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

Bastien Mussard, János G. Ángyán; Georg Jansen CRM², Université de Lorraine, Nancy, France

$$E_c^{\mathsf{AC-FDT}} = -rac{1}{2}\int_0^1\!dlpha\int_{-\infty}^\infty\!rac{d\omega}{2\pi i}\,\mathrm{Tr}\left\{\mathbb{\Pi}_lpha(\omega)\mathbb{V}-\mathbb{\Pi}_0(\omega)\mathbb{V}
ight\}$$

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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 $E = \int d\alpha P_{\alpha} \mathbf{V}$ (JCTC2011)
- dielectric-matrix formulation
- ▶ plasmon formula $E = \sum \omega_{RPA} \omega_{LDA}$ (rather limited)
- Ricatti equations and rCCD E=tr(BT) (explored)

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

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Flavors (Exchange)

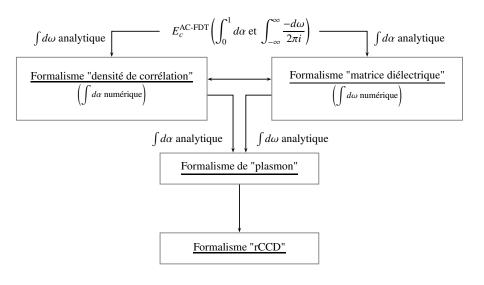
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+Approximations (in each formulations, for each flavors...)



What you (may) know
$$E_c^{\text{RPA}} = -\frac{1}{2} \int_0^1 d\alpha \int_{-\infty}^\infty \frac{d\omega}{2\pi i} \operatorname{Tr} \left\{ \mathbb{I}_{\alpha}(\omega) \mathbb{V} - \mathbb{I}_0(\omega) \mathbb{V} \right\}$$

$$\Pi_{0}(\omega) = -(\mathbb{A}_{0} - \omega \mathbb{A})^{-1}$$

$$\mathbb{A}_{0} = \begin{pmatrix} \epsilon & \mathbf{0} \\ \mathbf{0} & \epsilon \end{pmatrix} \qquad \mathbb{A} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -1 \end{pmatrix}$$

$$\Pi_{0}(\omega) = -(\Lambda_{0} - \omega \Delta)^{-1}$$

$$\Lambda_{0} = \begin{pmatrix} \epsilon & \mathbf{0} \\ \mathbf{0} & \epsilon \end{pmatrix} \qquad \Delta = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}$$

$$\Pi_{0}(\omega) = \begin{pmatrix} -(\epsilon - \omega \mathbf{1})^{-1} & \mathbf{0} \\ \mathbf{0} & -(\epsilon + \omega \mathbf{1})^{-1} \end{pmatrix} = \begin{pmatrix} \mathbf{\Pi}_{0}^{+} & \mathbf{0} \\ \mathbf{0} & \mathbf{\Pi}_{0}^{-} \end{pmatrix}$$

$\boxed{ \mathbb{\Pi}_0(\omega) {=} {-} (\mathbb{A}_0 {-} \omega \mathbb{A})^{-1} } \qquad \boxed{ (\mathbb{\Pi}_\alpha)^{-1} {=} (\mathbb{\Pi}_0)^{-1} {-} \alpha \mathbb{V} }$

$$\begin{bmatrix} \mathbb{I}_{0}(\omega) = -(\mathbb{N}_{0} - \omega \mathbb{Z})^{-1} \\ \mathbb{N}_{0} = \begin{pmatrix} \epsilon & \mathbf{0} \\ \mathbf{0} & \epsilon \end{pmatrix} & \mathbb{A} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix} \\ \mathbb{\Pi}_{0}(\omega) = \begin{pmatrix} -(\epsilon - \omega \mathbf{1})^{-1} & \mathbf{0} \\ \mathbf{0} & -(\epsilon + \omega \mathbf{1})^{-1} \end{pmatrix} = \begin{pmatrix} \mathbf{\Pi}_{0}^{+} & \mathbf{0} \\ \mathbf{0} & \mathbf{\Pi}_{0}^{-} \end{pmatrix}$$

$$\square_0(\omega) = -(\wedge_0 - \omega \wedge)^{-1}$$

$$\begin{bmatrix}
\Pi_{0}(\omega) = -(\mathbb{A}_{0} - \omega \mathbb{A})^{-1} \\
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\Pi_{0}(\omega) = \begin{pmatrix} -(\epsilon - \omega \mathbf{1})^{-1} & \mathbf{0} \\ \mathbf{0} & -1 \end{pmatrix} = \begin{pmatrix} \Pi_{0}^{+} & \mathbf{0} \\ \mathbf{0} & -1 \end{pmatrix}$$

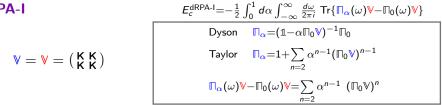
What you (may) know $E_c^{\text{RPA}} = -\frac{1}{2} \int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \operatorname{Tr} \left\{ \mathbb{I}_{\alpha}(\omega) \mathbb{V} - \mathbb{I}_0(\omega) \mathbb{V} \right\}$

$$\begin{bmatrix} \Pi_0(\omega) \! = \! -(\mathbb{A}_0 - \omega \mathbb{A})^{-1} \\ \mathbb{A}_0 \! = \! \begin{pmatrix} \epsilon & \mathbf{0} \\ \mathbf{0} & \epsilon \end{pmatrix} & \mathbb{A} \! = \! \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix} \\ \Pi_0(\omega) \! = \! \begin{pmatrix} -(\epsilon \! - \! \omega \mathbf{1})^{-1} & \mathbf{0} \\ \mathbf{0} & -(\epsilon \! + \! \omega \mathbf{1})^{-1} \end{pmatrix} \! = \! \begin{pmatrix} \Pi_0^+ & \mathbf{0} \\ \mathbf{0} & \Pi_0^- \end{pmatrix} \\ \end{bmatrix} \\ \mathbb{V} \! = \! \begin{pmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \mathbf{K} \end{pmatrix} \quad \text{or} \quad \mathbb{V} \! = \! \begin{pmatrix} \mathbf{A}' & \mathbf{B} \\ \mathbf{B} & \mathbf{A}' \end{pmatrix}$$

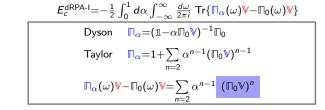
The goals

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

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



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



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

$$\Pi_0 = \Pi_0^+ + \Pi_0^-$$

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

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

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

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

$$\Pi_{\alpha}(\omega) \mathbb{V} - \Pi_{0}(\omega) \mathbb{V} = \sum_{n=2} \alpha^{n-1} (\Pi_{0} \mathbb{V})^{n}$$

$$\operatorname{Tr}\{(\Pi_0 \, \mathbb{V})^n\} = \operatorname{Tr}\left\{ \left(\begin{array}{cc} \Pi_0^+ \mathsf{K} & \Pi_0^+ \mathsf{K} \\ \Pi_0^- \mathsf{K} & \Pi_0^- \mathsf{K} \end{array} \right)^n \right\} = \operatorname{tr}\{(\Pi_0 \mathsf{K})^n\}$$

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

 $\mathbb{V} = \mathbb{V} = (\mathbf{K} \mathbf{K})$

 $\Pi_0 = \Pi_0^+ + \Pi_0^-$

Taylor $\Pi_{\alpha} = 1 + \sum_{n=2}^{\infty} \alpha^{n-1} (\Pi_0 \mathbb{V})^{n-1}$ $\Pi_{\alpha}(\omega) \vee -\Pi_{0}(\omega) \vee = \sum_{n=2} \alpha^{n-1} (\Pi_{0} \vee)^{n}$

 $\operatorname{Tr}\{(\Pi_0 \, \mathbb{V})^n\} = \operatorname{Tr}\left\{ \left(\begin{array}{cc} \Pi_0^+ \mathbf{K} & \Pi_0^+ \mathbf{K} \\ \Pi_0^- \mathbf{K} & \Pi_0^- \mathbf{K} \end{array} \right)^n \right\} = \operatorname{tr}\{(\Pi_0 \mathbf{K})^n\}$

 $E_c^{\mathsf{dRPA-I}} = -\frac{1}{2} \int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \operatorname{tr} \left\{ \sum_{r=2}^{\infty} \alpha^{r-1} \left(\mathbf{\Pi}_0 \mathbf{K} \right)^r \right\}$ $E_c^{\mathsf{dRPA-I}} = -\frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \operatorname{tr} \left\{ \sum_{n} \frac{\left(\Pi_0 \mathbf{K} \right)^n}{n} \right\}$

$$E_c^{\mathsf{dRPA-I}} = rac{1}{2} \int_{-\infty}^{\infty} rac{d\omega}{2\pi i} \operatorname{tr}\left\{ \operatorname{Log}\left(\mathbf{1} - \mathbf{\Pi}_0 \mathbf{K}\right) + \mathbf{\Pi}_0 \mathbf{K} \right\}$$

$$\mathbf{V} = (\mathbf{K} \mathbf{K} \mathbf{K})$$

$$\mathbf{W} = \left(\begin{smallmatrix} \mathbf{A}' & \mathbf{B} \\ \mathbf{B} & \mathbf{A}' \end{smallmatrix} \right)$$

 $(SX) \qquad E_c^{dRPA-II} = -\frac{1}{2} \int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \operatorname{Tr}\{\Pi_{\alpha}(\omega) \mathbb{W} - \Pi_0(\omega) \mathbb{W}\}$ $(SX) \qquad \qquad \mathbb{I}_{\alpha} = (\mathbb{1} - \alpha \Pi_0 \mathbb{W})^{-1} \Pi_0$

Taylor
$$\Pi_{\alpha} = (\mathbb{I} - \alpha \mathbb{I}_1)^{\vee}$$
 \mathbb{I}_0

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

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

$$V = (K K)$$

$$\mathbf{W} = \left(egin{array}{cc} \mathbf{A}' & \mathbf{B} \\ \mathbf{B} & \mathbf{A}' \end{array}
ight)$$

 $(SX) \qquad E_{c}^{dRPA-II} = -\frac{1}{2} \int_{0}^{1} d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \operatorname{Tr}\{\Pi_{\alpha}(\omega) \mathbb{W} - \Pi_{0}(\omega) \mathbb{W}\}$ $K \setminus K \setminus K \setminus B \quad Dyson \quad \Pi_{\alpha} = (\mathbb{1} - \alpha \Pi_{0} \mathbb{V})^{-1} \Pi_{0}$ $Taylor \quad \Pi_{\alpha} = 1 + \sum_{n=2} \alpha^{n-1} (\Pi_{0} \mathbb{V})^{n-1}$ $\Pi_{\alpha}(\omega) \mathbb{W} - \Pi_{0}(\omega) \mathbb{W} = \sum_{n=2} \alpha^{n-1} (\Pi_{0} \mathbb{V})^{n-1} \Pi_{0} \mathbb{W}$

$$\begin{aligned} \mathbb{V} &= \left(\begin{smallmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \mathbf{K} \end{smallmatrix} \right) \\ \mathbf{W} &= \left(\begin{smallmatrix} \mathbf{A}' & \mathbf{B} \\ \mathbf{B} & \mathbf{A}' \end{smallmatrix} \right) \\ \mathbf{W} &= \left(\begin{smallmatrix} \mathbf{B} & \mathbf{B} \\ \mathbf{B} & \mathbf{B} \end{smallmatrix} \right) + \left(\begin{smallmatrix} \mathbf{A}' - \mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}' - \mathbf{B} \end{smallmatrix} \right) \end{aligned}$$

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

$$) \mathbb{W} - \mathbb{I}_0(\omega) \mathbb{W} = \sum_{n=1}^{\infty} \alpha^{n-1}$$

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

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

$$\operatorname{Tr} \left\{ \left(\begin{array}{cc} \Pi_0^+ \mathsf{K} & \Pi_0^+ \mathsf{K} \\ \Pi_0^- \mathsf{K} & \Pi_0^- \mathsf{K} \end{array} \right)^{n} \right\}$$

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

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

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

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

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

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

 $\Pi_{\alpha}(\omega) \mathbb{W} - \Pi_{0}(\omega) \mathbb{W} = \sum_{n=2}^{\infty} \alpha^{n-1} \left(\Pi_{0} \mathbb{V} \right)^{n-1} \Pi_{0} \mathbb{W}$

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

 $\mathsf{Tr} \left\{ \begin{pmatrix} \Pi_0^+ \mathsf{K} & \Pi_0^+ \mathsf{K} \\ \Pi_0^- \mathsf{K} & \Pi_0^- \mathsf{K} \end{pmatrix}^{n-1} \left[\begin{pmatrix} \Pi_0^+ \mathsf{B} & \Pi_0^+ \mathsf{B} \\ \Pi_0^- \mathsf{B} & \Pi_0^- \mathsf{B} \end{pmatrix} + \begin{pmatrix} \Pi_0^+ (\mathsf{A}' - \mathsf{B}) & \mathbf{0} \\ \mathbf{0} & \Pi_0^- (\mathsf{A}' - \mathsf{B}) \end{pmatrix} \right] \right\}$

 $\mathsf{tr}\big\{(\Pi_0\mathsf{K})^{n-1}\Pi_0\mathsf{B}\big\} + \mathsf{tr}\big\{\big(\Pi_0^+\mathsf{K}(\Pi_0\mathsf{K})^{n-2}\Pi_0^+ + \Pi_0^-\mathsf{K}(\Pi_0\mathsf{K})^{n-2}\Pi_0^-\big)(\mathsf{A}'-\mathsf{B})\big\}$

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

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

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

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

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

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

$$\bigcap_{\alpha}(\omega)$$

 $\Pi_{\alpha}(\omega) \mathbb{W} - \Pi_{0}(\omega) \mathbb{W} = \sum_{n=2} \alpha^{n-1} (\Pi_{0} \mathbb{V})^{n-1} \Pi_{0} \mathbb{W}$

$$\operatorname{Tr} \left\{ \left(\begin{array}{cc} \Pi_0^+ \mathsf{K} & \Pi_0^+ \mathsf{K} \\ \Pi^- \mathsf{K} & \Pi^- \mathsf{K} \end{array} \right)^{n} \right\}$$

B
$$\Pi_0^+$$
B \ $\left(\Pi_0^+(A'-B) \quad 0 \quad \right)$

$$\mathsf{Tr} \Bigg\{ \left(\frac{\Pi_0^+ \mathsf{K} \ \Pi_0^+ \mathsf{K}}{\Pi_0^- \mathsf{K} \ \Pi_0^- \mathsf{K}} \right)^{n-1} \left[\left(\frac{\Pi_0^+ \mathsf{B} \ \Pi_0^+ \mathsf{B}}{\Pi_0^- \mathsf{B} \ \Pi_0^- \mathsf{B}} \right) + \left(\frac{\Pi_0^+ (\mathsf{A}' - \mathsf{B})}{0 \ \Pi_0^- (\mathsf{A}' - \mathsf{B})} \right) \right] \Bigg\}$$

$$\operatorname{Tr}\left\{ \left(\begin{array}{cc} \Pi_0 & \mathbf{K} & \Pi_0 & \mathbf{K} \\ \Pi_0 & \mathbf{K} & \Pi_0 & \mathbf{K} \end{array} \right) \quad \left[\left(\begin{array}{cc} \Pi_0 & \mathbf{B} & \Pi_0 & \mathbf{B} \\ \Pi_0 & \mathbf{B} & \Pi_0 & \mathbf{B} \end{array} \right) + \left(\begin{array}{cc} \Pi_0 & \mathbf{A} & -\mathbf{B} \end{pmatrix} & \mathbf{0} \\ \mathbf{0} & \Pi_0 & (\mathbf{A}' - \mathbf{B}) \end{array} \right) \right] \right\}$$

 $\mathsf{tr} \big\{ (\Pi_0 \mathsf{K})^{n-1} \Pi_0 \mathsf{B} \big\} + \mathsf{tr} \big\{ \big(\Pi_0^+ \mathsf{K} (\Pi_0 \mathsf{K})^{n-2} \Pi_0^+ + \Pi_0^- \mathsf{K} (\Pi_0 \mathsf{K})^{n-2} \Pi_0^- \big) (\mathsf{A}' - \mathsf{B}) \big\}$

$$\begin{split} \mathbb{V} &= \left(\begin{smallmatrix} \mathbf{K} & \mathbf{K} \\ \mathbf{K} & \mathbf{K} \end{smallmatrix} \right) \\ \mathbb{W} &= \left(\begin{smallmatrix} \mathbf{A}' & \mathbf{B} \\ \mathbf{B} & \mathbf{A}' \end{smallmatrix} \right) \\ \mathbb{W} &= \left(\begin{smallmatrix} \mathbf{B} & \mathbf{B} \\ \mathbf{B} & \mathbf{B} \end{smallmatrix} \right) + \left(\begin{smallmatrix} \mathbf{A}' - \mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}' - \mathbf{B} \end{smallmatrix} \right) \end{split}$$

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

 $\mathsf{tr} \big\{ (\Pi_0 \mathsf{K})^{n-1} \Pi_0 \mathsf{B} \big\} + \mathsf{tr} \big\{ \big(\Pi_0^+ \mathsf{K} (\Pi_0 \mathsf{K})^{n-2} \Pi_0^+ + \Pi_0^- \mathsf{K} (\Pi_0 \mathsf{K})^{n-2} \Pi_0^- \big) (\mathsf{A}' - \mathsf{B}) \big\}$

 $E_c^{\mathrm{dRPA-IIa}} = -\frac{1}{2} \int_0^1 d\alpha \int_{-\infty}^\infty \frac{d\omega}{2\pi} \mathrm{tr} \left\{ \sum_{n=0}^\infty \alpha^{n-1} \left(\Pi_0 \mathbf{K} \right)^{n-1} \Pi_0 \mathbf{B} \right\}.$

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

 $\Pi_{\alpha}(\omega) \mathbb{W} - \Pi_{0}(\omega) \mathbb{W} = \sum_{n=2} \alpha^{n-1} \left(\Pi_{0} \mathbb{V} \right)^{n-1} \Pi_{0} \mathbb{W}$

 $\mathsf{Tr} \left\{ \begin{pmatrix} \Pi_0^+ \mathsf{K} & \Pi_0^+ \mathsf{K} \\ \Pi_0^- \mathsf{K} & \Pi_0^- \mathsf{K} \end{pmatrix}^{n-1} \left[\begin{pmatrix} \Pi_0^+ \mathsf{B} & \Pi_0^+ \mathsf{B} \\ \Pi_0^- \mathsf{B} & \Pi_0^- \mathsf{B} \end{pmatrix} + \begin{pmatrix} \Pi_0^+ (\mathsf{A}' - \mathsf{B}) & \mathbf{0} \\ \mathbf{0} & \Pi_0^- (\mathsf{A}' - \mathsf{B}) \end{pmatrix} \right] \right\}$

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

$$\begin{split} & \operatorname{Tr} \left\{ \begin{pmatrix} \Pi_0^+ \mathsf{K} \ \Pi_0^+ \mathsf{K} \\ \Pi_0^- \mathsf{K} \ \Pi_0^- \mathsf{K} \end{pmatrix}^{n-1} \left[\begin{pmatrix} \Pi_0^+ \mathsf{B} \ \Pi_0^+ \mathsf{B} \\ \Pi_0^- \mathsf{B} \ \Pi_0^- \mathsf{B} \end{pmatrix} + \begin{pmatrix} \Pi_0^+ (\mathsf{A}' - \mathsf{B}) & \mathbf{0} \\ \mathbf{0} & \Pi_0^- (\mathsf{A}' - \mathsf{B}) \end{pmatrix} \right] \right\} \\ & \operatorname{tr} \left\{ (\Pi_0 \mathsf{K})^{n-1} \Pi_0 \mathsf{B} \right\} + \operatorname{tr} \left\{ \left(\Pi_0^+ \mathsf{K} (\Pi_0 \mathsf{K})^{n-2} \Pi_0^+ + \Pi_0^- \mathsf{K} (\Pi_0 \mathsf{K})^{n-2} \Pi_0^- \right) (\mathsf{A}' - \mathsf{B}) \right\} \\ & E_c^{\mathsf{dRPA-IIa}} = -\frac{1}{2} \int_0^1 d\alpha \int_{-\infty}^\infty \frac{d\omega}{2\pi} \operatorname{tr} \left\{ \sum_{k=0}^\infty \alpha^{n-1} \left(\Pi_0 \mathsf{K} \right)^{n-1} \Pi_0 \mathsf{B} \right\}. \end{split}$$

 $E_c^{\text{dRPA-II}} = -\frac{1}{2} \int_0^1 d\alpha \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \operatorname{Tr}\{\Pi_{\alpha}(\omega) \mathbb{W} - \Pi_{0}(\omega) \mathbb{W}\}$

 $\Pi_{\alpha}(\omega) \mathbb{W} - \Pi_{0}(\omega) \mathbb{W} = \sum_{n=2} \alpha^{n-1} (\Pi_{0} \mathbb{V})^{n-1} \Pi_{0} \mathbb{W}$

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

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

dRPA-II (SX)

 $\mathbb{V} = (\mathbf{K} \mathbf{K})$

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

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

Clear link to SOSEX
 B = K − K': you can write « E_c^{dRPA-IIa} = E_c^{dRPA-I} − term »

 $E_c^{ ext{dRPA-IIa}} = rac{1}{2} \int rac{d\omega}{2\pi} ext{tr} \left\{ ext{Log} \left(ext{I} - \Pi_0 ext{K}
ight) ext{K}^{-1} ext{B} + \Pi_0 ext{B}
ight\}$

second-order approximation to dRPA-IIa is MP2

$$\mathsf{RPAx-I}$$
$$\mathsf{W} = \left(\begin{smallmatrix} \mathsf{A} \\ \mathsf{E} \end{smallmatrix}\right)$$

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

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

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

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

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

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

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

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

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

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

$$\mathbb{D}yson \quad \mathbb{\Pi}_{\alpha} = (\mathbb{1} - \alpha \mathbb{\Pi}_{0} \mathbb{W})^{-1} \mathbb{\Pi}_{0}$$

$$\mathbb{T}_{\alpha} = 1 + \sum_{n=2} \alpha^{n-1} (\mathbb{\Pi}_{0} \mathbb{W})^{n-1}$$

$$\mathbb{\Pi}_{\alpha} = \mathbb{I}_{\alpha} = 1 + \sum_{n=2} \alpha^{n-1} (\mathbb{\Pi}_{0} \mathbb{W})^{n-1} \mathbb{\Pi}_{0} = 1 + \sum_{n=2} \alpha^{n-1} (\mathbb{\Pi}_{0} \mathbb{W})^{n-1} = 1 + \sum_{n$$

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

RPAx-I

$$\begin{pmatrix} \Pi_0^+ B & \Pi_0^+ B \\ \Pi_0^- B & \Pi_0^- B \end{pmatrix}^{n-1} + \sum_{p=1}^{n-1} \begin{pmatrix} \Pi_0^+ B & \Pi_0^+ B \\ \Pi_0^- B & \Pi_0^- B \end{pmatrix}^{n-1-p} \begin{pmatrix} \Pi_0^+ (A'-B) & 0 \\ 0 & \Pi_0^- (A'-B) \end{pmatrix} \begin{pmatrix} \Pi_0^+ B & \Pi_0^+ B \\ \Pi_0^- B & \Pi_0^- B \end{pmatrix}^{p-1}$$

$$\left(\frac{\Pi_0^+ B \ \Pi_0^+ B}{\Pi_0^- B \ \Pi_0^- B} \right)^{n-1} + \sum_{\rho=1}^{n-1} \left(\frac{\Pi_0^+ B \ \Pi_0^+ B}{\Pi_0^- B \ \Pi_0^- B} \right)^{n-1-\rho} \left(\frac{\Pi_0^+ (A'-B)}{0 \ \Pi_0^- (A'-B)} \right) \left(\frac{\Pi_0^+ B \ \Pi_0^+ B}{\Pi_0^- B \ \Pi_0^- B} \right)^{\rho-1}$$

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

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

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

$$\mathbb{D}yson \quad \mathbb{\Pi}_{\alpha} = (\mathbb{1} - \alpha \mathbb{\Pi}_{0} \mathbb{W})^{-1} \mathbb{\Pi}_{0}$$

$$\mathbb{T}_{\alpha} = 1 + \sum_{n=2} \alpha^{n-1} (\mathbb{\Pi}_{0} \mathbb{W})^{n-1}$$

$$\mathbb{\Pi}_{\alpha} = (\mathbb{1} - \alpha \mathbb{\Pi}_{0} \mathbb{W})^{n-1} \mathbb{\Pi}_{0} \mathbb{W}$$

$$\mathbb{\Pi}_{\alpha} = (\mathbb{1} - \alpha \mathbb{\Pi}_{0} \mathbb{W})^{n-1} \mathbb{\Pi}_{0} \mathbb{W}$$

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

RPAx-I

$$\left(\begin{array}{ccc} \Pi_0^+ B & \Pi_0^+ B \\ \Pi_0^- B & \Pi_0^- B \end{array} \right)^{n-1} + \sum_{\rho=1}^{n-1} \left(\begin{array}{ccc} \Pi_0^+ B & \Pi_0^+ B \\ \Pi_0^- B & \Pi_0^- B \end{array} \right)^{n-1-\rho} \left(\begin{array}{ccc} \Pi_0^+ (A'-B) & 0 \\ 0 & \Pi_0^- (A'-B) \end{array} \right) \left(\begin{array}{ccc} \Pi_0^+ B & \Pi_0^+ B \\ \Pi_0^- B & \Pi_0^- B \end{array} \right)^{\rho-1}$$

 $\mathbb{W} = \begin{pmatrix} \mathbf{A}' & \mathbf{B} \\ \mathbf{B} & \mathbf{A}' \end{pmatrix}$ Dyson $\Pi_{\alpha} = (\mathbb{1} - \alpha \Pi_0 \mathbb{W})^{-1} \Pi_0$ Taylor $\Pi_{\alpha} = 1 + \sum_{n=2}^{\infty} \alpha^{n-1} (\Pi_0 \mathbb{W})^{n-1}$ $\mathbb{W} = \left(\begin{smallmatrix} \mathbf{B} & \mathbf{B} \\ \mathbf{B} & \mathbf{B} \end{smallmatrix} \right) + \left(\begin{smallmatrix} \mathbf{A}' - \mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}' - \mathbf{B} \end{smallmatrix} \right)$ $\Pi_{\alpha}(\omega) \bigvee - \Pi_{0}(\omega) \bigvee = \sum_{n=2} \alpha^{n-1} (\Pi_{0} \bigvee)^{n-1} \Pi_{0} \bigvee$ $\mathbf{V} = (\mathbf{K} \mathbf{K})$

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

RPAx-I

$$egin{aligned} \left(oldsymbol{\Pi}_0 \, oldsymbol{\mathsf{B}} \, oldsymbol{\Pi}_0 \, oldsymbol{\mathsf{B}} \, oldsymbol{\mathsf{H}}_0 \, oldsymbol{\mathsf{H}}_0 \, oldsymbol{\mathsf{B}} \, oldsymbol{\mathsf{H}}_0 \,$$

 $\mathbb{W} = \begin{pmatrix} \mathbf{B} \ \mathbf{B} \\ \mathbf{B} \ \mathbf{B} \end{pmatrix} + \begin{pmatrix} \mathbf{A}' - \mathbf{B} \ \mathbf{0} \\ \mathbf{0} \ \mathbf{A}' - \mathbf{B} \end{pmatrix}$ $\mathbb{V} = (\mathbf{K} \mathbf{K})$ $\left(\begin{array}{c} \Pi_0^+ B \ \Pi_0^+ B \\ \Pi_0^- B \ \Pi_0^- B \end{array} \right)^{n-1} + \sum_{p=1}^{n-1} \left(\begin{array}{c} \Pi_0^+ B \ \Pi_0^+ B \\ \Pi_0^- B \ \Pi_0^- B \end{array} \right)^{n-1-p} \left(\begin{array}{c} \Pi_0^+ (A'-B) \ 0 \\ 0 \end{array} \right) \left(\begin{array}{c} \Pi_0^+ B \ \Pi_0^+ B \\ \Pi_0^- B \ \Pi_0^- B \end{array} \right)^{p-1}$

RPAx-I

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

$$\begin{array}{c} \mathbf{0} \\ \mathbf{A}' - \mathbf{B} \end{array} \right) \qquad \begin{array}{c} \mathsf{Taylor} \qquad \mathbb{I}_{\alpha} = 1 + \sum_{n=2} \alpha^{n-1} (\mathbb{I}_0 \mathbb{W})^{n-1} \\ \mathbb{I}_{\alpha}(\omega) \mathbb{V} - \mathbb{I}_0(\omega) \mathbb{V} = \sum_{n=2} \alpha^{n-1} (\mathbb{I}_0 \mathbb{W})^{n-1} \mathbb{I}_0 \mathbb{V} \end{array}$$

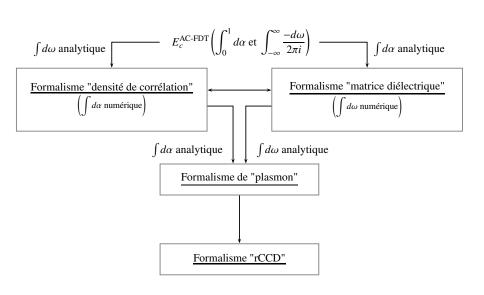
 $E_c^{\mathsf{RPAx-I}} = -\frac{1}{2} \int_0^1 d\alpha \int_{-\infty}^\infty \frac{d\omega}{2\pi} \mathsf{tr} \left\{ \sum_{n=0}^\infty \alpha^{n-1} (\mathbf{\Pi}_0 \mathbf{B})^{n-1} \mathbf{\Pi}_0 \mathbf{K} \right\}.$

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

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

$$E_c^{ extsf{RPAx-I}} = rac{1}{2} \int rac{d\omega}{2\pi} extsf{tr} \left\{ extsf{Log} \left(extsf{I} - oldsymbol{\Pi}_0 extbf{B}
ight) extbf{B}^{-1} extbf{K} + oldsymbol{\Pi}_0 extbf{K}
ight\}$$

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



- 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 $f(A) = P.f(D).P^{-1}$)