Motivation

- Non-conserving $G^{\text{LDA}} W^{\text{LDA}}$ has been successful in calculating quasi-particle (QP) band gap: Why?
  - Schindlmayr: $G^{\text{LDA}} W^{\text{LDA}}$ violates particle number conservation. [PRB 56, 3528 (1997)]
  - Schöne and Eguiluz: conserving $GW$ overshoots the gap by the amount LDA underestimates it. [PRL 85, 2410 (2000)]
  - Do we have a conserving theory capable of producing good gap?

- Deep core electrons play almost no role: True?

- Polarization from 3d core states is responsible to switch Ge from direct gap (no gap) to indirect gap: True?

- Is pseudo-potential designed for performing QP calculation?
Finite Temperature Many-Body Perturbation Theory (MBPT)

\[ \Sigma = -G^2 \]

\[ \Sigma = \bigcirc - \bigcirc + \Sigma \]

\[ L = \bigcirc + \bigcirc \]

\[ \Lambda = \triangle + \Lambda \]

Baym-Kadanoff Conserving Scheme:

- \( \Sigma \) is \( \Phi \) derivable.
- Dyson equation is solved self-consistently. (\( \Sigma = \Sigma[G] \))
- All microscopic conservation laws are guaranteed!

Ex: Shielded Interaction Approximation (SIA): (GW form)

\[ \Phi_{\text{SIA}} : \frac{1}{2} - \frac{1}{2} \bigcirc - \frac{1}{4} \bigcirc - \frac{1}{6} \bigcirc - \frac{1}{8} \bigcirc - \cdots \]

\[ \Sigma_{\text{SIA}} : \bigcirc - \bigcirc - \bigcirc - \bigcirc - \bigcirc - \cdots \]

\[ W_{\text{SIA}} : \cdots = \cdots + \bigcirc \]
New Implementation

- All-electron and full-potential:
  - Realistic wave functions (*oscillations* near atomic sites)
  - Core (and semi-core) states explicitly included in $\Sigma$
  - Applicable to systems with localized $d$-states (Physical temperature effect $\rightarrow$ finite temperature formalism)

- Matsubara time:
  - Bounded and continuous $\rightarrow$ cutoff- and modeling-free
  - Capable of treating shallow core states or highly excited states (no exponential growth)
  - Applicable beyond $GW$
  - Real algorithms $\rightarrow \sim 5$ times more efficient
### Results: QP Band Gap of Si within $GW$

**Effect of Self-consistency**

<table>
<thead>
<tr>
<th></th>
<th>abs. gap (eV)</th>
<th>direct gap (eV)</th>
<th>occupied bandwidth (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Landolt-Börnstein (exp)</td>
<td>1.17</td>
<td>3.4</td>
<td>12.5 ± 0.6</td>
</tr>
<tr>
<td>present work (LDA, FLAPW)</td>
<td>0.52</td>
<td>2.53</td>
<td>12.22</td>
</tr>
<tr>
<td>Hybertsen and Louie</td>
<td>1.29</td>
<td>3.35</td>
<td>12.04</td>
</tr>
<tr>
<td>Schöne and Egiluz</td>
<td>1.34</td>
<td>3.27</td>
<td>11.65</td>
</tr>
<tr>
<td>Schöne and Egiluz (SC)</td>
<td>1.91</td>
<td>4.02</td>
<td>13.10</td>
</tr>
<tr>
<td>present work (all e')</td>
<td>0.85</td>
<td>3.12</td>
<td>12.15</td>
</tr>
<tr>
<td>present work (all e', SC)</td>
<td>1.03</td>
<td>3.48</td>
<td>13.53</td>
</tr>
</tbody>
</table>

### Results: QP Band Gap of Si within $G^{LDA}W^{LDA}$

**All-electron vs. Pseudo-potential**

<table>
<thead>
<tr>
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<tr>
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<tr>
<td>Rohlfing, Krüger, and Pollmann</td>
<td>1.17</td>
</tr>
<tr>
<td>Rojas, Godby, and Needs</td>
<td>1.29</td>
</tr>
<tr>
<td>Fleszar and Hanke</td>
<td>1.19</td>
</tr>
<tr>
<td>Schöne and Egiluz *</td>
<td>1.34</td>
</tr>
<tr>
<td>Arnaud and Alouani (~all e', PAW)</td>
<td>1.00</td>
</tr>
<tr>
<td>Hamada, Hwang, and Freeman (~all e', LAPW)</td>
<td>1.01</td>
</tr>
<tr>
<td>present work (all e', LAPW)</td>
<td>0.85</td>
</tr>
</tbody>
</table>

~all e': $\Sigma$ from core $\approx V^{LDA}[n_{\text{valence + core}}] - V^{LDA}[n_{\text{valence}}]$ $\Rightarrow$ $\sim -0.15\text{ eV}$ error

* discrepancy due to oscillation of WF is also found in dynamical response.

(N31.008, Z13.010)
Results: QP Band Structure of Si within $G^{LDA}_W^{LDA}$
Effect of Core Contribution

- Full calculation
- Exclude core $\Sigma_F$ contribution

at the level of $G^{LDA}_W^{LDA}$ → Band gap decreases by 0.9 eV!
semi-conductor → metal?

Results: Dynamical Response of Ge
Effect of 3d Semi-Core Contribution

Ge
$q // (111)$
$q = 0.10 \text{ Å}^{-1}$

$V^* \chi$

Energy (eV)

All-Electron, Conserving Investigation of the Band Gap of Si and Ge
**Conclusion**

- The success of non-conserving $G^{LDA} W^{LDA}$ calculations is helped by large compensation between effects from lack of:
  - core contribution to self-energy
  - oscillations in wave functions when evaluating $\langle k_1 | \Sigma | k_2 \rangle$
  - self-consistency
- Deep core states play an important role in defining the QP band gap through exchange process with the valence states.
- Omission of oscillations of the wave functions near the atomic sites have sizeable impact on the QP band gap.
- Self-consistency is necessary in our conserving calculation to produce satisfactory gap.
- Polarization from 3d core states in Ge has almost no effect on the QP band structure within $GW$ approximation.
- Further improvement requires processes beyond $GW$ diagram.