GW@ exciting

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- Implementation
  - Program workflow
  - Product basis representation
  - Matrix form of GW equations
- Usage
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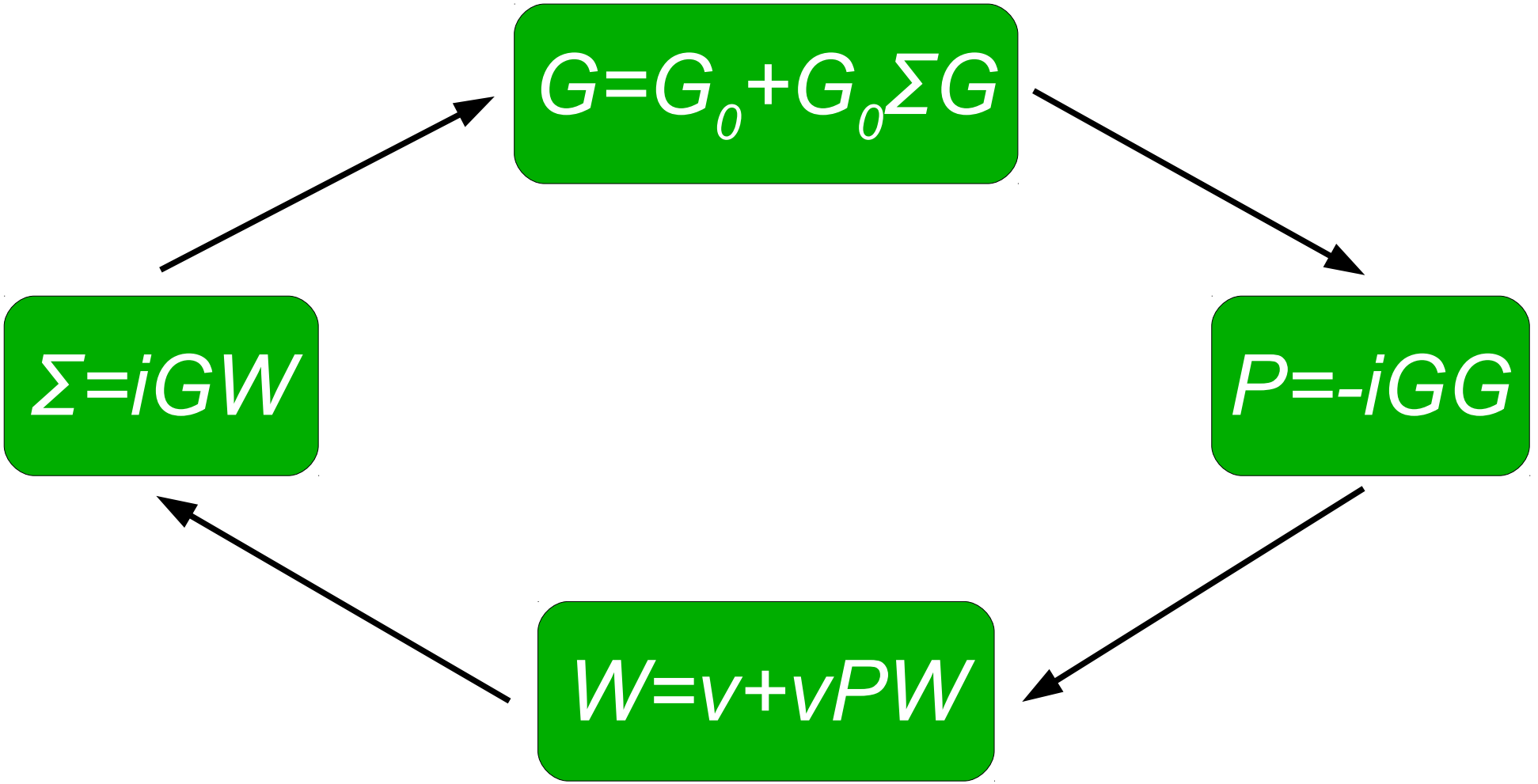
  - Convergence control

Introduction

GW approximation



L. Hedin, Phys. Rev. 139, A796 (1965)
L. Hedin and B. I. Lundqvist, Solid State Phys. 23, 1 (1969)

G_0W_0 approximation

Kohn-Sham (KS) eigenvalues

DFT exchange-correlation potential

$$\epsilon_{n\mathbf{k}}^{\mathrm{qp}} = \epsilon_{n\mathbf{k}} + \left\langle \psi_{n\mathbf{k}}(\mathbf{r}) \left| \Re\left[\Sigma\left(\mathbf{r}, \mathbf{r}'; \epsilon_{n\mathbf{k}}^{\mathrm{qp}}\right)\right] - V^{\mathrm{xc}}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}') \right| \psi_{n\mathbf{k}}(\mathbf{r}') \right\rangle$$

KS eigenfunctions

M. Hybertsen and S. Louie, PRB 34, 5390 (1986)

G_0W_0 approximation

Non-interacting Green's function

$$G_0(\mathbf{r}, \mathbf{r}'; \omega) = \sum_{n\mathbf{k}} \frac{\psi_{n\mathbf{k}}(\mathbf{r})\psi^*_{n\mathbf{k}}(\mathbf{r}')}{\omega - \tilde{\epsilon}_{n\mathbf{k}}}$$

$$\tilde{\epsilon}_{n\mathbf{k}} \equiv \epsilon_{n\mathbf{k}} + i\eta \, \mathrm{sgn}(\epsilon_F - \epsilon_{n\mathbf{k}})$$

G_0W_0 approximation

P

Polarizability in the random phase approximation (RPA)

$$P_0(\mathbf{r},\mathbf{r}';\omega) = \sum_{n\mathbf{k},m\mathbf{k}'} f(\epsilon_{n\mathbf{k}})\left[1-f(\epsilon_{m\mathbf{k}'})\right]\psi_{n\mathbf{k}}(\mathbf{r})\psi^*_{m\mathbf{k}'}(\mathbf{r})\psi^*_{n\mathbf{k}}(\mathbf{r}')\psi_{m\mathbf{k}'}(\mathbf{r}')$$

$$\times\left\{\frac{1}{\omega-\epsilon_{m\mathbf{k}'}+\epsilon_{n\mathbf{k}}+i\eta}-\frac{1}{\omega+\epsilon_{m\mathbf{k}'}-\epsilon_{n\mathbf{k}}-i\eta}\right\}$$

$f(\epsilon_{n\mathbf{k}})$ – Fermi distribution function

G_0W_0 approximation

Dynamically screened Coulomb potential

W

$$W_0(\mathbf{r},\mathbf{r}';\omega) = \int \varepsilon^{-1}(\mathbf{r},\mathbf{r}_1;\omega)\, v(\mathbf{r}_1,\mathbf{r}')\, d\mathbf{r}_1$$

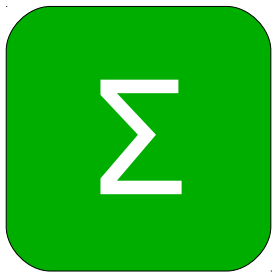
Dielectric function

$$\varepsilon(\mathbf{r},\mathbf{r}';\omega) = \delta(\mathbf{r},\mathbf{r}') - \int v(\mathbf{r},\mathbf{r}_1)\, P_0(\mathbf{r}_1,\mathbf{r}';\omega)\, d\mathbf{r}_1$$

$v(\mathbf{r},\mathbf{r}') = 1/|\mathbf{r}-\mathbf{r}'|$ – (bare) Coulomb potential

G_0W_0 approximation

$$W_0^c(\mathbf{r},\mathbf{r}';\omega) = W_0(\mathbf{r},\mathbf{r}';\omega) - v(\mathbf{r},\mathbf{r}')$$



Exchange self-energy:

$$\Sigma^x(\mathbf{r},\mathbf{r}') = \frac{i}{2\pi}\int G_0(\mathbf{r},\mathbf{r}';\omega')v(\mathbf{r}',\mathbf{r})e^{i\omega'\eta}d\omega'$$

$$= -\sum_{n\mathbf{k}} f_{n\mathbf{k}}\psi_{n\mathbf{k}}(\mathbf{r})v(\mathbf{r}',\mathbf{r})\psi^*_{n\mathbf{k}}(\mathbf{r}')$$

Correlation self-energy:

$$\Sigma^c(\mathbf{r},\mathbf{r}';\omega) = \frac{i}{2\pi}\int G_0(\mathbf{r},\mathbf{r}';\omega+\omega')W_0^c(\mathbf{r}',\mathbf{r};\omega')\,d\omega'$$

GW approximation

G_0W_0

$$\epsilon_{n\mathbf{k}}^{\mathrm{qp}} = \epsilon_{n\mathbf{k}} + \left\langle \psi_{n\mathbf{k}}(\mathbf{r}) \middle| \Re\left[\Sigma\left(\mathbf{r}, \mathbf{r}'; \epsilon_{n\mathbf{k}}^{\mathrm{qp}}\right)\right] - V^{\mathrm{xc}}(\mathbf{r})\,\delta(\mathbf{r}-\mathbf{r}') \middle| \psi_{n\mathbf{k}}(\mathbf{r}') \right\rangle$$

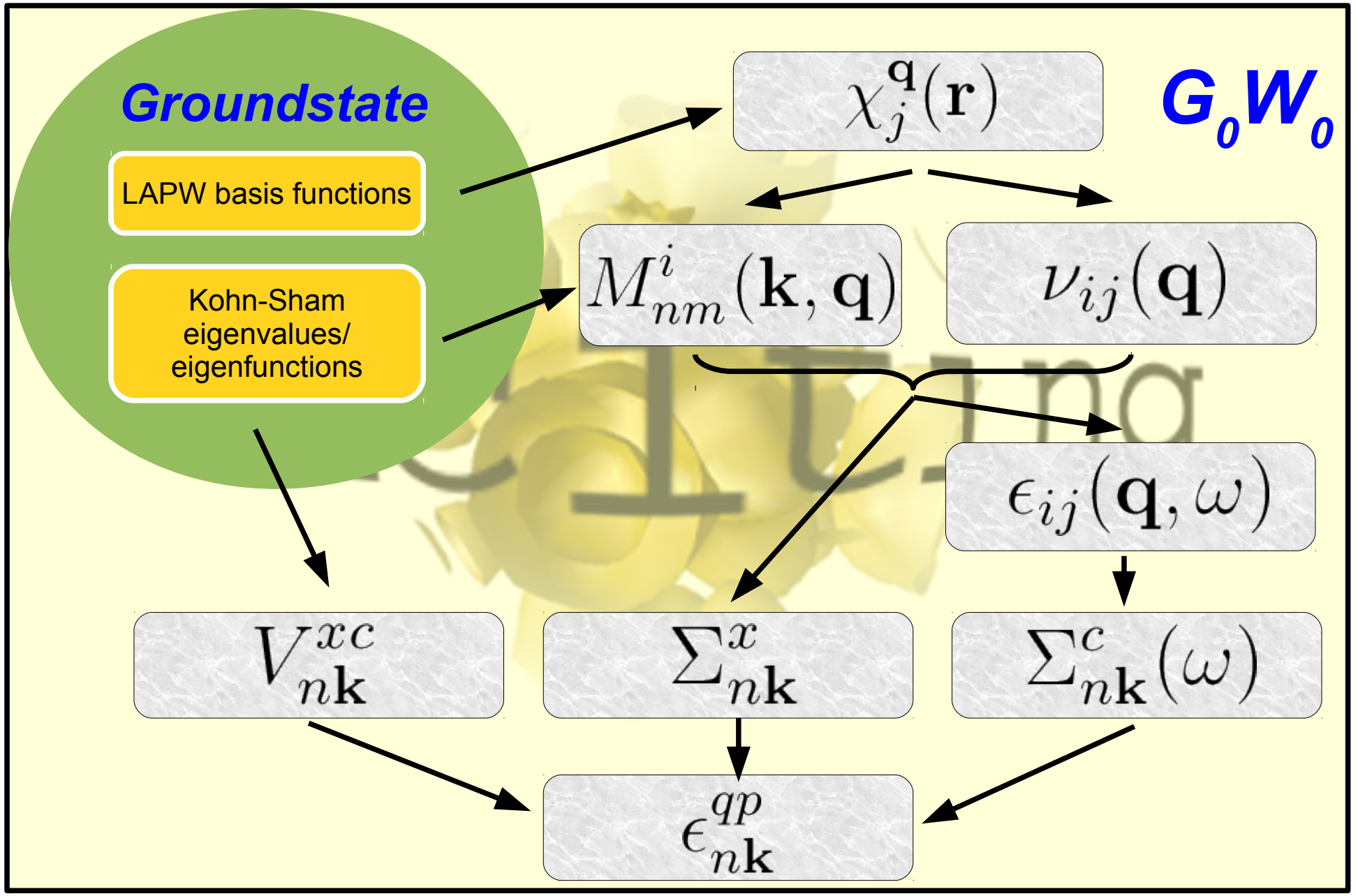
Think of self-consistency?

- Partial: G_0W, GW_0
- Full (e.g. QSGW):

$$\left[-\frac{1}{2}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r}) + V_H(\mathbf{r})\right]\Psi_{n\mathbf{k}}(\mathbf{r}) + \int \Sigma(\mathbf{r}, \mathbf{r}'; E_{n\mathbf{k}}^{\mathrm{qp}})\,\Psi_{n\mathbf{k}}(\mathbf{r}')d\mathbf{r}' = E_{n\mathbf{k}}^{\mathrm{qp}}\,\Psi_{n\mathbf{k}}(\mathbf{r})$$

Implementation

Program flowchart



Product-basis representation

$$P_0\left(\mathbf{r},\mathbf{r}';\omega\right)=\sum_{nm}\sum_{\mathbf{k},\mathbf{q}}F_{nm}(\mathbf{k},\mathbf{q};\omega)\psi_{n\mathbf{k}}(\mathbf{r})\psi^*_{m\mathbf{k}-\mathbf{q}}(\mathbf{r})\psi^*_{n\mathbf{k}}(\mathbf{r}')\psi_{m\mathbf{k}-\mathbf{q}}(\mathbf{r}')$$

$$\psi_{n\mathbf{k}}(\mathbf{r})\,\psi^*_{m\mathbf{k}-\mathbf{q}}(\mathbf{r})=\sum_i M^i_{nm}(\mathbf{k},\mathbf{q})\,\chi^{\mathbf{q}}_i(\mathbf{r})$$

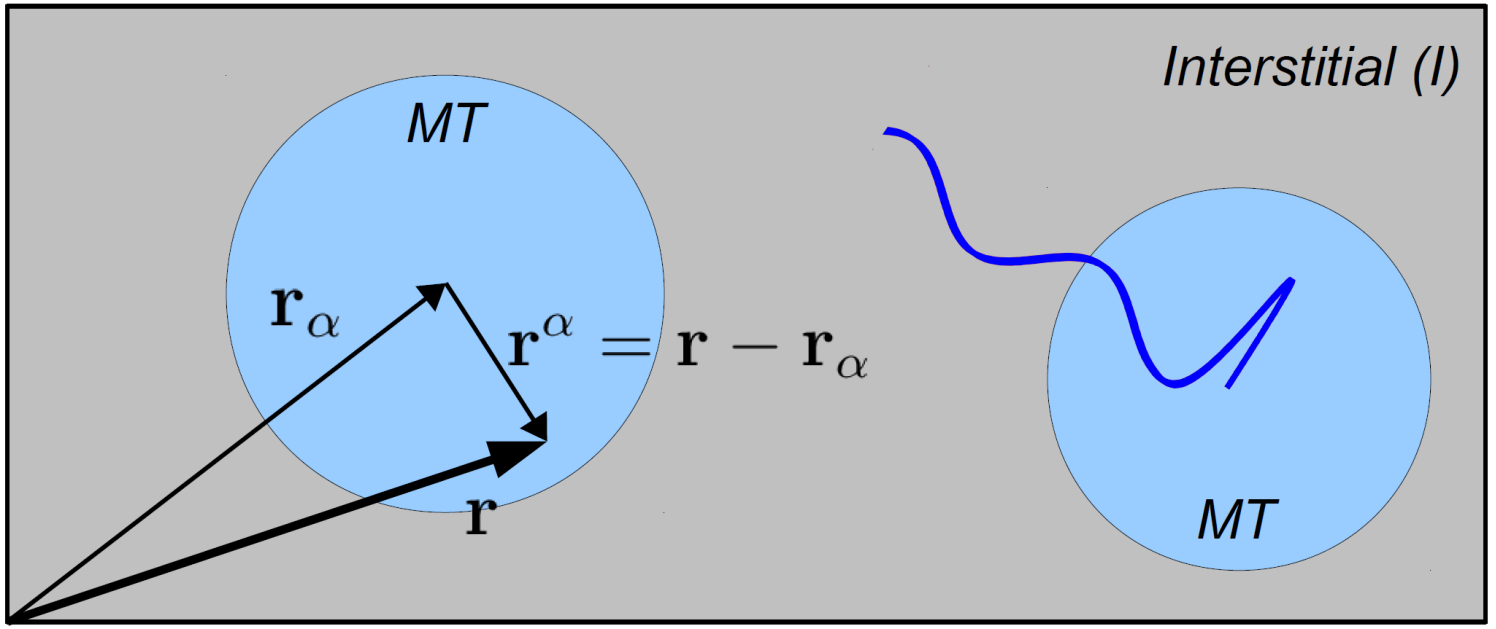
Matrix form:

$$P_{ij}(\mathbf{q},\omega)\equiv\int_V\int_V\left[\chi^{\mathbf{q}}_i(\mathbf{r})\right]^*P(\mathbf{r},\mathbf{r}';\omega)\chi^{\mathbf{q}}_j(\mathbf{r}')d\mathbf{r}d\mathbf{r}'$$

$$=\sum_{\mathbf{k}}^{BZ}\sum_{nm}F_{nm}(\mathbf{k},\mathbf{q};\omega)M^i_{nm}(\mathbf{k},\mathbf{q})\left[M^j_{nm}(\mathbf{k},\mathbf{q})\right]^*$$

LAPW basis

$$\phi_{\mathbf{k}+\mathbf{G}}(\mathbf{r}) = \begin{cases} \sum_{lm} \left[A_{lm}(\mathbf{k}+\mathbf{G}) u_l(r^\alpha, E_l) + ... \right] Y_{lm}(\mathbf{r}^\alpha) & , r^\alpha \leqslant R^\alpha_{MT} \\ \frac{1}{\Omega} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} & , \mathbf{r} \in I \end{cases}$$



Mixed basis

MT region

- Use only $u_{\alpha l}(r^\alpha)$ with $l \leq l_{\max}^{\mathrm{MB}}$
- Neglect $\dot{u}_{\alpha l}(r)$
- $v_{\alpha NL}(r^\alpha) = u_{\alpha l}(r^\alpha) u_{\alpha l'}(r^\alpha) \;:\; |l - l'| \leq L \leq l + l'$
- Form orthonormal basis + eliminate linearly dependent products
- Take in account the translational symmetry

$$\gamma^{\mathbf{q}}_{\alpha NLM}(\mathbf{r}) = \frac{1}{\sqrt{N_c}} \sum_{\mathbf{R}} e^{i\mathbf{q}\cdot(\mathbf{r}_\alpha + \mathbf{R})} v_{\alpha NL}(r^\alpha) Y_{LM}(\hat{\mathbf{r}}^\alpha)$$

F. Aryasetiawan and O. Gunnarsson, Phys. Rev. B 49, 16214 (1994)
T. Kotani and M. van Schilfgaarde, Solid State Comm. 121, 461 (2002)

Mixed basis

Interstitial region

- Overlap matrix

$$\mathbb{O}_{\mathbf{G}\mathbf{G}'} = \frac{1}{\Omega}\int_{\Omega} \theta_I(\mathbf{r})\, e^{i(\mathbf{G}-\mathbf{G}')\cdot\mathbf{r}}\, d^3r$$

- Diagonalize

$$\sum_{\mathbf{G}'} \mathbb{O}_{\mathbf{G}\mathbf{G}'} S_{\mathbf{G}'i} = \lambda_i^I\, S_{\mathbf{G}i}$$

- Build an orthonormal basis set:

$$P_i^{\mathbf{q}}(\mathbf{r}) \equiv \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G}}^{G_{max}^{MB}} \tilde{S}_{\mathbf{G}i} e^{i(\mathbf{G}+\mathbf{q})\cdot\mathbf{r}} \theta_I(\mathbf{r}) \text{ , where } \tilde{S}_{\mathbf{G}i} \equiv \frac{S_{\mathbf{G}i}}{\sqrt{\lambda_i^I}}$$

Mixed basis

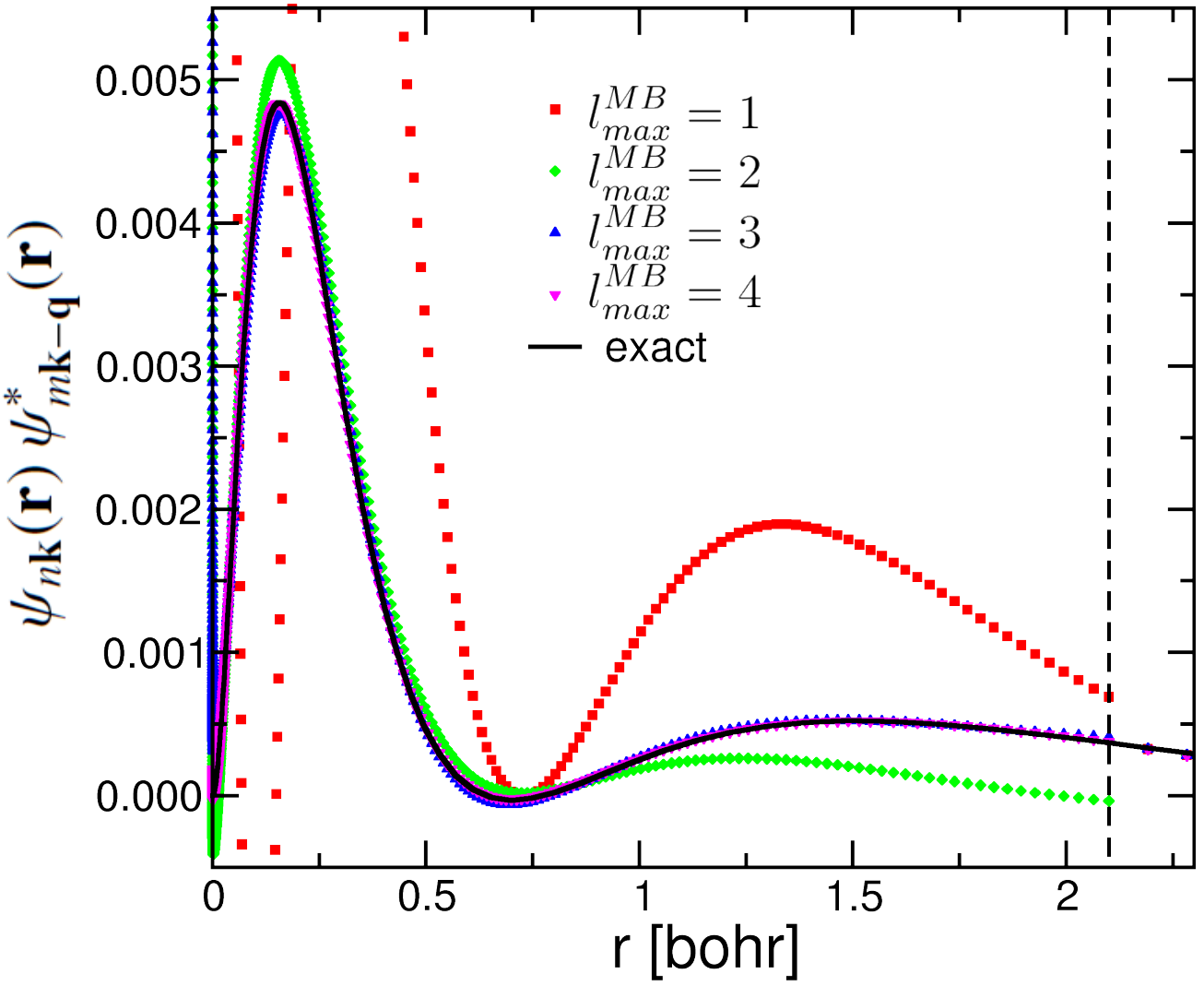
$$\left\{\chi_j^{\mathbf{q}}(\mathbf{r})\right\} \equiv \left\{\gamma_{\alpha NLM}^{\mathbf{q}}(\mathbf{r}), P_i^{\mathbf{q}}(\mathbf{r})\right\}$$

$$M_{nm}^{i}(\mathbf{k},\mathbf{q}) \equiv \int_{\Omega} \left[\chi_i^{\mathbf{q}}(\mathbf{r})\, \psi_{m\mathbf{k}-\mathbf{q}}(\mathbf{r})\right]^{*} \psi_{n\mathbf{k}}(\mathbf{r}) d^3 r$$

Mixed basis

Completeness test: MT region

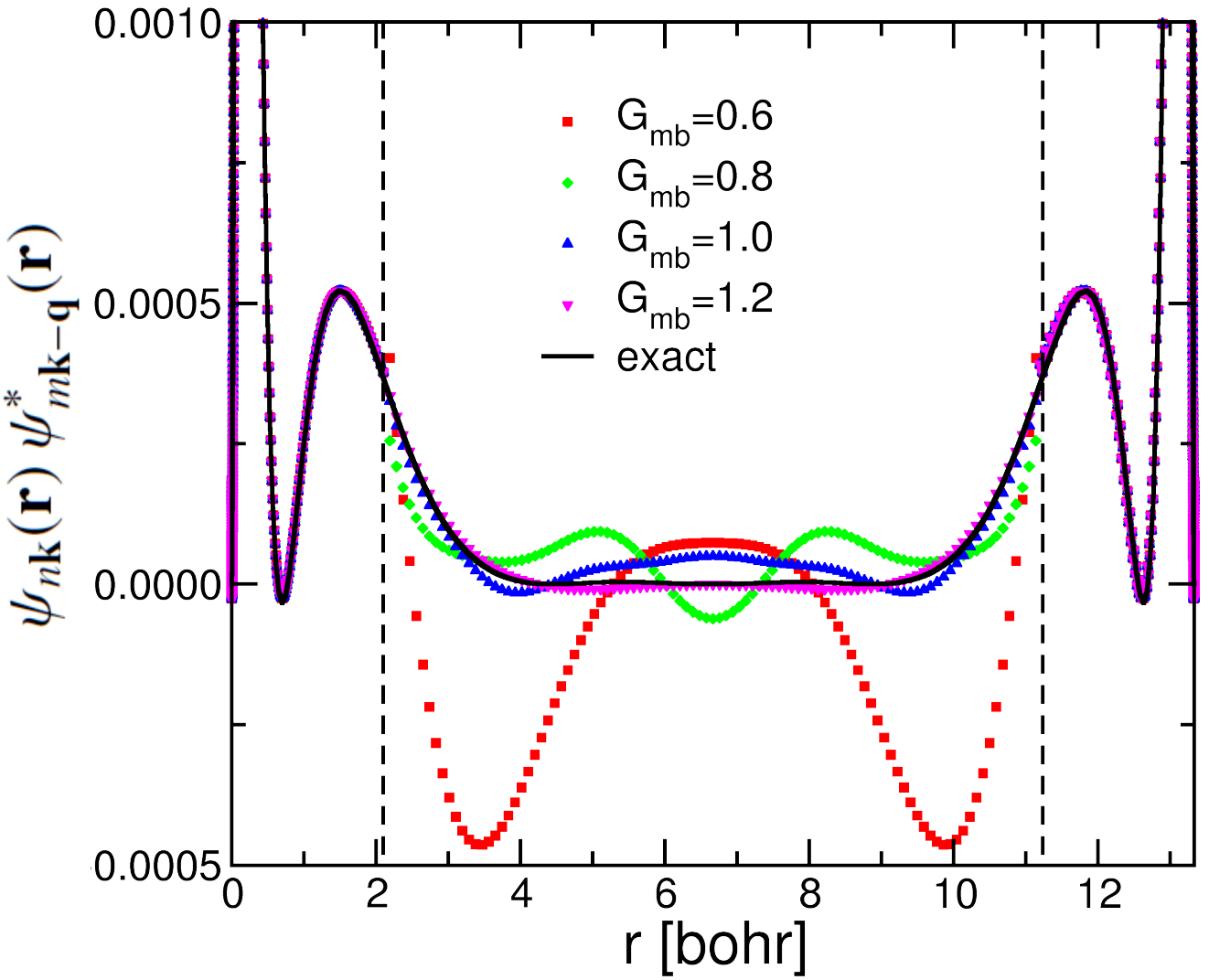
Si, **k**=(0,0,0),**k-q**=(0,0,1), n=5, m=4



Mixed basis

Completeness test: Interstitial

Si, **k**=(0,0,0),**k-q**=(0,0,1), n=5, m=4



$$G_{MB} = \frac{G_{max}^{MB}}{G_{max}^{LAPW}}$$

G_0W_0 equations in matrix form

Coulomb potential

$$\nu_{ij}(\mathbf{q}) = \int_V \int_V \left[\chi_i^{\mathbf{q}}(\mathbf{r})\right]^* \nu(\mathbf{r},\mathbf{r}')\chi_j^{\mathbf{q}}(\mathbf{r}')d\mathbf{r}d\mathbf{r}'$$

Special treatment for the case $\mathbf{q} \to 0$

Exchange part of the self-energy

$$\Sigma^x_{n\mathbf{k}} = -\sum_{\mathbf{q}}^{BZ}\sum_{ij}\nu_{ij}(\mathbf{q})\sum_{m}^{occ}\left[M^i_{nm}(\mathbf{k},\mathbf{q})\right]^* M^j_{nm}(\mathbf{k},\mathbf{q})$$

G_0W_0 equations in matrix form

Polarizability

$$P_{ij}(\mathbf{q},\omega) = \sum_{\mathbf{k}}^{BZ} \sum_{n}^{occ} \sum_{m}^{unocc} F_{nm}(\mathbf{k},\mathbf{q};\omega) M^{i}_{nm}(\mathbf{k},\mathbf{q}) \left[M^{j}_{nm}(\mathbf{k},\mathbf{q})\right]^{*}$$

`/input/gw/@nempty`

Generalized tetrahedron method (LIBBZINT library):

`/input/gw/@ngridq` + `/input/gw/@vqloff`

G_0W_0 equations in matrix form

Dielectric function

$$\epsilon_{ij}(\mathbf{q},\omega) = \delta_{ij} - \sum_{lm} \nu_{il}^{\frac{1}{2}}(\mathbf{q}) P_{lm}(\mathbf{q},\omega) \nu_{mj}^{\frac{1}{2}}(\mathbf{q})$$

Correlation term of the screened Coulomb potential

$$W_{ij}^{c}(\mathbf{q},\omega) = \sum_{lm} \nu_{il}^{\frac{1}{2}}(\mathbf{q}) \left[\epsilon_{lm}^{-1}(\mathbf{q},\omega) - \delta_{lm}\right] \nu_{mj}^{\frac{1}{2}}(\mathbf{q})$$

G_0W_0 equations in matrix form

Correlation part of the self-energy

$$X_{nm}(\mathbf{k},\mathbf{q};\omega) \equiv \sum_{ij} \left[M^i_{nm}(\mathbf{k},\mathbf{q})\right]^* W^c_{ij}(\mathbf{q},\omega) M^j_{nm}(\mathbf{k},\mathbf{q})$$

$$\Sigma^c_{n\mathbf{k}}(\omega) = \frac{i}{2\pi} \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+unocc} \int_{-\infty}^{\infty} d\omega' \frac{X_{nm}(\mathbf{k},\mathbf{q};\omega')}{\omega + \omega' - \tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}}}$$

`/input/gw/freqgrid`

Integral over imaginary frequency: $\omega = iu$

$$\Sigma^c_{n\mathbf{k}}(iu) = \frac{1}{N_c} \sum_{\mathbf{q}}^{BZ} \sum_{m} \int_0^{\infty} \frac{du'}{2\pi} X_{nm}(\mathbf{k},\mathbf{q};iu') \frac{2\left(\epsilon_{m\mathbf{k}-\mathbf{q}} - iu\right)}{u'^2 + \left(\epsilon_{m\mathbf{k}-\mathbf{q}} - iu\right)^2}$$

Analytic continuation onto the real frequency axis

G_0W_0 quasi-particle energy

$$\epsilon^{qp}_{n\mathbf{k}} = \epsilon_{n\mathbf{k}} + Z_{n\mathbf{k}} \left[\Sigma^x_{n\mathbf{k}} + \Re\Sigma^c_{n\mathbf{k}}(\epsilon_{n\mathbf{k}}) - V^{xc}_{n\mathbf{k}} \right]$$

KS energies

Diagonal matrix elements of the exchange-correlation potential

$$Z_{n\mathbf{k}} = \left[1 - \frac{\partial}{\partial\omega} \Re\Sigma^c_{n\mathbf{k}}(\omega) \Big|_{\epsilon_{n\mathbf{k}}} \right]^{-1}$$

QP renormalization factor

Usage

Input file

Groundstate

```
<groundstate
   rgkmax="8.0"
   ngridk="8 8 8"
   gmaxvr="14"
   xctype="LDA_PW"
>
</groundstate>
```

Quality of the starting ("zero order") potential, eigenvalues, eigenvectors

Input file

GW

```
<gw
   taskname="g0w0"
    ...
    <mixbasis
        lmaxmb="3"
        epsmb="1.0d-4"
        gmb="1.0"
    ></mixbasis>
    ...
    <barecoul ... ></barecoul>
    ...
    <selfenergy ... ></selfenergy>
    ...
    <freqgrid ... ></freqgrid>

</gw>
```

Type of calculations:

- "band" - QP band-structure plot
- "dos" - QP density of states

...

Input file

GW

```
<gw

    taskname="g0w0"
    ...
    <mixbasis
       lmaxmb="3"
       epsmb="1.0d-4"
       gmb="1.0"
    ></mixbasis>
    ...
    <barecoul ... ></barecoul>
    ...
    <selfenergy ... ></selfenergy>
    ...
    <freqgrid ... ></freqgrid>

</gw>
```

Quality of
the product basis

Input file

GW

```
<gw

    taskname="g0w0"

    ...

    <mixbasis
        lmaxmb="3"
        epsmb="1.0d-4"
        gmb="1.0"
    ></mixbasis>
    ...
    <barecoul ... ></barecoul>
    ...
    <selfenergy ... ></selfenergy>
    ...
    <freqgrid ... ></freqgrid>

</gw>
```

Parameters for more "advanced" usage

Output

GW_INFO.OUT

```
================================================================================
=                              Main GW output file                             =
================================================================================


********************************************************************************
*                              GW input parameters                             *
********************************************************************************


 GW taskname:

   g0w0 - G0W0 run

--------------------------------------------------------------------------------

 Frequency integration parameters:
 Number of frequencies:           16
 Cutoff frequency:    1.00000000000000
 Grid type:
   gaule2 - Grid for double Gauss-Legendre quadrature,
            from 0 to freqmax and from freqmax to infinity
 Convolution method:
   imfreq : weights calculated for imaginary frequecies

--------------------------------------------------------------------------------

 Correlation self-energy parameters:
...
```

Output

EVALQP.DAT

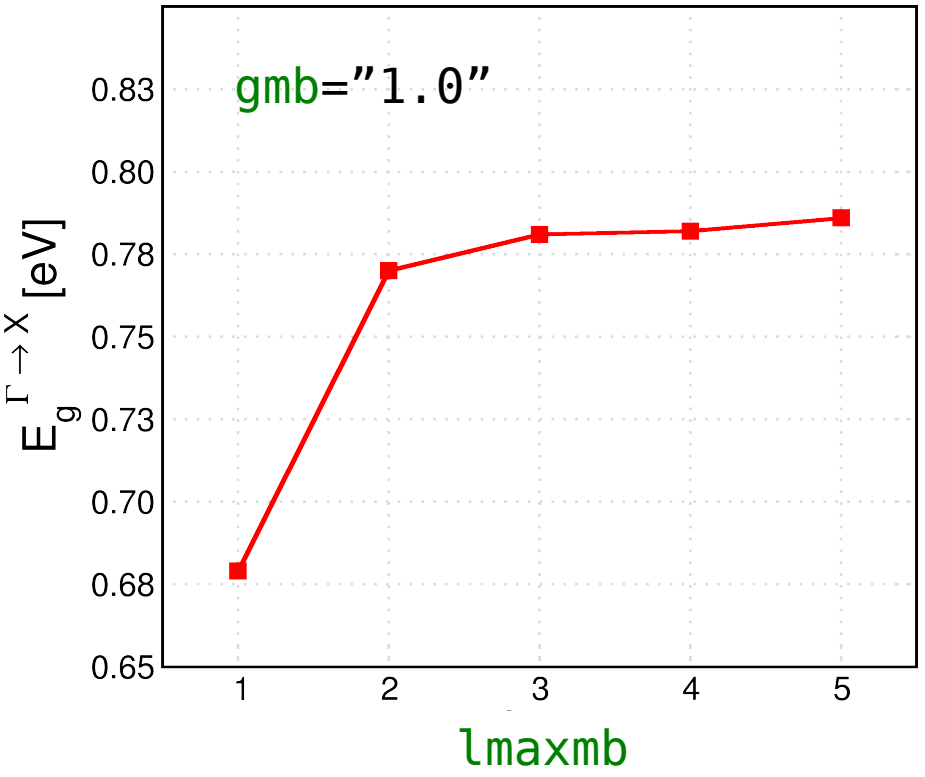
```
k-point #     1:    0.000000    0.000000    0.000000    0.125000
 state    E_KS      E_HF       E_GW       Sx         Sc         Vxc         DE_HF       DE_GW       Znk
   1    -0.24974   -0.48679   -0.46467   -0.69023    0.21961   -0.45318   -0.23704   -0.21493    0.78986
   2     0.19048    0.09502   -0.00819   -0.59347    0.09863   -0.49801   -0.09546   -0.19867    0.78709
   3     0.19048    0.09502   -0.00856   -0.59347    0.09817   -0.49801   -0.09546   -0.19904    0.78439
   4     0.19048    0.09502   -0.00861   -0.59347    0.09811   -0.49801   -0.09546   -0.19909    0.78417
   5     0.28272    0.48340    0.11444   -0.23178   -0.15909   -0.43246    0.20068   -0.16828    0.79071
   6     0.28272    0.48340    0.11444   -0.23178   -0.15912   -0.43246    0.20068   -0.16828    0.79120
   7     0.28272    0.48340    0.11493   -0.23178   -0.15857   -0.43246    0.20068   -0.16779    0.79254
   8     0.30752    0.54184    0.14817   -0.32549   -0.18035   -0.55982    0.23433   -0.15934    0.77472
   9     0.47138    0.68975    0.29754   -0.12737   -0.18501   -0.34573    0.21836   -0.17385    0.81888
  10     0.47467    0.69897    0.31363   -0.16335   -0.17396   -0.38765    0.22430   -0.16104    0.79701

k-point #     2:    0.000000    0.000000    0.500000    0.500000
 state    E_KS      E_HF       E_GW       Sx         Sc         Vxc         DE_HF       DE_GW       Znk
   1    -0.16372   -0.36830   -0.37099   -0.68347    0.19693   -0.47889   -0.20458   -0.20727    0.79924
   2    -0.06718   -0.21348   -0.27030   -0.58829    0.14380   -0.44199   -0.14630   -0.20312    0.78162
   3     0.14633    0.04672   -0.05214   -0.58597    0.10306   -0.48636   -0.09961   -0.19847    0.77887
   4     0.14633    0.04672   -0.05241   -0.58597    0.10271   -0.48636   -0.09961   -0.19875    0.77972
   5     0.24226    0.44139    0.07439   -0.26439   -0.15708   -0.46352    0.19912   -0.16788    0.79173

...
```

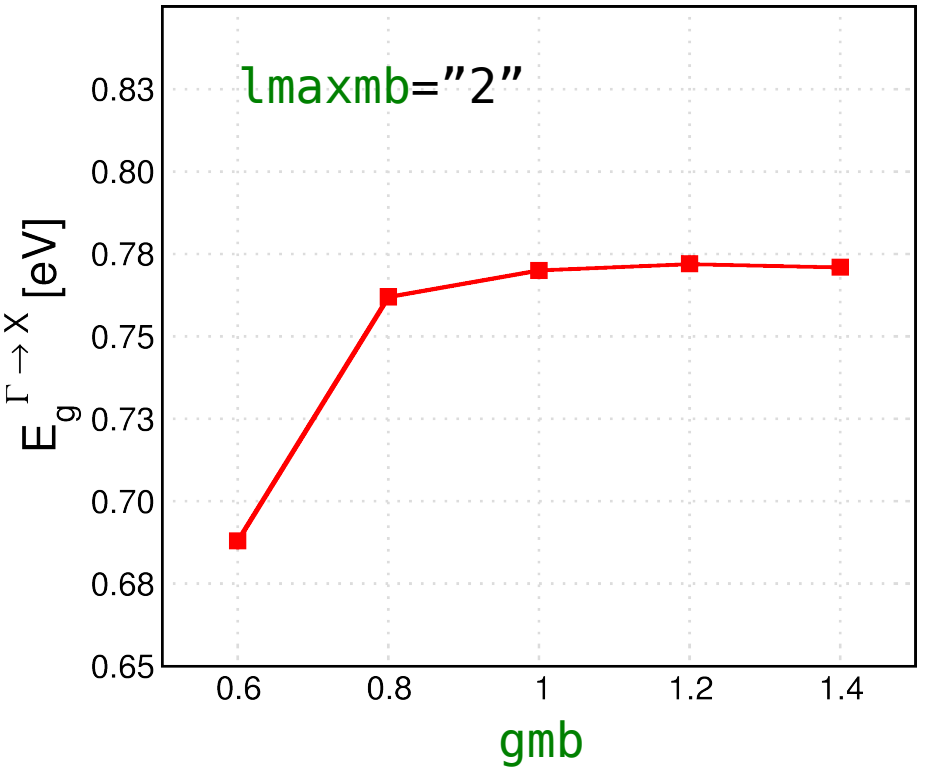
Convergence control

Product basis

`/input/gw/mixbasis/@lmaxmb` `/input/gw/mixbasis/@gmb`

`nempty="17", ngridk="2 2 2"`

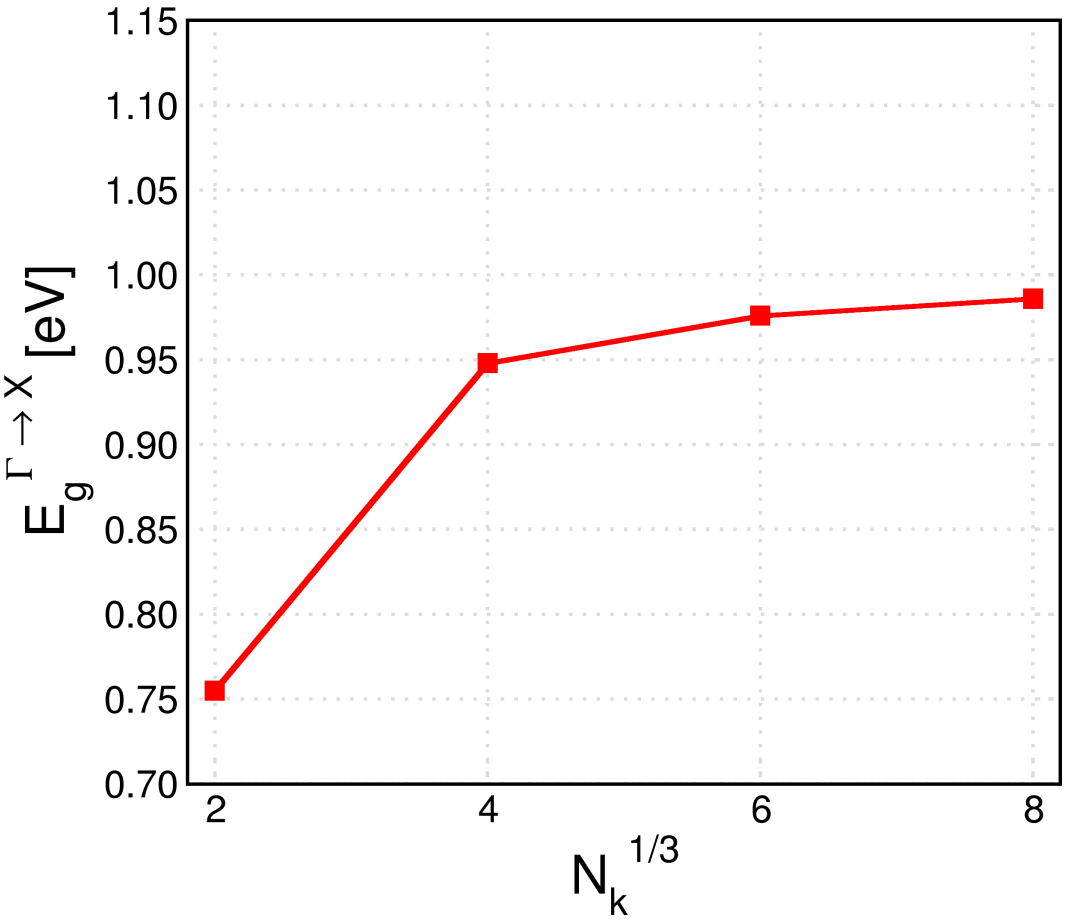




Convergence control

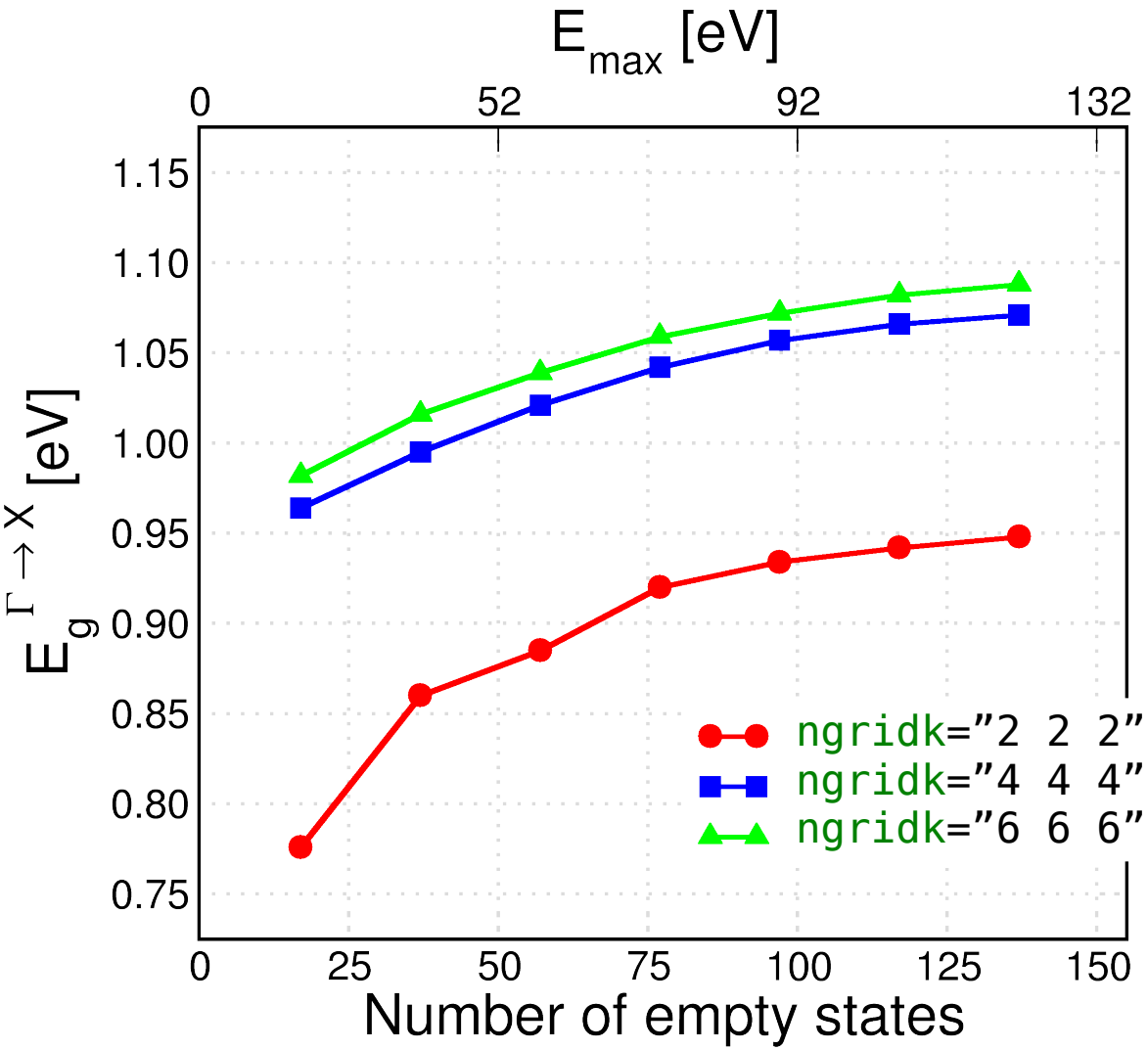
k / q -point grids: `/input/groundstate/@ngridk`

```
lmaxmb="3", gmb="1.0", nempty="17"
```



Convergence control

Number of unoccupied states: `/input/groundstate/@nempty`



BSE@GW

```
<gw
    taskname=”skip”
</gw>
```

Signal to use QP spectrum in XS calculations

```
<xs>
    xstype=”BSE”
    ngridk=”4 4 4”
    ngridq=”4 4 4”
    nempty=”100”
    ...
    <BSE
        bsetype="singlet"
        nstlbse="1 5 1 4"
        nstlbsemat="1 5 1 4"
    />
    ...
</xs>
```

How exciting?

exciting

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Electronic Bandstructure From GW

by Dmitrii Nabok for exciting *carbon*

Purpose: In this tutorial you will learn how to perform a basic G_0W_0 calculation. As an example, the electronic bandstructure of bulk Si is calculated. Notice that **self-consistent GW** is not yet implemented in **exciting**.

Fold

Table of Contents

0. Define relevant environment variables