An Heuristic approach to GW
The Dielectric Concept

The Kubo Formula

The Statically Screened Hatree Fock approximation
The QUASIPARTICLE concept and a dielectric approach to GW
Electron removal

Before

vacuum

conduction

valence

\[ E_N \]

After

\[ E_{N-1} \]
WHAT IS THE QUASIPARTICLE BAND GAP

Electron addition

before

vacuum

conduction

valence

after

\[ E_N \]

\[ E_{N+1} \]
So what?! Why is DFT correlation not enough?

Correlation is the effect of the mutual interaction of particles beyond the simple electrostatic and statistic effects.

\[ V_c = V_c[\rho](\vec{r}) \]

DFT

MBPT
The “dielectric way” to the MB problem

\[ \delta \rho(\vec{r}) = - \phi^{\text{ext}}(\vec{r}) = \int d\vec{r}' |\vec{r} - \vec{r}'|^{-1} \delta \rho(\vec{r}) \]
The Kubo Formula

\[ H_{tot} = H + H^{ext}(t) = H + \sum_i \phi^{ext}(\mathbf{r}_i, t) = H + \int d\mathbf{r} \rho(\mathbf{r}) \phi^{ext}(\mathbf{r}, t) \]

The external potential “induces” a (time-dependent) density perturbation

\[ \rho^{ind}(t) = \langle \Phi(t) | \hat{\rho} | \Phi(t) \rangle - \langle \Phi | \hat{\rho} | \Phi \rangle \]

\[ |\Phi(t)\rangle = |\Phi_0\rangle + \int_{-\infty}^{t} dt' H^{ext}_{I}(t') |\Phi(t)\rangle \approx |\Phi_0\rangle + \int_{-\infty}^{t} dt' H^{ext}_{I}(t') |\Phi_0\rangle \]

\[ \rho^{ind}(r, t) = \int_{-\infty}^{t} dt' \int d\mathbf{r}' \chi_{\rho\rho}(\mathbf{r}\mathbf{r}', t-t') \phi^{ext}(t') \]

With the causal response function

\[ \chi_{\rho\rho}(\mathbf{r}\mathbf{r}', t) \equiv -i \langle [\rho_{I}(\mathbf{r}, t), \rho_{I}(\mathbf{r}')] \rangle = -i \langle [\delta\rho_{I}(\mathbf{r}, t), \delta\rho_{I}(\mathbf{r}')] \rangle \]
The "dielectric way" to the MB problem

\[ \delta \rho^{\text{ind}}(\vec{r},t) = \int d\vec{r}' |\vec{r} - \vec{r}'|^{-1} \rho^{\text{ind}}(\vec{r},t) \]

\[ \delta H_{mf}(t) \equiv \int dr (\phi^{\text{ind}}(r,t) + \phi^{\text{ext}}(r,t)) \rho(\vec{r},t) \approx \int dr (\phi^{\text{ind}}(r,t) + \phi^{\text{ext}}(r,t)) \rho^{\text{ext}}(r) \]

\[ \int dr \phi^{\text{ind}}(r,t) \rho^{\text{ext}}(r) = \int \rho^{\text{ext}}(r_1) v(r_1-r_2) \chi(r_2,r_3,t) v(r_3-r_4) \rho^{\text{ext}}(r_4) \]
The “dielectric way” to the MB problem

\[ \delta H_{mf}(t) = \int \rho^{ext}(r) W(r,r',t) \rho^{ext}(r') \]

\[ W(r,r',t) = v(r-r') + \int v(r-r_1) \chi(r_1,r_2,t) v(r_2-r') \]
The "dielectric way" to the MB problem

\[
\left[ h(x) + V_H(x) \right] \phi_{nk}(x) + \int dx' \sum_f(x, x') \phi_{nk}(x') = \epsilon_{nk}^{hf} \phi_{nk}(x)
\]

Quantistic

\[ \Sigma_f(x, x') = \sum_{n'k', mp} \frac{\phi_{n'k'}(x) \phi_{mp}(x')}{|x - x'|} \frac{\phi_{n'k'}(x') \phi_{n'k'}(x')}{|x - x'|} \]

Classical

\[ V_H(x) = \int dx' \sum_{n'k'} \phi_{n'k'}(x') \phi_{n'k'}(x') \]

\[ \Sigma_{hf}(x, x') \rightarrow \Sigma_{GW}(x, x') \]

\[ \Sigma_{GW}(x, x') \approx \sum_{n'k', mp} \phi_{n'k'}(x) \phi_{mp}(x') W(x, x') \]
The "dielectric way" to the MB problem

\[ H = \sum_i h(x_i) + \frac{1}{2} \sum_{i \neq j} |x_i - x_j|^{-1} \]
1. Many-body perturbation theory calculations using the yambo code
2. Yambo: an ab initio tool for excited state calculations