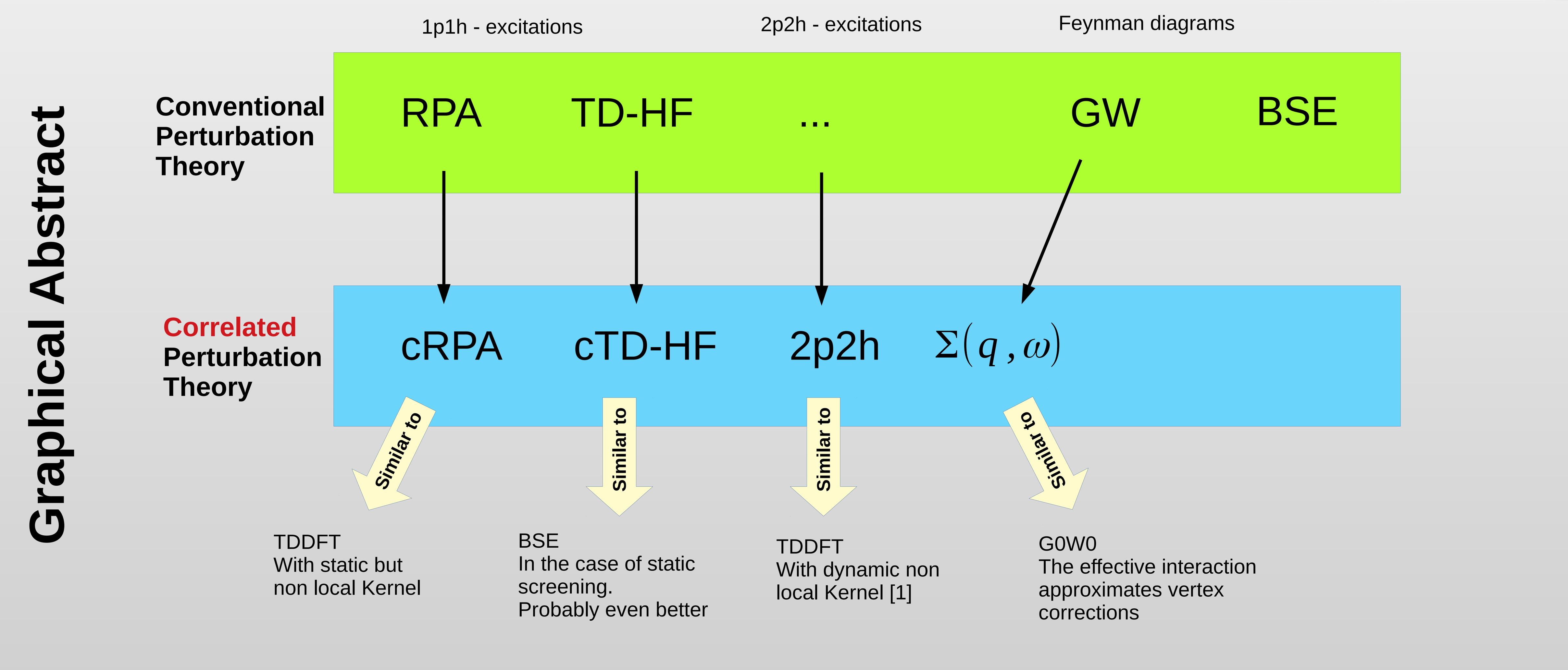
Time Dependent Perturbation theory in a correlated basis

Martin Panholzer
Johannes Kepler University Linz, Institute for Theoretical Physics, 4040 Linz, Austria
Email: Martin.panholzer@jku.at, homepage: www.mpanholzer.com



The Correlated Basis

For more details see e.g. [4,8]

$$|\Psi_{\mathbf{m}}\rangle = \frac{F\,|\Phi_{\mathbf{m}}\rangle}{\langle\Phi_{\mathbf{m}}|F^\dagger F|\Phi_{\mathbf{m}}\rangle^{1/2}}$$

Jastrow correlation factor

Excited Slater determinant e.g. $|\Phi_{ph}\rangle = a_p^\dagger a_h|\Phi_0\rangle$

Normalization

non orthogonal

$$M_{\mathbf{m,n}} = \langle\Psi_{\mathbf{m}}|\Psi_{\mathbf{n}}\rangle \equiv \delta_{\mathbf{m,n}} + N_{\mathbf{m,n}}\,,$$
$$H'_{\mathbf{m,n}} = \langle\Psi_{\mathbf{m}}|H'|\Psi_{\mathbf{n}}\rangle$$
$$\equiv W_{\mathbf{m,n}} + \frac{1}{2}\left(H_{\mathbf{m,m}} + H_{\mathbf{n,n}} - 2H_{\mathbf{o,o}}\right)M_{\mathbf{m,n}}\,.$$

$$M_{p'h',ph} \approx \delta_{p,p'}\delta_{h,h'} + \langle hp'|\Gamma_{\rm dd}|ph'\rangle_a$$

Including exchange

$$H'_{p'h',ph} \approx \delta_{p,p'}\delta_{h,h'}\,e_{ph} + \langle hp'|W|ph'\rangle_a + \frac{1}{2}\left[e_{ph} + e_{p'h'}\right]\langle hp'|\Gamma_{\rm dd}|ph'\rangle_a$$

$$e_{ph} = e(p) - e(h)$$
$$e(q) = \frac{\hbar^2 q^2}{2m} + u(q)$$
$$u(q) = -\sum_k n(k)V_F(q-k)$$

$$S(q) = S_F(q)\left[1 + \Gamma_{\rm dd}(q)\,S_F(q)\right]$$
$$V_F(q) = W(q) \approx -\frac{\hbar^2 q^2}{2mS_F(q)}\Gamma_{dd}(q)$$

Time Dependent HF in our correlated basis

Ansatz:

$$\left|\Psi_t\right\rangle \propto \frac{1}{\mathcal{N}^{1/2}(t)}F\exp\left[\tfrac{1}{2}U(t)\right]\left|\Phi_0\right\rangle$$

$$U(t) \equiv \sum_{ph}\delta u_{ph}^{(1)}(t)\,a_p^\dagger a_h$$

$$\mathcal{L}(t) = \langle\Psi(t)|\,H + H_{\rm ext}(t) - {\rm i}\,\hbar\frac{\partial}{\partial t}\,|\Psi(t)\rangle$$

Minimal action principle

Equations of Motion:

$$\begin{bmatrix} \mathbf{A} - \hbar\omega\mathbf{M} - i\eta & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A}^* + \hbar\omega\mathbf{M}^* + i\eta \end{bmatrix}\begin{pmatrix}\delta u^{(1+)}\\ \delta u^{(1-)}\end{pmatrix} = \begin{pmatrix}\rho_{ph,0}\\ \rho_{0,ph}\end{pmatrix}h_{ext}(q,\omega)$$

Not diagonal

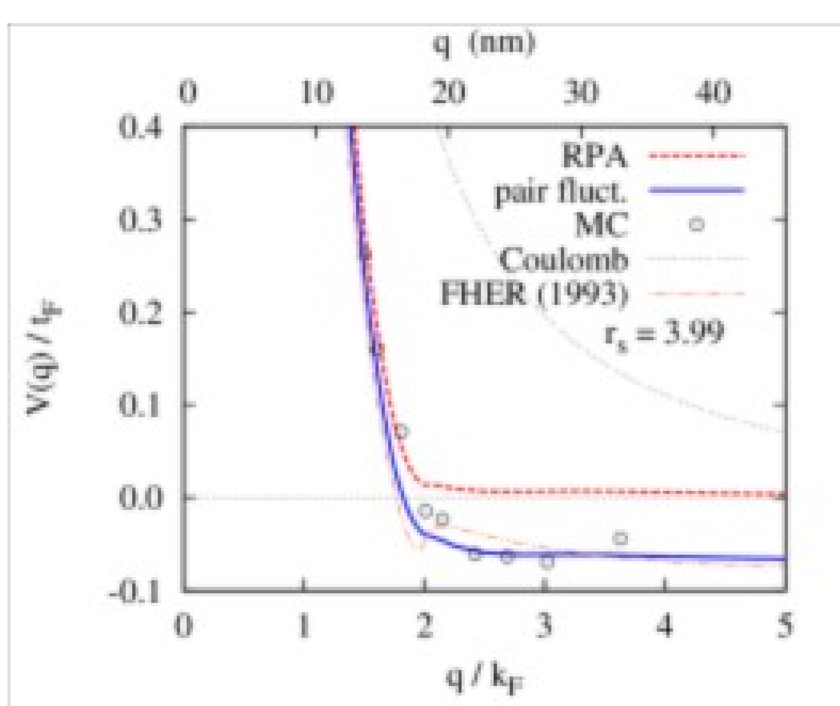
$$A_{ph,p'h'} = e_{ph}\delta_{pp'}\delta_{hh'} + H_{ph,p'h'}$$
$$B_{ph,p'h'} = H_{php'h',0}$$
$$M_{ph,p'h'} = \delta_{pp'}\delta_{hh'} + N_{ph,p'h'}$$

cRPA - Neglect Exchange

- Non interacting single particle energy $e(q) \approx \frac{\hbar^2 q^2}{2m}$
- Still off-diagonal in Energy, Solution: Coordinate Transform

→ The result, for the linear response, is identical to RPA, except the Coulomb interaction is replaced by an effective interaction

$$V_{ph}(q) = \frac{\hbar^2 q^2}{4m}\left(\frac{1}{S(q)^2} - \frac{1}{S_F(q)^2}\right)$$

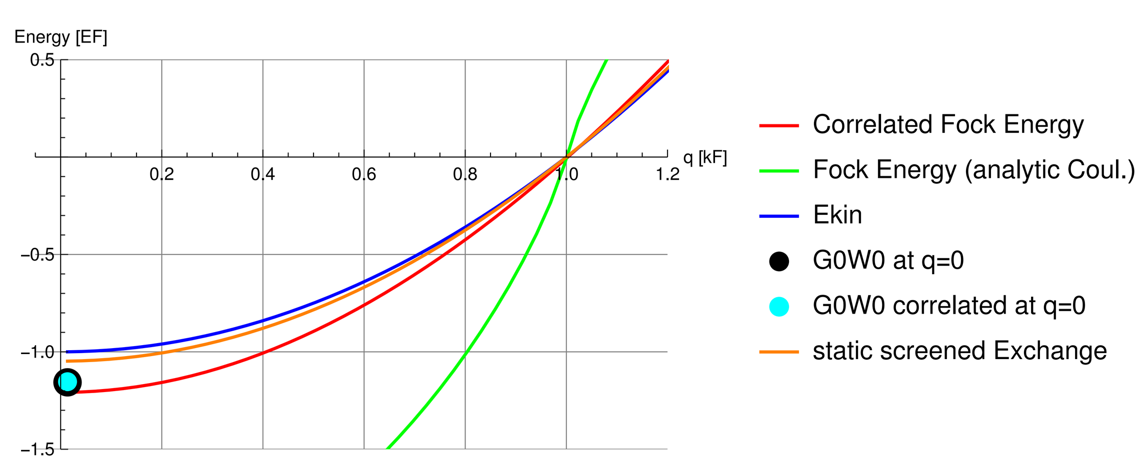


cTD-HF - Including Exchange

- Single particle energy including the correlated Fock-term $e(q) = \frac{\hbar^2 q^2}{2m} + u(q)$
- Do the same transformation as in cRPA
- And a few approximations

→ The result is numerically similar to BSE

$$V_F(q) = -\frac{\hbar^2 q^2}{2mS_F(q)^2}\left(\frac{S(q)}{S_F(q)} - 1\right)$$



References

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Der Wissenschaftsfonds.

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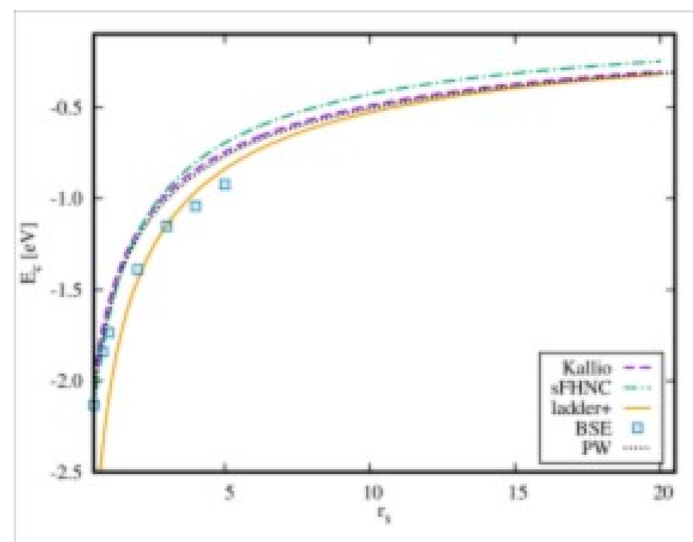
The Ground State

$$|\psi\rangle = F\,|\Phi_0\rangle \qquad F = \prod_{1\le i<j\le N} f(r_{ij}) = e^{\frac{1}{2}\sum_{i<j}u(r_{ij})}$$

Optimal Correlation function

$$\frac{\delta}{\delta u(r)}\frac{\langle\psi|\,H\,|\psi\rangle}{I_{00}} = 0$$

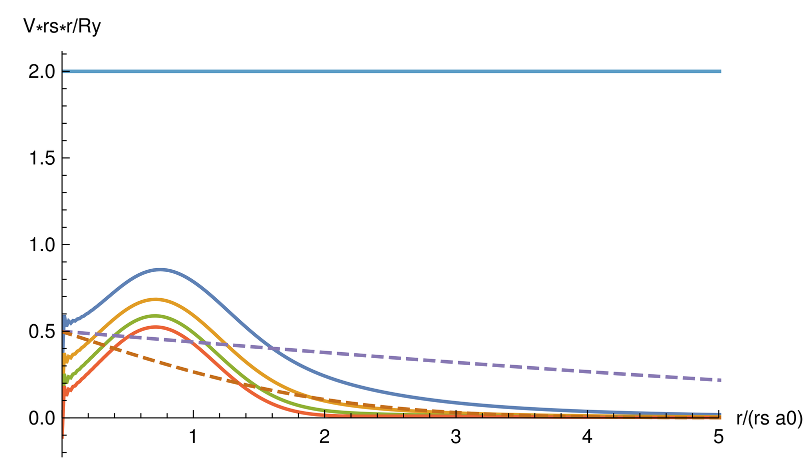


The Slater-determinat

- For HEG: plane wave SD
- For inhomogeneous systems: generalized HF equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(r) + V_H(r)\right]\phi_i(r) - \frac{1}{\nu}\int dr' V_F(r,r')\rho_1(r,r')\phi_i(r') = e_i\phi_i(r)$$

Looks very similar to **hybrid functionals** in generalized KS
→ Compare the Fock potential V_F to e.g. HSE06

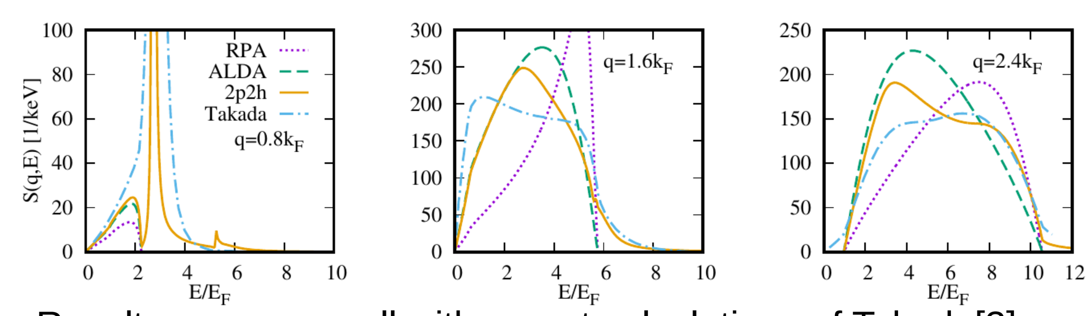


Beyond cTDHF- 2p2h kernel

Optimize also two particle two hole excitations

$$U(t) \equiv \sum_{ph}\delta u_{ph}^{(1)}(t)\,a_p^\dagger a_h + \frac{1}{2}\sum_{pp'hh'}\delta u_{pp'hh'}^{(2)}(t)\,a_p^\dagger a_{p'}^\dagger a_{h'}a_h$$

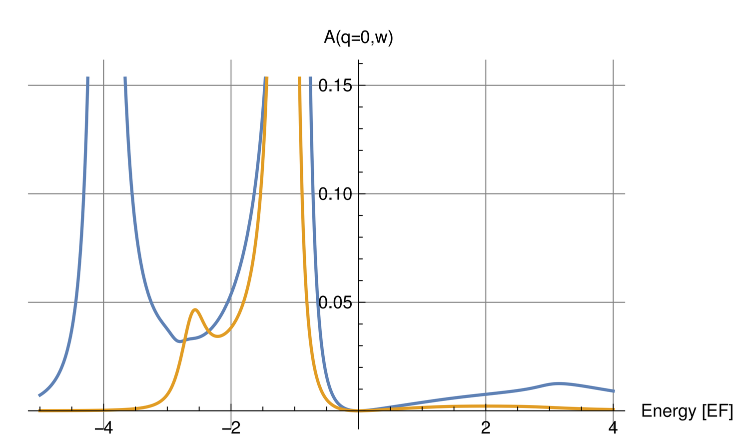
The result can be cast into a TDDFT picture leading to a non local dynamic exchange correlation potential [1]:



Result compares well with recent calculations of Takada[3] and yields the **double plasmon!**
The kernel can be downloaded at:
https://etsf.polytechnique.fr/research/connector/2p2h-kernel

Self-energy beyond cFock

$$W_c(q,\omega) = V_F(q) + V_F^2(q)\frac{\chi^0(q,\omega)}{1 - V_{ph}(q)\chi^0(q,\omega)}$$



Conclusion

- Conventional PT can be enhanced by replacing the Coulomb interaction with an effective one.
- Results comparable to most advanced methods, possibility to predict new physics[2].
- The effective interactions can be expressed in terms of the static structure factor, derived from CBF methods.
- For static structure factor input use either MC or FHNC results (see github.com/mpanho/FHNC_3D)

Outlook

- Extend to in-homogeneous systems
  - → Use the HEG results in a clever way
  - → Do the full in-homogeneous calculation

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