On the merging of DF(P)T and Many-Body Perturbation theory: a practical scheme

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Outline

(1) The DFT and MB perspectives
(2) Self-Consistency and screening in MBPT
(3) A practical scheme for DF(P)T–MBPT merging
The DF(P)T and MBPT perspectives compared (I)

\[ h_{DFT} = \left[ \frac{-\nabla^2}{2} + V_{\text{ion}}(r) + V_{\text{Hxc}}(r) \right] \]

\[ \Sigma_{\text{MBPT}} = \Sigma[G_{ks}] - V_{xc} \]

\[ H[[R]] = H[[R_0]] + \sum_R \nabla_R V_{\text{ion}}[[R]] \cdot u_R + \frac{1}{2} \sum_{R R'} \nabla_R \nabla_{R'} V_{\text{ion}}[[R]] \cdot u_R u_{R'} \]

\[ \Delta E_i^{(2)} = \frac{1}{2} \sum_{R R'} \langle i | \nabla_R \nabla_{R'} V_{\text{ion}}[[R]] | i \rangle \langle \tilde{u}_R \tilde{u}_{R'} \rangle \neq \Delta E_i^{(2)} = \frac{1}{2} \sum_{R R'} \langle i | \nabla_R \nabla_{R'} V_{\text{scf}}[[R]] | i \rangle \langle u_R u_{R'} \rangle \]

“bare” ≠ “dressed”
The DFPT and MBPT perspectives compared (II)

\[ \sum_R \nabla_R V_{ion}([R]) \cdot u_R \approx \tilde{g} c^+ c (\tilde{b} + \tilde{b}^+) \]

\[ \sum_R \nabla_R V_{scf}([R]) \cdot u_R \approx g c^+ c (b + b^+) \]
The "strategy": merge a purely MB approach with DFPT "ingredients" avoiding double-counting and over-screening.
DF(P)T in a nutshell

\[ \{ R \} \rightarrow \{ R + u_R \} \]
\[ H\{ R \} \rightarrow H\{ R = R_o \} + \delta H^{(1)}_{scf} + \delta H^{(2)}_{scf} \]

\[ \partial_u^2 \Delta E_i(T) \approx \left\{ \frac{1}{2} \langle i | V^{(2)}_{scf} (r) | i \rangle + \sum_{j \neq i} \frac{| \langle i | V^{(1)}_{scf} (r) | j \rangle |^2}{(E_j - E_i)} \right\} (2N+1) \]

Heine-Allen-Cardona Theory

Static (& purely electronic) screening
Non diagonal DW
Test-Particle dielectric function to mimic vertex corrections

No phonon frequencies (= adiabatic ansatz)
The diagrammatic way (I)  

Bare el  

Bare ph  

Bare e–e interaction  

\[ V_{\text{ion}}^{(2)}(r) \quad V_{\text{ion}}^{(1)}(r) \]

Oops! In DFPT this is 0!

Oops! In MBPT self-consistency is also screening!

1st order  

2nd order
The diagrammatic way (II)

MBPT

\[
\int \epsilon_{TC, e-e}^{-1}(rr', \omega) V_{ion}^{(1)}(r')
\]

\[
\int \epsilon_{TC, TOTAL}^{-1}(rr') V_{ion}^{(2)}(r')
\]

DFPT

\[
\int \epsilon_{TP}^{-1}(rr') V_{ion}^{(1)}(r')
\]

\[
\int \partial_u \left[ \epsilon_{TP}^{-1}(rr') V_{ion}^{(1)}(r') \right]
\]
Some comments on the translational invariance

\[ \Delta E_i(\{R \to R+u\}T) = \Delta E_i(T) \]

\[ \approx D_{ph}(\omega=0) \approx \frac{\omega_{ph}}{(i\theta^+)^2 + \omega^2_{ph}} = 0 \]

\[ \Sigma_i(\{R \to R+u\}, \omega, T) \neq \Sigma_i(\omega, T) \]

\[ \neq 0 \]
A practical way to merge MBPT and DF(P)T

\[ \Sigma_i(\omega, T) \approx \left( \right) \]

\[ \frac{\epsilon_{TP}^{-1} \approx \epsilon_{TC}^{-1}} {\tilde{\Gamma}} \]

WARNING! Use of MBPT self-consistency must be done selectively to avoid over-screening!

Conclusions

DF(P)T and MBPT can be merged but...

Use of MBPT self-consistency must be done selectively to avoid over-screening!

Tricky use of translational invariance

Different dielectric screening in MBPT can lead to additional problems in low-dimensional systems

Diagrams beyond Fan and DW should be evaluated (is Migdal’s applying?)
People...

... & all diagrams have been drawn by hand