_i(s_0), \quad s > s_0,$$

which in turn allows us to integrate the flow equation for the off-diagonal matrix elements. We obtain

$$\left\langle i\left|\hat{H}_{od}(s)\right|j\right\rangle \approx \left\langle i\left|\hat{H}_{od}(s_0)\right|j\right\rangle e^{-(E_i-E_j)^2(s-s_0)}, \quad s > s_0$$

i.e., the off-diagonal matrix elements are suppressed exponentially.

Application of SRG to the pairing model

```
#------------------------------------------------------------------------------
# Main program
#------------------------------------------------------------------------------

def main():
    g     = 1.
    delta = 2.

    H0    = Hamiltonian(delta, g)
    dim   = H0.shape[0]

    # calculate exact eigenvalues
    eigenvalues = eigvalsh(H0)

    # turn initial Hamiltonian into a linear array
    y0  = reshape(H0, -1)

    # flow parameters for snapshot images
    flowparams = array([0.,0.001,0.01,0.05,0.1, 1., 5., 10.])

    # integrate flow equations - odeint returns an array of solutions,
    # which are 1d arrays themselves
    ys  = odeint(derivative, y0, flowparams, args=(dim,))

    # reshape individual solution vectors into dim x dim Hamiltonian
    # matrices
    Hs  = reshape(ys, (-1, dim,dim))

    data = []
    for h in Hs:
        data.append(diag(h))
    data = list(zip(*data))

    print(len(Hs))

    plot_diagonals(data, eigenvalues, flowparams, delta, g)
    plot_snapshots(Hs, flowparams, delta, g)

    return
```

```
# Hamiltonian for the pairing model
def Hamiltonian(delta,g):

    H = array(
        [[2*delta-g,    -0.5*g,     -0.5*g,     -0.5*g,    -0.5*g,          0.],
         [   -0.5*g, 4*delta-g,     -0.5*g,     -0.5*g,        0.,     -0.5*g ],
         [   -0.5*g,    -0.5*g,  6*delta-g,         0.,    -0.5*g,     -0.5*g ],
         [   -0.5*g,    -0.5*g,         0.,  1*6*delta-g,    -0.5*g,     -0.5*g ],
         [   -0.5*g,        0.,     -0.5*g,     -0.5*g, 8*delta-g,     -0.5*g ],
         [       0.,    -0.5*g,     -0.5*g,     -0.5*g,    -0.5*g, 10*delta-g ]]
      )

    return H

# commutator of matrices
def commutator(a,b):
    return dot(a,b) - dot(b,a)

# derivative / right-hand side of the flow equation
def derivative(y, t, dim):

    # reshape the solution vector into a dim x dim matrix
    H = reshape(y, (dim, dim))

    # extract diagonal Hamiltonian...
    Hd  = diag(diag(H))

    # ... and construct off-diagonal the Hamiltonian
    Hod = H-Hd

    # calculate the generator
    eta = commutator(Hd, Hod)

    # dH is the derivative in matrix form
    dH  = commutator(eta, H)

    # convert dH into a linear array for the ODE solver
    dy = reshape(dH, -1)

    return dy
```