I. Motivations

♣ Implementation of the HK theorem starting from self-consistent $G(E)$

♣ Exercise to build the notion of QP and s.p. strength $S(E)$ explicitly into DFT

♣ Include more explicitly long-range correlations via partial occupation numbers

♣ Start from $G(E)$ and define the $0^{th}$ and $1^{st}$ energy-weighted moment of $S(E)$

$$[G(E)]^{-1} = [G_0(E)]^{-1} - \Sigma(E)$$

$$S(E) = \frac{1}{2i\pi} \text{sign}(\epsilon_F - E) ([G(E)] - [G(E)]^\dagger)$$

$$\rho = \rho^- + \rho^+ = \int_{-\infty}^{\epsilon_F} dE S(E) + \int_{\epsilon_F}^{+\infty} dE S(E) = I$$

$$M = M^- + M^+ = \int_{-\infty}^{\epsilon_F} dE E S(E) + \int_{\epsilon_F}^{+\infty} dE E S_{ij}(E) = H_0 + V_{HF}[\rho^-]$$

$$E_0^N = \frac{1}{2} Tr \left[ H_0 \rho^- + M^- \right] / 2$$

♣ Split $S(E) = S_{QP}(E) + S_B(E)$ and model the background $\rho_B$ and $M_B$ as functionals of $\rho^-$

♣ Rely on the extension of HK theorem / full density matrix $\rho^-$; Gilbert, PRB (1975)
II. Implementation: QP-DFT equations

Using \( \rho_{QP} = I - \rho_B[\rho^-] \) and \( M_{QP} = M - M_B[\rho^-] \), one obtains a generalized eigenvalue problem

\[
\left\{ H_0 + V_{HF}[\rho^-] - M_B[\rho^-] \right\} u_{QP,j}^{[n]} = \epsilon_{QP,j}^{[n]} (I - \rho_B[\rho^-]) u_{QP,j}^{[n]}
\]

\[
\rho_{[n+1]}^- = \sum_{j=1}^{N} z_{QP,j}^{[n]} z_{QP,j}^{[n]} + \rho_B[\rho^-]
\]

\[
E_0^N = \frac{1}{2} \sum_{j=1}^{N} z_{QP,j}^{[n]} H_0 + \epsilon_{QP,j} z_{QP,j} + \frac{1}{2} Tr \left( H_0 \rho_B[\rho^-] + M_B[\rho^-] \right)
\]

\( z_{QP,j} = (I - \rho_B[\rho^-]) u_{QP,j} \) denotes a QP orbital / \( z_{QP,j}^{[n]} z_{QP,j} \leq 1 \) and \( \rho_{QP} = \sum_{j=1}^{N} z_{QP,j} z_{QP,j}^{[n]} \)

III. Comments

\( \rho_B^\pm = M_B^\pm = 0 \); \( z_{QP,j} = u_{QP,j} \) is an orthonormal set

\( \rho_B^\pm = 0 \) but \( M_B^\pm \neq 0 \); \( z_{QP,j} = u_{QP,j} \) is an orthonormal set and \( M_B = V_F - V_{xc} \)

General scheme introduces partial occupation numbers BUT \( z_{QP,j} \) are NOT natural orbitals

Splitting relies on the idea that the background is due to "universal" \( e^- - e^- \) correlations

However, the splitting into \( QP + B \) is not unique

Beyond \( E_{xc}[\rho^-] \), one must model \( \rho_B[\rho^-] \) ⇒ unexplored territory (additional phenomenology... )