All-electron GWA based on the PAW method:
Application to insulating materials

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Plan

I. The Projector Augmented Wave (PAW) method
   • Description of the basis set
   • Comparison with the FPLMTO optical spectra
   • The band gap problem

II. Implementation of the GW-PAW approximation
   • The quasiparticle (QP) equation
   • The self-energy within the GW approximation

III. Applications
   • QP energies of semiconductors and insulators
   • Effects of correlation on optical spectra
The PAW method

The Projector augmented-wave (PAW) method was introduced by Blöchl, 1994.

* Space representation

\[ |\Psi\rangle = |\tilde{\Psi}\rangle + |\Psi_{\text{aug}}\rangle - |\tilde{\Psi}_{\text{aug}}\rangle \]

Idea:

- Interstitial region
- Augmentation region
- Pseudopotential
- All-electron Potential

\[ |\Psi\rangle \]
The PAW method continued ...

LDA potential and $\tilde{v}_{eff}$ of Si on the (001) plan
The PAW method continued ...

1. Pseudopotential $\tilde{v} : |\tilde{\Psi}\rangle = \sum_G a_G |G\rangle$ (planes waves)

2. Atomic potential $v^a : |\Psi_{aug}\rangle = \sum_i c_i|\phi_i\rangle$ (partial waves)

3. Atomic Pseudopotential $\tilde{v}^a : |\tilde{\Psi}_{aug}\rangle = \sum_i c_i|\tilde{\phi_i}\rangle$ (partial pseudo-waves)

Crystal wave function :

$$|\Psi\rangle \overset{\text{def}}{=} |\tilde{\Psi}\rangle + \sum_i c_i|\phi_i\rangle - \sum_i c_i|\tilde{\phi_i}\rangle,$$

where the $c_i$ are to be determined.

Conditions to be satisfied:

- $r \in \Omega^{\text{int}} : \Psi(r) = \tilde{\Psi}(r)$  \hspace{1cm} (true by construction)
- $r \in \Omega^{\text{aug}} : \Psi(r) = \sum_i c_i\phi_i(r)$  \hspace{1cm} (desired equality)

Condition satisfied if: $\tilde{\Psi}(r) \neq \sum_i c_i\tilde{\phi_i}(r)$  \hspace{1cm} ($r \in \Omega^{\text{aug}}$)

The projectors $|\tilde{p}_i\rangle$ are defined as:

$$\langle r \in \Omega^{\text{int}} | \tilde{p}_i \rangle = 0 \quad \forall i$$

$$\langle \tilde{p}_j | \tilde{\phi}_i \rangle = \delta_{ij} \quad \forall i, j$$

$$\implies \langle r | \tilde{\phi}_i \rangle = \langle r | \phi_i \rangle \quad \text{if } r \in \Omega^{\text{int}}.$$
The PAW method continued...

The $c_i$ coefficients are then given by:

$$\langle \tilde{p}_j | \tilde{\Psi} \rangle = \sum_i c_i \langle \tilde{p}_j | \phi_i \rangle = c_j$$

The crystal wave function becomes:

$$|\Psi\rangle = |\tilde{\Psi}\rangle + \sum_i \langle \tilde{p}_i | \tilde{\Psi} \rangle (|\phi_i\rangle - |\tilde{\phi}_i\rangle)$$

$$= \left[ 1 + \sum_i (|\phi_i\rangle - |\tilde{\phi}_i\rangle) \langle \tilde{p}_i | \right] |\tilde{\Psi}\rangle = T |\tilde{\Psi}\rangle$$

The transformation operator $T$ is defined as:

$$T = 1 + \sum_i (|\phi_i\rangle - |\tilde{\phi}_i\rangle) \langle \tilde{p}_i |$$
Illustration of the PAW Augmentation

Example: $3s$, and $3p$ partial, pseudo-partial waves, and projectors of Si.

![Graph showing $3s$ and $3p$ waves with projectors and partial waves plotted against $r$ in bohr units.](image)
Expectation value of a local operator

Expectation value of a local one-particle operator

\[ \langle A \rangle = \sum_n \langle \tilde{\Psi}_n | A | \tilde{\Psi}_n \rangle + \sum_{i,j} D_{i,j} \langle \phi_i | A | \phi_j \rangle - \sum_{i,j} D_{i,j} \langle \phi_i | A | \phi_j \rangle \\
+ \sum_n \langle \Psi_c^* | A | \Psi_c \rangle \\
\]

with a one-center density matrix

\[ D_{i,j} = \sum_n \langle \tilde{p}_i \tilde{\Psi}_n \rangle \langle \tilde{\Psi}_n | \tilde{p}_j \rangle \]

and the core state contribution \( |\Psi_c^\rangle \).
Example: Electronic Density

Electronic density $n(r)$ is composed of a plane wave part $\tilde{n}(r)$ and two one-center components $n^1(r)$ and $\tilde{n}^1(r)$

$$n(r) = \tilde{n}(r) + n^1(r) - \tilde{n}^1(r)$$

$$= \sum_n f_n \tilde{\Psi}_n^*(r) \tilde{\Psi}_n(r) + \tilde{n}^c$$

$$+ \sum_{i,j} \phi_i^*(r) D_{i,j} \phi_j(r) + n^c$$

$$- \sum_{i,j} \tilde{\phi}_i^*(r) D_{i,j} \tilde{\phi}_j(r) - \tilde{n}^c$$

$$D_{i,j} = \sum_n \langle \tilde{p}_i | \tilde{\Psi}_n \rangle f_n \langle \tilde{\Psi} | \tilde{p}_j \rangle$$

where:

$$f_n = \text{occupation number (i.e. 0 or 1)}$$

The electronic density (like the wave function) is divided into:

- A plane-wave part
- Two partial expansions per atom in radial functions times spherical harmonics
PAW total energy

\[ E([\tilde{\Psi}_n], R_i) = \tilde{E} + E^1 - \tilde{E}^1 \]

Plane-wave part

\[ \tilde{E} = \sum_n f_n \langle \tilde{\Psi}_n \rangle - \frac{1}{2} \nabla^2 |\tilde{\Psi}_n\rangle \]

\[ + \frac{1}{2} \int d^3r \int d^3r' \frac{(\tilde{n}(r) + \hat{n}(r))(\tilde{n}(r') + \hat{n}(r'))}{|r - r'|} \]

\[ + \int d^3r \tilde{n}(r)\epsilon_{xc}(r, [\tilde{n}]) + \int d^3r \bar{v}(r)\tilde{n}(r) \]

One-center expansion of the plane-wave part

\[ \tilde{E}^1 = \sum_n D_{i,j} \langle \tilde{\phi}_i \rangle - \frac{1}{2} \nabla^2 |\tilde{\phi}_j\rangle \]

\[ + \frac{1}{2} \int d^3r \int d^3r' \frac{(\tilde{n}^1(r) + \hat{n}(r))(\tilde{n}^1(r') + \hat{n}(r'))}{|r - r'|} \]

\[ + \int d^3r \tilde{n}^1(r)\epsilon_{xc}(r, [\tilde{n}^1]) + \int d^3r \bar{v}(r)\tilde{n}^1(r) \]

One-center expansion of the true density

\[ E^1 = \sum_n D_{i,j} \langle \phi_i \rangle - \frac{1}{2} \nabla^2 |\phi_j\rangle \]

\[ + \frac{1}{2} \int d^3r \int d^3r' \frac{(n^1(r) + Z(r))(n^1(r') + Z(r'))}{|r - r'|} \]

\[ + \int d^3r n^1(r)\epsilon_{xc}(r, [n^1]) \]

The compensation charge density \( \hat{n} \) is such that \((n^1 + n^Z) - (\tilde{n}^1 + \hat{n})\) has vanishing electrostatic multipole moments \( \longrightarrow \) it does not interact with the charge outside \( \Omega^{aug} \).
Effective Hamiltonian

The total energy $E$ is stationary / variational parameters ($\tilde{\Psi}_{nk}$), with the condition insuring the total number $N$ of electrons

$$\sum_{m,k} f_{m,k} \langle \Psi_{mk} | \Psi_{mk} \rangle - N = 0.$$

The effective eigenvalue problem is then deduced from

$$\frac{\delta}{\delta \langle \tilde{\Psi}_{nk} \rangle} \left[ E - \epsilon_{nk} \left( \sum_{m,k} f_{m,k} \langle \tilde{\Psi}_{mk} | \tilde{O} | \tilde{\Psi}_{mk} \rangle - N \right) \right] = 0,$$

where $\epsilon_{nk}$ are Lagrange parameters. The variational calculus leads to the effective Schrödinger equation

$$\tilde{H} | \tilde{\Psi}_{nk} \rangle = \epsilon_{nk} \tilde{O} | \tilde{\Psi}_{nk} \rangle,$$

where the effective Hamiltonian is given by

$$\tilde{H} = -\frac{\nabla^2}{2} + \tilde{v}_{eff}(r) + \sum_{\tau,i,j} | \tilde{p}_{\tau i} \rangle \Gamma_{ij} \langle \tilde{p}_{\tau j} |,$$

The local term $\tilde{v}_{eff}$ is given by

$$\tilde{v}_{eff}(r) = \int dr' \tilde{n}(r') + \tilde{\hat{n}}(r') + \hat{n}(r) + v_{xc}[\tilde{n}(r)]$$

and the non local term is defined by the matrix elements

$$\Gamma_{ij} = H_{ij} - \tilde{H}_{ij},$$

where

$$H_{ij} = \langle \phi_{ij} \big| -\frac{\nabla^2}{2} + v_H (n_\tau + n_\tau Z) + v_\circ (r) + v_{xc}[n_\tau (r)] \big| \phi_{ij} \rangle,$$

and

$$\tilde{H}_{ij} = \langle \tilde{\phi}_{\tau i} \big| -\frac{\nabla^2}{2} + v_H [\tilde{n}_\tau + \tilde{n}_\tau] + v_\circ (r) + v_{xc}[\tilde{n}_\tau (r)] \big| \tilde{\phi}_{\tau j} \rangle.$$

The PAW (solid line) and the FPLMTO (dashed line) calculations are in good agreement. The local-field and the excitonic effects are not included in both calculations.
The DFT band-gap problem

- **Kohn-Sham Equation**

\[
[h_0(r) + V_{xc}(r)] \Psi_{nk}(r) = \epsilon_{nk} \Psi_{nk}(r)
\]

où \( h_0(r) = -\frac{\nabla^2}{2} + V_{ext}(r) + V_H(r) \)

- **LDA band gaps**

![Graph showing experimental versus calculated band gaps for various materials, with data points for LiF, LiCl, KCl, NaCl, C, Si, AlAs, InP, GaAs, and LDA (PAW).]
The DFT band-gap problem continued ...

The band gap $E_g$ is defined as the difference between the ionization energy and the electron affinity

$$E_g = [E^{(N-1)} - E^{(N)}] - [E^{(N)} - E^{(N+1)}] = I - A$$

where $E^{(N\pm1)}$ represents the energy of the fundamental state of a system of $N \pm 1$ electrons.

It was shown by Schlüter and Sham (PRL, 83) that the DFT band gap $\epsilon_{g}^{DFT}$ is not equal to the quasiparticle gap $E_g$

$$\Delta = E_g - \epsilon_{g}^{DFT} = E_g - [E_{N+1,DFT}^{(N)} - E_{N,DFT}^{(N)}]$$

$$= V_{XC}^{(N+1)}(r) - V_{XC}^{(N)}(r)$$
• **Self-energy** $\Sigma$

\[
\Sigma = \ldots
\]

• **Hartree-Fock band gaps**
The GWA (Hedin, 1965)

- **Kohn-Sham equation**
  \[
  [h_0(r) + V_{xc}(r)] \Psi_{nk}(r) = \epsilon_{nk} \Psi_{nk}(r)
  \]

- **Quasiparticle equation**
  \[
  h_0(r) \Psi_{nk}^{qp}(r) + \int d^3r' \Sigma(r, r', \epsilon_{nk}^{qp}) \Psi_{nk}^{qp}(r') = \epsilon_{nk}^{qp} \Psi_{nk}^{qp}(r)
  \]

- **Self-energy \( \Sigma \)**
  \[
  \Sigma(r, r', \omega) = \frac{i}{2\pi} \int d\omega' G(r, r', \omega + \omega') W(r, r', \omega') e^{i\delta \omega'}
  \]
  where the dynamical screened interaction \( W \) is defined by
  \[
  W(r, r', \omega) = \int dr'' \epsilon^{-1}(r, r'', \omega) v(r'', r')
  \]
  \( v \) represents the bare coulomb interaction and \( \epsilon^{-1} \) the inverse of the dielectric function.

Any two point function \( f(r, r') \) such as \( f(r+R, r'+R) = f(r, r') \) has the following Fourier transform
\[
  f(r, r', \omega) = \frac{1}{\Omega} \sum_{q, G, G'} e^{i(q+G)r} f_{GG'}(q, \omega) e^{-i(q+G')r'}
\]
\( q \in BZ, G \) a reciprocal vector, and \( \Omega \) the crystal volume.

The Fourier transform of the screened interaction \( W \) can be written as
\[
  W_{G, G'}(q, \omega) = 4\pi\frac{1}{|q + G|} \epsilon^{-1}_{G, G'}(q, \omega) \frac{1}{|q + G'|}
\]

The Green function \( G \) is computed within the LDA
\[
  G(r, r', \omega) = \lim_{\delta \to 0^+} \sum_{nk} \frac{\Psi_{nk}(r) \Psi_{nk}^*(r')}{\omega - \epsilon_{nk} + i\delta \text{sgn}(\epsilon_{nk} - \mu)}
\]
The self-energy can be written as
\[
\langle \Psi_m^k | \Sigma(\omega) | \Psi_{l^k} \rangle = \frac{1}{\Omega} \sum_q \sum_{G,G'} \sum_n M^n_{G'}(k,q) B^n_{G,G'}(k,q) \left[ M^n_{G}(k,q) \right]^* ,
\]
where
\[
B^n_{G,G'}(k,q) = \frac{i}{2\pi} \int d\omega' e^{i\delta\omega'} \frac{W_{G,G'}(q,\omega')}{\omega + \omega' - \epsilon_{nk-q} + i\delta \text{sgn}(\epsilon_{nk-q} - \mu)},
\]
and the matrix elements $M^n_{G}(k,q)$ are given by
\[
M^n_{G}(k,q) = \langle \Psi_{nk-q} | e^{-i(q+G)r} | \Psi_{mk} \rangle
\]
The self-energy can be decomposed into two terms which are integrated on the complex plan.
The first term is called the Hartree-Fock term and is given by
\[
\langle \Psi_m^k | \Sigma^{hf} | \Psi_{l^k} \rangle = -\frac{4\pi}{\Omega} \sum_{n_{occ}} \sum_q \sum_G M^n_{G}(k,q) \left[ M^n_{G}(k,q) \right]^* |q + G|^2 .
\]
The second term is called the correlation term and is given by
\[
\langle \Psi_m^k | \Sigma^{C}(\omega) | \Psi_{l^k} \rangle = \frac{1}{\Omega} \sum_q \sum_{G,G'} \sum_n M^n_{G}(k,q) \left[ M^n_{G}(k,q) \right]^* C^{k,q,n}_{G,G'}(\omega) ,
\]
where
\[
C^{k,q,n}_{G,G'}(\omega) = \frac{i}{2\pi} \int d\omega' \frac{W^C_{G,G'}(q,\omega')}{\omega + \omega' - \epsilon_{nk-q} + i\delta \text{sgn}(\epsilon_{nk-q} - \mu)},
\]
and where $W^C$ is given by
\[
W^C_{G,G'}(q,\omega') = W_{G,G'}(q,\omega') - v_{G,G'}
\]
• **Solution of the QP equation**

\[ \Psi_{mk}(r) = \sum_n \alpha_{mn}(k) \Psi_{nk}(r) \]

In practice, \( \alpha_{mn} \simeq \delta_{mn} \) (Hybertsen-Louie, 1986). Then the QP energies are provided by

\[ \epsilon_{mk}^{qp} = \epsilon_{mk} + \langle \Psi_{mk} | \Sigma(\epsilon_{mk}^{qp}) | \Psi_{mk} \rangle - \langle \Psi_{mk} | V_{xc}[n_v(r)] | \Psi_{mk} \rangle \]

assuming that \( V_{xc}^{\text{core}-\text{val}} \simeq V_{xc}[n_v + n_c] - V_{xc}[n_v] \)

• **Practical scheme**

\[ \epsilon_{mk}^{qp} - \epsilon_{mk} = Z_{mk} \times \left\{ \frac{\langle \Psi_{mk} | \Sigma(r, r', \epsilon_{mk}) | \Psi_{mk} \rangle}{-\langle \Psi_{mk} | V_{xc}(r) | \Psi_{mk} \rangle} \right\} \]

where the renormalization factor \( Z_{nk} \) is defined by

\[ Z_{nk} = [1 - \langle \Psi_{nk} | \frac{\partial}{\partial \omega} \Sigma(r, r', \epsilon_{nk}) | \Psi_{nk} \rangle]^{-1} \]

Since \( \frac{\partial}{\partial \omega} \Sigma < 0 \), the renormalization factor should be between 0 and 1.
Removal of the double counting

- **LDA decoupling:** $V_{xc}^{val} \sim V_{xc}[n_v + n_c] - V_{xc}[n_v]$

$$\epsilon_{mq}^{qp,1} = \left\{ \begin{array}{l}
\epsilon_{mk} + \langle \Psi_{mk} | \Sigma(r, r', \epsilon_{mq}^{qp,1}) | \Psi_{mk} \rangle \\
- \langle \Psi_{mk} | V_{xc}[n_v(r)] | \Psi_{mk} \rangle
\end{array} \right.$$

- **Hartree-Fock decoupling:** $V_{xc}^{val} \sim V_{X}^{c}$

$$\epsilon_{mq}^{qp,2} = \left\{ \begin{array}{l}
\epsilon_{mk} + \langle \Psi_{mk} | \Sigma(r, r', \epsilon_{mq}^{qp,2}) | \Psi_{mk} \rangle \\
- \langle \Psi_{mk} | V_{xc}[n_v(r) + n_c(r)] | \Psi_{mk} \rangle + \langle \Psi_{mk} | V_{X}^{c}(r, r') | \Psi_{mk} \rangle
\end{array} \right.$$

- **Results for silicon**

<table>
<thead>
<tr>
<th></th>
<th>$V_{xc}[n_v + n_c] - V_{X}^{c}$</th>
<th>$V_{xc}[n_v]$</th>
<th>$\epsilon_{mq}^{qp,2}$</th>
<th>$\epsilon_{mq}^{qp,1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma_{25'} v$</td>
<td>-11.60</td>
<td>-11.45</td>
<td>0.0</td>
<td>0.0</td>
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<tr>
<td>$\Gamma_{15c}$</td>
<td>-10.34</td>
<td>-10.19</td>
<td>3.15</td>
<td>3.15</td>
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<tr>
<td>$X_{4v}$</td>
<td>-10.85</td>
<td>-10.74</td>
<td>-3.05</td>
<td>-3.01</td>
</tr>
<tr>
<td>$X_{1c}$</td>
<td>-9.25</td>
<td>-9.15</td>
<td>1.10</td>
<td>1.15</td>
</tr>
<tr>
<td>$L_{3'} v$</td>
<td>-11.33</td>
<td>-11.20</td>
<td>-1.28</td>
<td>-1.26</td>
</tr>
<tr>
<td>$L_{1c}$</td>
<td>-10.39</td>
<td>-10.28</td>
<td>2.12</td>
<td>2.16</td>
</tr>
</tbody>
</table>
Comparison with plasmon-pole model

- **Homogeneous electron gas**
  \[
  \epsilon^{-1}(q, \omega) = 1 + A_q \left( \frac{1}{\omega - (\omega_q - i\delta)} - \frac{1}{\omega + (\omega_q - i\delta)} \right)
  \]

- **Calculation of parameters** $A_q$ and $\omega_q$
  1. Static limit of $\epsilon^{-1}(q, \omega)$
  2. Johnson sum rule
  \[
  \int_0^\infty d\omega \, \omega \, \text{Im} \left[ \epsilon^{-1}(q, \omega) \right] = -\frac{\pi}{2} \omega_p^2
  \]

- **Results for silicon**

<table>
<thead>
<tr>
<th></th>
<th>LDA</th>
<th>GW</th>
<th>GW with Plasmon-pole model</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Von der Linden et Horsch</td>
</tr>
<tr>
<td>$\Gamma_{25'}$</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$\Gamma_{15c}$</td>
<td>2.54</td>
<td>3.09</td>
<td>3.09</td>
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<tr>
<td>$X_{4v}$</td>
<td>-2.85</td>
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<tr>
<td>$X_{1c}$</td>
<td>0.61</td>
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<td>1.09</td>
</tr>
<tr>
<td>$L_{3'}$</td>
<td>-1.19</td>
<td>-1.16</td>
<td>-1.28</td>
</tr>
<tr>
<td>$L_{1c}$</td>
<td>1.44</td>
<td>2.05</td>
<td>2.09</td>
</tr>
</tbody>
</table>
Calculated quasiparticle energies of silicon using two different integration schemes. The results are in good agreement.
QP band structures

Band gap: LDA 0.5 eV; GW 1.12 eV; Expt. 1.17 eV

Band gap: LDA 4.75 eV; GW 8.24 eV; Expt. 8.69 eV
Band gap: **LDA 8.71 eV; GW 13.97 eV; Expt. 14.1 eV**

Band width F 2p: **LDA 3.17 eV; GW 3.76 eV; Expt. 3.5 eV**
GW band gaps

![Graph showing GW band gaps for various materials]

- **Experimental band gap (eV)**
  - 0 2 4 6 8 10 12 14

- **Calculated band gap (eV)**
  - LDA (PAW)
  - GWA (PAW)

- Materials:
  - LiF
  - LiCl
  - NaCl
  - KCl
  - AlAs
  - Si
  - C
  - InP
  - GaAs
Spectral function of silicon at $\Gamma$
Life time of the QP of Si at $\Gamma$

$$\tau_{nk} = 2 \times \text{Im} \left( \varepsilon_{nk}^{qp} \right)$$

![Graph showing the relationship between Re[$\varepsilon_{nk}^{qp}$] and $1/\tau_{nk}$](image_url)
Optical properties within RPA

- **RPA formulation**

\[ \epsilon(\omega) = \lim_{q \to 0} \epsilon_{0,0}(q, \omega) - \lim_{q \to 0} \sum_{G, G' \neq 0} \epsilon_{0,G}(q, \omega) \epsilon_{G,G'}^{-1}(q, \omega) \epsilon_{G',0}(q, \omega) \]

- **RPA dielectric function of Silicon**
The static dielectric function is obtained using the KK relations

$$\epsilon_\infty = 1 + \lim_{q \to 0} \frac{2}{\pi} P \int_0^\infty \frac{d\omega'}{\omega'} \frac{\epsilon_2(q, \omega')}{\omega'}$$
Excitonic effects (Hanke-Sham, 1975)

- Bethe-Salpeter equation

\[
\begin{align*}
S & = 1 \quad \begin{array}{c} \downarrow \end{array} \quad 2 \\
1' & \quad \begin{array}{c} \downarrow \end{array} \quad 2'
\end{align*}
\]

\[
\Xi
\]

\[
\Xi(3, 3', 4, 4') = i\delta(3, 4)\delta(3', 4')W(3, 3') - i\delta(3, 3')\delta(4, 4')v(3, 4)
\]

- Expression for the Kernel

\[
S = S^0 + S^0 \Xi S
\]

- Reformulation of the Bethe-Salpeter equation

\[
(\epsilon_{qp}^{ck} - \epsilon_{vp}^{ck}) A^\lambda_{vck} + \sum_{v', c', k'} \langle vck|\Xi|v'c'k'\rangle A^\lambda_{v'c'k'} = E_\lambda A^\lambda_{vck}
\]

- Macroscopic dielectric function

\[
\epsilon^{(2)}(\omega) = \lim_{q\to 0} \frac{4\pi^2}{\Omega} \times \frac{1}{q^2} \times \sum \left| \sum_{ck} \langle vke^{-iq.r}|ck\rangle A^\lambda_{vck} \right|^2 \delta(\omega - E_\lambda)
\]
Excitonic effects (Hanke-Sham, 1975)

- Silicon

\[ \varepsilon_\omega (\omega) = \varepsilon_\infty + \frac{g^2}{\varepsilon_\infty} \text{ when } r \to \infty \]
Semiconductors of type III-V and diamond

electron-hole attraction: \( \frac{e^2}{\varepsilon_\infty r} \) when \( r \to \infty \)
Ionic insulators

<table>
<thead>
<tr>
<th></th>
<th>Band gap</th>
<th>Position of the first excitonic peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>GW</td>
<td>Expt</td>
<td>Theory</td>
</tr>
<tr>
<td>KCl</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>8.24</td>
<td>8.69 7.44 7.79 7.6</td>
</tr>
</tbody>
</table>

- Interacting
- Non interacting
- Expt (300 K)
Conclusion

Results

- GW-PAW $\Rightarrow \epsilon_{nk}^{qp}$ in good agreement with experiment
- $\epsilon_{nk}^{qp} \Rightarrow$ Calculation of the optical properties
- Excitonic effects crucial $\Rightarrow$ Bethe-Salpeter equation

Outlooks

- Extension to more complex systems
- Selfconsistent GW-DMFT
- Determination of XAS spectra