Dielectric matrix formulation of correlation energies in the Random Phase Approximation (RPA) : inclusion of exchange effects

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What you (may) know

$$E_c^{\text{AC-FDT}} = -\frac{1}{2}\int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i}\ \mathrm{Tr}\left\{\mathbb{\Pi}_\alpha(\omega)\mathbb{V} - \mathbb{\Pi}_0(\omega)\mathbb{V}\right\}$$

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Flavors (Exchange)

- *direct* or *exchange* RPA
- *single-bar* or *double-bar*

This yields the flavors : dRPA-I, dRPA-II, RPAx-I, RPAx-II

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Formulations (Integrals)

- *density-matrix* formulation $E = \int d\alpha\, \mathbf{P}_\alpha \mathbf{V}$ (JCTC2011)
- *dielectric-matrix* formulation
- *plasmon* formula $E = \sum \omega_{\text{RPA}} - \omega_{\text{LDA}}$ (rather limited)
- *Ricatti equations* and *rCCD* $E = \mathrm{tr}(\mathbf{BT})$ (explored)

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+Approximations (in each formulations, for each flavors...)

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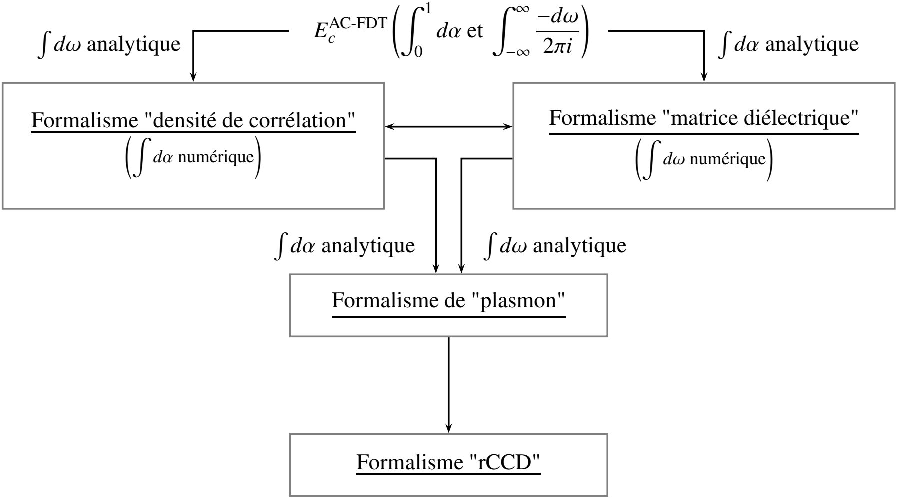

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$$\mathbb{\Pi}_0(\omega) = -(\mathbb{\Lambda}_0 - \omega\mathbb{\Delta})^{-1}$$

$$\mathbb{\Lambda}_0 = \begin{pmatrix} \boldsymbol{\epsilon} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\epsilon} \end{pmatrix} \qquad \mathbb{\Delta} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}$$

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The goals

- analytical integration over the coupling constant α
- reduce the dimensions of the operations involved (« Tr » to « tr »)
- all sums up to the use of :

$$(1-\alpha x)^{-1} = 1 + \sum_{n=2} \alpha^{n-1} x^{n-1} \quad \text{and} \quad \text{Log}(1-x) + x = \sum_{n=2} \frac{x^n}{n}$$

dRPA-I

$$E_c^{\text{dRPA-I}} = -\frac{1}{2}\int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i}\ \mathrm{Tr}\{\mathbb{\Pi}_\alpha(\omega)\mathbb{V} - \mathbb{\Pi}_0(\omega)\mathbb{V}\}$$

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$$\mathrm{Tr}\{(\mathbb{\Pi}_0\, \mathbb{V})^n\} = \mathrm{Tr}\left\{ \begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{K} & \mathbf{\Pi}_0^+\mathbf{K} \\ \mathbf{\Pi}_0^-\mathbf{K} & \mathbf{\Pi}_0^-\mathbf{K} \end{pmatrix}^n \right\} = \mathrm{tr}\{(\mathbf{\Pi}_0\mathbf{K})^n\}$$

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$$\text{Tr}\left\{ \begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{K} & \mathbf{\Pi}_0^+\mathbf{K} \\ \mathbf{\Pi}_0^-\mathbf{K} & \mathbf{\Pi}_0^-\mathbf{K} \end{pmatrix}^{n-1} \left[\begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix} + \begin{pmatrix} \mathbf{\Pi}_0^+(\mathbf{A}'-\mathbf{B}) & \mathbf{0} \\ \mathbf{0} & \mathbf{\Pi}_0^-(\mathbf{A}'-\mathbf{B}) \end{pmatrix} \right] \right\}$$

$$\text{tr}\left\{(\mathbf{\Pi}_0\mathbf{K})^{n-1}\mathbf{\Pi}_0\mathbf{B}\right\} + \text{tr}\left\{\left(\mathbf{\Pi}_0^+\mathbf{K}(\mathbf{\Pi}_0\mathbf{K})^{n-2}\mathbf{\Pi}_0^+ + \mathbf{\Pi}_0^-\mathbf{K}(\mathbf{\Pi}_0\mathbf{K})^{n-2}\mathbf{\Pi}_0^-\right)(\mathbf{A}'-\mathbf{B})\right\}$$

$$E_c^{\text{dRPA-IIa}} = -\frac{1}{2}\int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \text{tr}\left\{ \sum_{n=2}^{\infty} \alpha^{n-1} (\mathbf{\Pi}_0\mathbf{K})^{n-1}\, \mathbf{\Pi}_0\mathbf{B} \right\}.$$

dRPA-II (SX)

$$E_c^{\text{dRPA-II}} = -\frac{1}{2}\int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i}\, \mathrm{Tr}\{\mathbb{\Pi}_\alpha(\omega)\mathbb{W} - \mathbb{\Pi}_0(\omega)\mathbb{W}\}$$

$$\mathbb{V} = \begin{pmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \mathbf{K} \end{pmatrix}$$

$$\mathbb{W} = \begin{pmatrix} \mathbf{A}' & \mathbf{B} \\ \mathbf{B} & \mathbf{A}' \end{pmatrix}$$

$$\mathbb{W} = \begin{pmatrix} \mathbf{B} & \mathbf{B} \\ \mathbf{B} & \mathbf{B} \end{pmatrix} + \begin{pmatrix} \mathbf{A}'-\mathbf{B} & 0 \\ 0 & \mathbf{A}'-\mathbf{B} \end{pmatrix}$$

Dyson $\quad \mathbb{\Pi}_\alpha = (\mathbb{1} - \alpha \mathbb{\Pi}_0 \mathbb{V})^{-1}\mathbb{\Pi}_0$

Taylor $\quad \mathbb{\Pi}_\alpha = 1 + \sum_{n=2} \alpha^{n-1} (\mathbb{\Pi}_0\mathbb{V})^{n-1}$

$$\mathbb{\Pi}_\alpha(\omega)\mathbb{W} - \mathbb{\Pi}_0(\omega)\mathbb{W} = \sum_{n=2} \alpha^{n-1}\, (\mathbb{\Pi}_0\mathbb{V})^{n-1}\mathbb{\Pi}_0\mathbb{W}$$

$$\mathrm{Tr}\left\{ \begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{K} & \mathbf{\Pi}_0^+\mathbf{K} \\ \mathbf{\Pi}_0^-\mathbf{K} & \mathbf{\Pi}_0^-\mathbf{K} \end{pmatrix}^{n-1} \left[\begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix} + \begin{pmatrix} \mathbf{\Pi}_0^+(\mathbf{A}'-\mathbf{B}) & \mathbf{0} \\ \mathbf{0} & \mathbf{\Pi}_0^-(\mathbf{A}'-\mathbf{B}) \end{pmatrix} \right] \right\}$$

$$\mathrm{tr}\left\{(\mathbf{\Pi}_0\mathbf{K})^{n-1}\mathbf{\Pi}_0\mathbf{B}\right\} + \mathrm{tr}\left\{\left(\mathbf{\Pi}_0^+\mathbf{K}(\mathbf{\Pi}_0\mathbf{K})^{n-2}\mathbf{\Pi}_0^+ + \mathbf{\Pi}_0^-\mathbf{K}(\mathbf{\Pi}_0\mathbf{K})^{n-2}\mathbf{\Pi}_0^-\right)(\mathbf{A}'-\mathbf{B})\right\}$$

$$E_c^{\text{dRPA-IIa}} = -\frac{1}{2}\int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathrm{tr}\left\{ \sum_{n=2}^{\infty} \alpha^{n-1} (\mathbf{\Pi}_0\mathbf{K})^{n-1}\, \mathbf{\Pi}_0\mathbf{B} \right\}.$$

$$E_c^{\text{dRPA-IIa}} = \frac{1}{2}\int \frac{d\omega}{2\pi} \mathrm{tr}\left\{ \mathrm{Log}\left(\mathbf{I} - \mathbf{\Pi}_0\mathbf{K}\right)\mathbf{K}^{-1}\mathbf{B} + \mathbf{\Pi}_0\mathbf{B} \right\}$$

- clear link to SOSEX
- $\mathbf{B} = \mathbf{K} - \mathbf{K}'$: you can write « $E_c^{\text{dRPA-IIa}} = E_c^{\text{dRPA-I}} - \text{term}$ »
- second-order approximation to dRPA-IIa is MP2

RPAx-I

$$\mathbb{W} = \begin{pmatrix} \mathbf{A}' & \mathbf{B} \\ \mathbf{B} & \mathbf{A}' \end{pmatrix}$$

$$\mathbb{W} = \begin{pmatrix} \mathbf{B} & \mathbf{B} \\ \mathbf{B} & \mathbf{B} \end{pmatrix} + \begin{pmatrix} \mathbf{A}'-\mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}'-\mathbf{B} \end{pmatrix}$$

$$\mathbb{V} = \begin{pmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \mathbf{K} \end{pmatrix}$$

$$E_c^{\text{dRPA-II}} = -\frac{1}{2} \int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \, \mathrm{Tr}\{\Pi_\alpha(\omega)\mathbb{V} - \Pi_0(\omega)\mathbb{V}\}$$

Dyson $\quad \Pi_\alpha = (\mathbb{1} - \alpha \Pi_0 \mathbb{W})^{-1} \Pi_0$

Taylor $\quad \Pi_\alpha = 1 + \sum_{n=2} \alpha^{n-1} (\Pi_0 \mathbb{W})^{n-1}$

$$\Pi_\alpha(\omega)\mathbb{V} - \Pi_0(\omega)\mathbb{V} = \sum_{n=2} \alpha^{n-1} \; (\Pi_0 \mathbb{W})^{n-1} \Pi_0 \mathbb{V}$$

RPAx-I

$$E_c^{\text{dRPA-II}} = -\frac{1}{2}\int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i}\, \mathrm{Tr}\{\mathbb{\Pi}_\alpha(\omega)\mathbb{V} - \mathbb{\Pi}_0(\omega)\mathbb{V}\}$$

$$\mathbb{W} = \begin{pmatrix} \mathbf{A}' & \mathbf{B} \\ \mathbf{B} & \mathbf{A}' \end{pmatrix}$$

$$\mathbb{W} = \begin{pmatrix} \mathbf{B} & \mathbf{B} \\ \mathbf{B} & \mathbf{B} \end{pmatrix} + \begin{pmatrix} \mathbf{A}'-\mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}'-\mathbf{B} \end{pmatrix}$$

$$\mathbb{V} = \begin{pmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \mathbf{K} \end{pmatrix}$$

Dyson $\mathbb{\Pi}_\alpha = (\mathbb{1} - \alpha\mathbb{\Pi}_0\mathbb{W})^{-1}\mathbb{\Pi}_0$

Taylor $\mathbb{\Pi}_\alpha = 1 + \sum_{n=2} \alpha^{n-1}(\mathbb{\Pi}_0\mathbb{W})^{n-1}$

$$\mathbb{\Pi}_\alpha(\omega)\mathbb{V} - \mathbb{\Pi}_0(\omega)\mathbb{V} = \sum_{n=2} \alpha^{n-1}\, (\mathbb{\Pi}_0\mathbb{W})^{n-1}\mathbb{\Pi}_0\mathbb{V}$$

$$\begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix}^{n-1} + \sum_{p=1}^{n-1} \begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix}^{n-1-p} \begin{pmatrix} \mathbf{\Pi}_0^+(\mathbf{A}'-\mathbf{B}) & \mathbf{0} \\ \mathbf{0} & \mathbf{\Pi}_0^-(\mathbf{A}'-\mathbf{B}) \end{pmatrix} \begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix}^{p-1}$$

RPAx-I

$$E_c^{\text{dRPA-II}} = -\frac{1}{2}\int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i}\, \mathrm{Tr}\{\mathbb{\Pi}_\alpha(\omega)\mathbb{V} - \mathbb{\Pi}_0(\omega)\mathbb{V}\}$$

$$\mathbb{W} = \begin{pmatrix} \mathbf{A}' & \mathbf{B} \\ \mathbf{B} & \mathbf{A}' \end{pmatrix}$$

$$\mathbb{W} = \begin{pmatrix} \mathbf{B} & \mathbf{B} \\ \mathbf{B} & \mathbf{B} \end{pmatrix} + \begin{pmatrix} \mathbf{A}'-\mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}'-\mathbf{B} \end{pmatrix}$$

$$\mathbb{V} = \begin{pmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \mathbf{K} \end{pmatrix}$$

Dyson $\mathbb{\Pi}_\alpha = (\mathbb{1} - \alpha\mathbb{\Pi}_0\mathbb{W})^{-1}\mathbb{\Pi}_0$

Taylor $\mathbb{\Pi}_\alpha = 1 + \sum_{n=2} \alpha^{n-1}(\mathbb{\Pi}_0\mathbb{W})^{n-1}$

$$\mathbb{\Pi}_\alpha(\omega)\mathbb{V} - \mathbb{\Pi}_0(\omega)\mathbb{V} = \sum_{n=2} \alpha^{n-1} \boxed{(\mathbb{\Pi}_0\mathbb{W})^{n-1}\mathbb{\Pi}_0\mathbb{V}}$$

$$\begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix}^{n-1} + \sum_{p=1}^{n-1} \begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix}^{n-1-p} \begin{pmatrix} \mathbf{\Pi}_0^+(\mathbf{A}'-\mathbf{B}) & \mathbf{0} \\ \mathbf{0} & \mathbf{\Pi}_0^-(\mathbf{A}'-\mathbf{B}) \end{pmatrix} \begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix}^{p-1}$$

RPAx-I

$$E_c^{\text{dRPA-II}} = -\frac{1}{2}\int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i}\, \mathrm{Tr}\{\mathbb{\Pi}_\alpha(\omega)\mathbb{V} - \mathbb{\Pi}_0(\omega)\mathbb{V}\}$$

$$\mathbb{W} = \begin{pmatrix} \mathbf{A}' & \mathbf{B} \\ \mathbf{B} & \mathbf{A}' \end{pmatrix}$$

$$\mathbb{W} = \begin{pmatrix} \mathbf{B} & \mathbf{B} \\ \mathbf{B} & \mathbf{B} \end{pmatrix} + \begin{pmatrix} \mathbf{A}'-\mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}'-\mathbf{B} \end{pmatrix}$$

$$\mathbb{V} = \begin{pmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \mathbf{K} \end{pmatrix}$$

Dyson $\quad \mathbb{\Pi}_\alpha = (\mathbb{1} - \alpha\mathbb{\Pi}_0\mathbb{W})^{-1}\mathbb{\Pi}_0$

Taylor $\quad \mathbb{\Pi}_\alpha = 1 + \sum_{n=2} \alpha^{n-1}(\mathbb{\Pi}_0\mathbb{W})^{n-1}$

$$\mathbb{\Pi}_\alpha(\omega)\mathbb{V} - \mathbb{\Pi}_0(\omega)\mathbb{V} = \sum_{n=2} \alpha^{n-1} \boxed{(\mathbb{\Pi}_0\mathbb{W})^{n-1}\mathbb{\Pi}_0\mathbb{V}}$$

$$\begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix}^{n-1} + \sum_{p=1}^{n-1} \begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix}^{n-1-p} \begin{pmatrix} \mathbf{\Pi}_0^+(\mathbf{A}'-\mathbf{B}) & \mathbf{0} \\ \mathbf{0} & \mathbf{\Pi}_0^-(\mathbf{A}'-\mathbf{B}) \end{pmatrix} \begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix}^{p-1}$$

$$E_c^{\text{RPAx-I}} = -\frac{1}{2}\int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathrm{tr}\left\{ \sum_{n=2}^{\infty} \alpha^{n-1} (\mathbf{\Pi}_0\mathbf{B})^{n-1}\, \mathbf{\Pi}_0\mathbf{K} \right\}.$$

RPAx-I

$$E_c^{\text{dRPA-II}} = -\frac{1}{2}\int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i}\, \mathrm{Tr}\{\mathbb{\Pi}_\alpha(\omega)\mathbb{V} - \mathbb{\Pi}_0(\omega)\mathbb{V}\}$$

$$\mathbb{W} = \begin{pmatrix} \mathbf{A}' & \mathbf{B} \\ \mathbf{B} & \mathbf{A}' \end{pmatrix}$$

$$\mathbb{W} = \begin{pmatrix} \mathbf{B} & \mathbf{B} \\ \mathbf{B} & \mathbf{B} \end{pmatrix} + \begin{pmatrix} \mathbf{A}'-\mathbf{B} & 0 \\ 0 & \mathbf{A}'-\mathbf{B} \end{pmatrix}$$

$$\mathbb{V} = \begin{pmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \mathbf{K} \end{pmatrix}$$

Dyson $\quad \mathbb{\Pi}_\alpha = (\mathbb{1} - \alpha\mathbb{\Pi}_0\mathbb{W})^{-1}\mathbb{\Pi}_0$

Taylor $\quad \mathbb{\Pi}_\alpha = 1 + \sum_{n=2} \alpha^{n-1}(\mathbb{\Pi}_0\mathbb{W})^{n-1}$

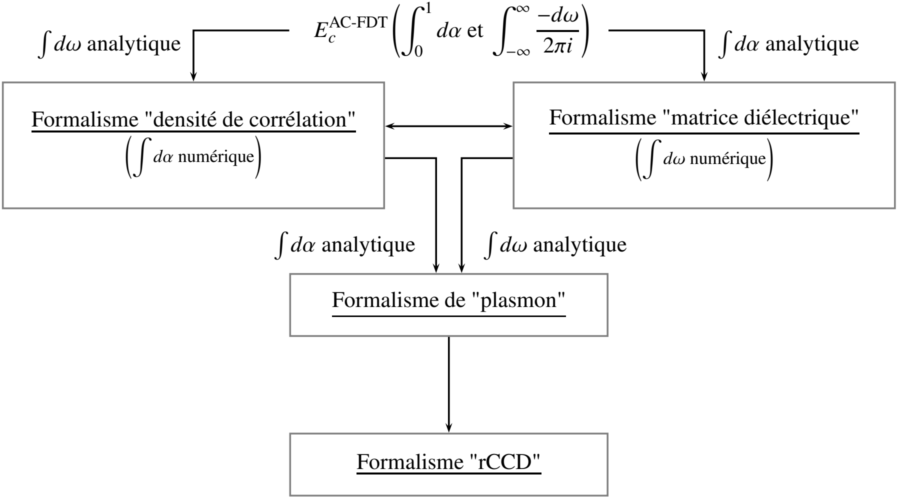
$$\mathbb{\Pi}_\alpha(\omega)\mathbb{V} - \mathbb{\Pi}_0(\omega)\mathbb{V} = \sum_{n=2} \alpha^{n-1} \boxed{(\mathbb{\Pi}_0\mathbb{W})^{n-1}\mathbb{\Pi}_0\mathbb{V}}$$

$$\begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix}^{n-1} + \sum_{p=1}^{n-1} \begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix}^{n-1-p} \begin{pmatrix} \mathbf{\Pi}_0^+(\mathbf{A}'-\mathbf{B}) & 0 \\ 0 & \mathbf{\Pi}_0^-(\mathbf{A}'-\mathbf{B}) \end{pmatrix} \begin{pmatrix} \mathbf{\Pi}_0^+\mathbf{B} & \mathbf{\Pi}_0^+\mathbf{B} \\ \mathbf{\Pi}_0^-\mathbf{B} & \mathbf{\Pi}_0^-\mathbf{B} \end{pmatrix}^{p-1}$$

$$E_c^{\text{RPAx-I}} = -\frac{1}{2}\int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\mathrm{tr}\left\{\sum_{n=2}^{\infty} \alpha^{n-1}\left(\mathbf{\Pi}_0\mathbf{B}\right)^{n-1}\mathbf{\Pi}_0\mathbf{K}\right\}.$$

$$E_c^{\text{RPAx-I}} = \frac{1}{2}\int \frac{d\omega}{2\pi}\mathrm{tr}\left\{\mathrm{Log}\left(\mathbf{I} - \mathbf{\Pi}_0\mathbf{B}\right)\mathbf{B}^{-1}\mathbf{K} + \mathbf{\Pi}_0\mathbf{K}\right\}$$

- similar to Hesselmann's RPAX2
- can be obtain in a « RPAx-IIa »way
- second-order is MP2


$E_c^{\text{AC-FDT}}\left(\int_0^1 d\alpha \text{ et } \int_{-\infty}^{\infty} \frac{-d\omega}{2\pi i}\right)$
$\int d\omega$ analytique
$\int d\alpha$ analytique
Formalisme "densité de corrélation"
$\left(\int d\alpha \text{ numérique}\right)$
Formalisme "matrice diélectrique"
$\left(\int d\omega \text{ numérique}\right)$
$\int d\alpha$ analytique
$\int d\omega$ analytique
Formalisme de "plasmon"
Formalisme "rCCD"

- computational realization
  (symmetric expressions, logarithm/power series, DF)
- numerical frequency integration
  (Clenshaw-Curtis
  parameter a based on analytical integration of a diagonal model)

- (might be cleaner with $f(A) = P.f(D).P^{-1}$)