II. CI + MBPT

1. $\mathbf{P}, \mathbf{Q}$-decomposition.

$$\mathbf{I} = \mathbf{P} + \mathbf{Q}; \qquad \mathbf{P}^2 = \mathbf{P}; \qquad \mathbf{Q}^2 = \mathbf{Q}.$$

$$\mathbf{H\Psi} = E\mathbf{\Psi} \quad \Longrightarrow \quad \begin{cases} \mathbf{PHP}\ \mathbf{\Psi} + \mathbf{PHQ}\ \mathbf{\Psi} = E\ \mathbf{P\Psi}, \\ \mathbf{QHQ}\ \mathbf{\Psi} + \mathbf{QHP}\ \mathbf{\Psi} = E\ \mathbf{Q\Psi}. \end{cases}$$

The formal solution of the lower equation has the form

$$\mathbf{Q\Psi} = \mathbf{R}_Q(E)\ (\mathbf{QHP})\ \mathbf{\Psi},$$
$$\mathbf{R}_Q(E) = (\mathbf{Q}(E - \mathbf{H})\mathbf{Q})^{-1}.$$

Substituting it into the upper equation we arrive at:

$$\begin{cases} \mathbf{P}\left(\mathbf{H} + \mathbf{\Sigma}(E)\right)\mathbf{P}\ \mathbf{\Psi} = E\ \mathbf{P}\Psi, \\ \mathbf{\Sigma}(E) = (\mathbf{PHQ})\ \mathbf{R}_Q(E)\ (\mathbf{QHP}). \end{cases}$$

Normalization condition for the solutions of this equation can be **approximately** written as follows:

$$\langle \mathbf{P\Psi}_i | \mathbf{1} - \partial_E \mathbf{\Sigma}(E) | \mathbf{P\Psi}_k \rangle_{E=E_{av}} = \delta_{i,k},$$

where it is assumed that that $E_i \approx E_k \approx E_{av}$.

2. Main idear of the method:

- Construct operator $\mathbf{\Sigma}(E)$ by means of the MBPT.
- Solve the eigenvalue equation in the $\mathbf{P}$-subspace with the effective Hamiltonian $\mathbf{H}_{\text{eff}} = \mathbf{H} + \mathbf{\Sigma}$ using the CI technique.

III. MPBT part

We need to calculate the operator

$$\mathbf{\Sigma}(E) = (\mathbf{PHQ})\ \mathbf{R}_Q(E)\ (\mathbf{QHP}),$$

where $\mathbf{P}$ is a subspace which correspond to the frozen core with the wave function

$$\mathbf{\Psi}_c = \frac{1}{\sqrt{N_c!}} det\left\{\phi_1\phi_2\cdots\phi_{N_c}\right\},$$
$$h_{\mathrm{DF}}\phi_n = \varepsilon_n\phi_n.$$

In the second quantization formalism it can be written as:

$$|\phi_n\rangle = a_n^\dagger|0\rangle,$$
$$\mathbf{\Psi}_c = a_1^\dagger a_2^\dagger\cdots a_{N_c}^\dagger|0\rangle.$$

Let us define now the many-body Dirac-Fock operator as

$$\mathbf{H}_{\mathrm{DF}} = \sum_n \varepsilon_n a_n^\dagger a_n + \mathrm{Const},$$

and fix the constant from a condition:

$$\langle\mathbf{\Psi}_c|\mathbf{H}_{\mathrm{DF}}|\mathbf{\Psi}_c\rangle = \langle\mathbf{\Psi}_c|\mathbf{H}|\mathbf{\Psi}_c\rangle \equiv E_c.$$

Note that such definition of $\mathbf{H}_{\mathrm{DF}}$ means that

$$\mathbf{H}_{\mathrm{DF}}\mathbf{\Psi}_c = E_c\mathbf{\Psi}_c.$$

As far as $\mathbf{\Psi}_c$ is the eigenfunction of $\mathbf{H}_{\mathrm{DF}}$,

$$\mathbf{P}\mathbf{H}_{\mathrm{DF}}\mathbf{Q} = \mathbf{Q}\mathbf{H}_{\mathrm{DF}}\mathbf{P} = 0.$$

Thus

$$\mathbf{\Sigma}(E) = (\mathbf{P}\mathbf{V}'\mathbf{Q})\ \mathbf{R}_Q(E)\ (\mathbf{Q}\mathbf{V}'\mathbf{P}),$$

where $\mathbf{V}' \equiv \mathbf{H} - \mathbf{H}_{\mathrm{DF}}$ is the residual field operator.

Now we can use the usual expansion in $\mathbf{V}'$ for the Green's function

$$\frac{1}{E-\mathbf{H}} = \frac{1}{E-\mathbf{H}_{\mathrm{DF}}} + \frac{1}{E-\mathbf{H}_{\mathrm{DF}}}\ \mathbf{V}'\ \frac{1}{E-\mathbf{H}}$$

to form the perturbation series for the operator $\mathbf{\Sigma}(E)$.

IV. Expectation Values and Transition Amplitudes

With the help of the effective Hamiltonian $\mathbf{H}_{\text{eff}} = \mathbf{H} + \mathbf{\Sigma}(E)$ we can find only the projection $\mathbf{\Phi}$ of the wave function $\mathbf{\Psi}$:

$$\left.\begin{aligned} \mathbf{\Phi} &= \mathbf{P\Psi} \\ \mathbf{Q\Psi} &= \mathbf{R}_Q(E)\mathbf{V'P\Phi} \end{aligned}\right\} \Longrightarrow \mathbf{\Psi} = (\mathbf{P} + \mathbf{R}_Q(E)\mathbf{V'P})\mathbf{\Phi}.$$

The amplitude of the arbitrary operator $\mathbf{A}$ can be written as:

$$A_{2,1} = \langle \mathbf{\Psi}_2 | \mathbf{A} | \mathbf{\Psi}_1 \rangle \equiv \langle \mathbf{\Phi}_2 | \mathbf{A}_{\text{eff}} | \mathbf{\Phi}_1 \rangle,$$

where

$$\begin{aligned} \mathbf{A}_{\text{eff}} = \mathbf{PAP} &+ \mathbf{PV'R}_Q(E_2)\mathbf{AP} + \mathbf{PAR}_Q(E_1)\mathbf{V'P} \\ &+ \mathbf{PV'R}_Q(E_2)\mathbf{AR}_Q(E_1)\mathbf{V'P}. \end{aligned}$$

In this equation we have **exact** Green's functions $\mathbf{R}_Q(E)$. One can show that the following approximate expression holds true:

$$\mathbf{A}_{\text{eff}} \approx \mathbf{PAP} + \mathbf{PV'R}_Q^{\text{DF}}(E_2)\mathbf{A}^{\text{RPA}}\mathbf{P} + \mathbf{PA}^{\text{RPA}}\mathbf{R}_Q^{\text{DH}}(E_1)\mathbf{V'P},$$

where Green's functions are taken in the Dirac-Fock approximation and operator is taken in the Random-Phase approximation.