"Accurate effective masses from first principles"

Laflamme Janssen, Jonathan ; Gonze, Xavier

Abstract

The accurate ab initio description of effective masses is of key interest in the design of materials with high mobility. However, up to now, they have been calculated using finite-difference estimation of density functional theory (DFT) electronic band curvatures. To eliminate the numerical noise inherent to finite-difference and obtain an approach that is more suitable for material design using high throughput computing, we develop a method allowing to obtain the curvature of DFT bands using Density-Functional Perturbation Theory (DFPT), taking a change of wavevector as a perturbation. Also, the inclusion of G$_0$W$_0$ corrections to DFT bands in our method will be presented.

Document type : *Communication à un colloque (Conference Paper)*

Référence bibliographique

Laflamme Janssen, Jonathan ; Gonze, Xavier. *Accurate effective masses from first principles.* APS March Meeting 2015 (San Antonio, TX, USA, du 02/03/2015 au 06/03/2015).

Accurate effective masses from first principles

Jonathan Laflamme Janssen* and Xavier Gonze

Institute of Condensed Matter and Nanosciences (IMCN/NAPS), Université catholique de Louvain

*jonathan.laflamme@uclouvain.be

Université catholique de Louvain

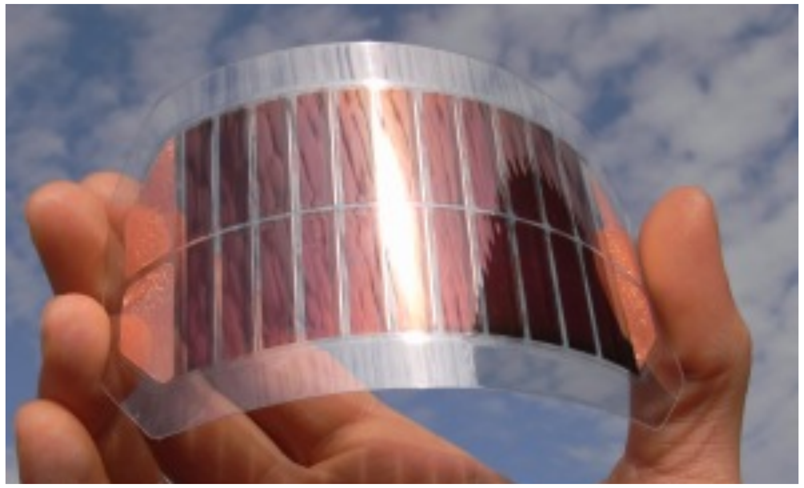
Effective masses

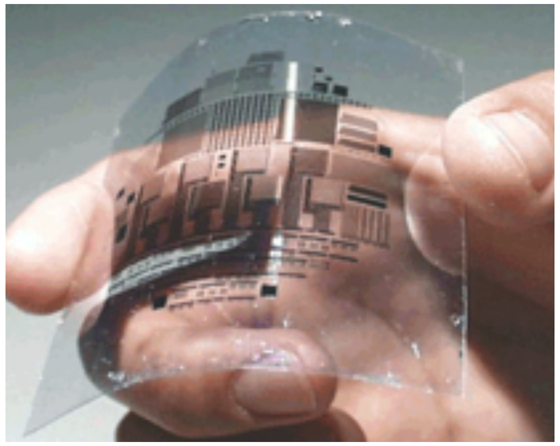
Effective masses

- design materials with better mobility for electronic applications

Effective masses

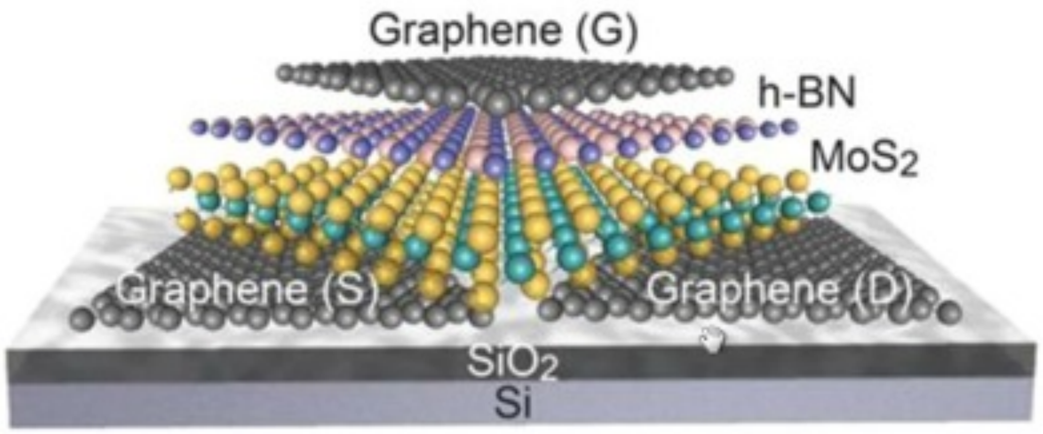
- design materials with better mobility for electronic applications
  - organic semiconductors





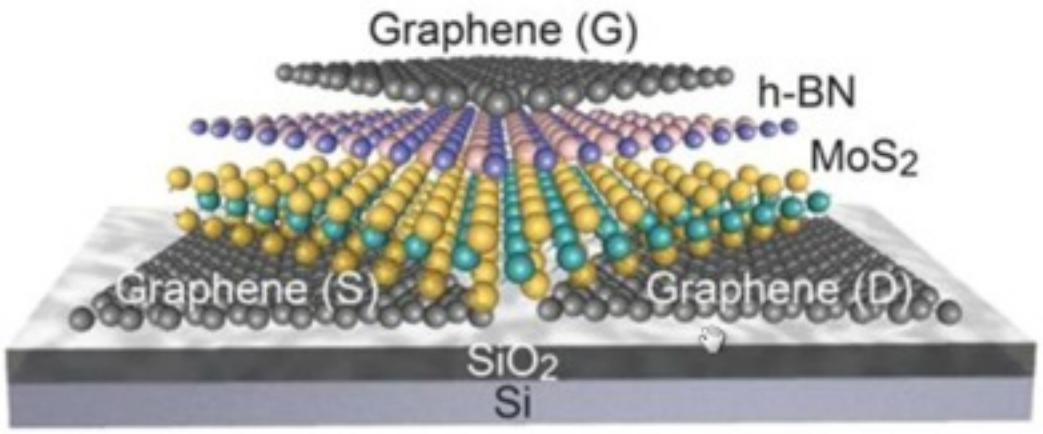
Effective masses

- design materials with better mobility for electronic applications
  - organic semiconductors
  - next generation CPUs



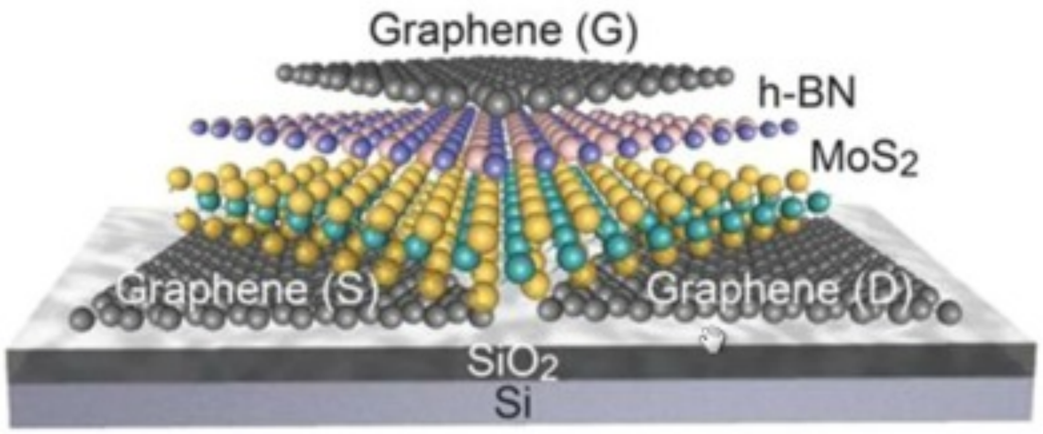
Effective masses

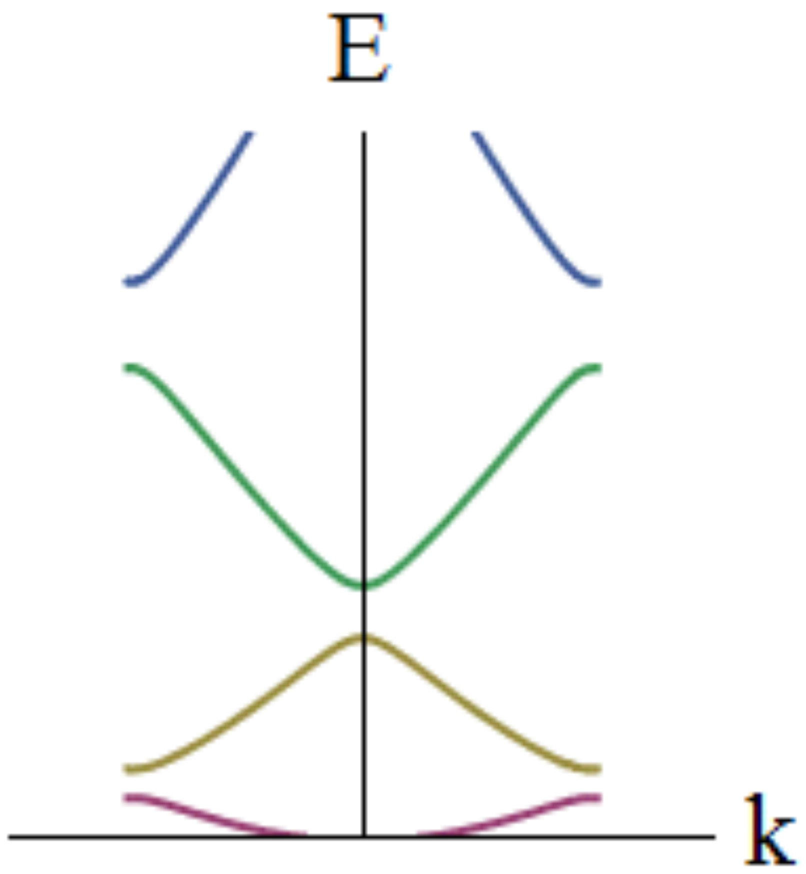
- design materials with better mobility for electronic applications
  - organic semiconductors
  - next generation CPUs
  - transparent conducting oxides (TCOs)
    better μ : both higher conductivity and transparency



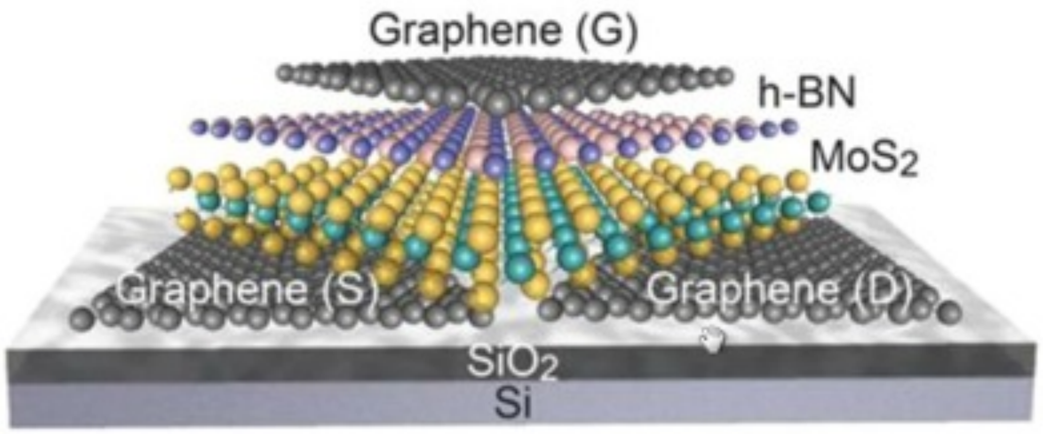
Effective masses

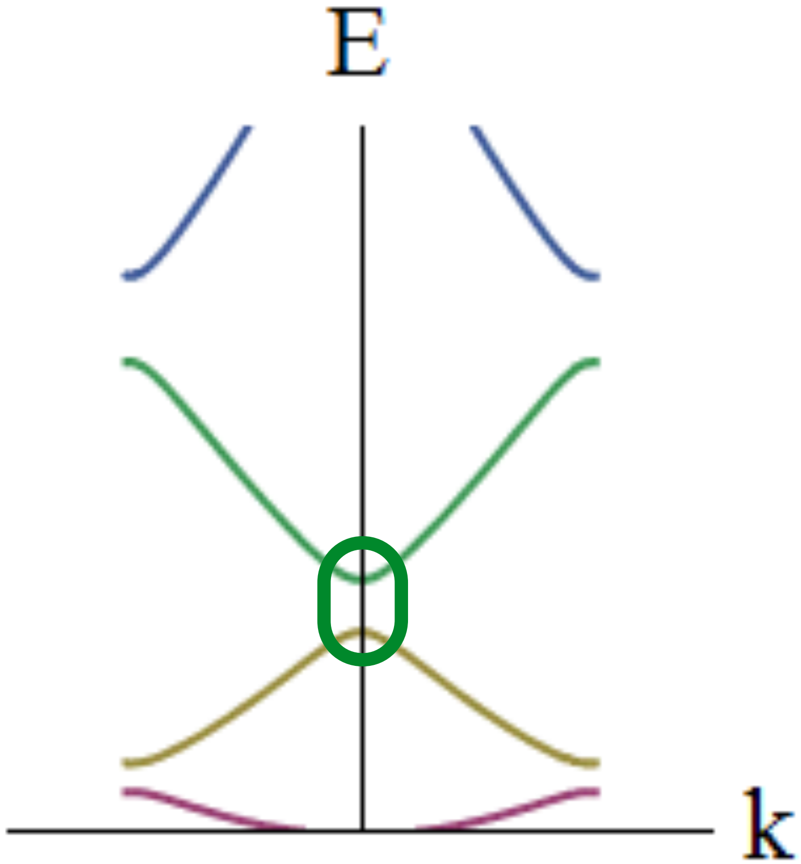
- design materials with better mobility for electronic applications
  - organic semiconductors
  - next generation CPUs
  - transparent conducting oxides (TCOs)
    better μ : both higher conductivity and transparency





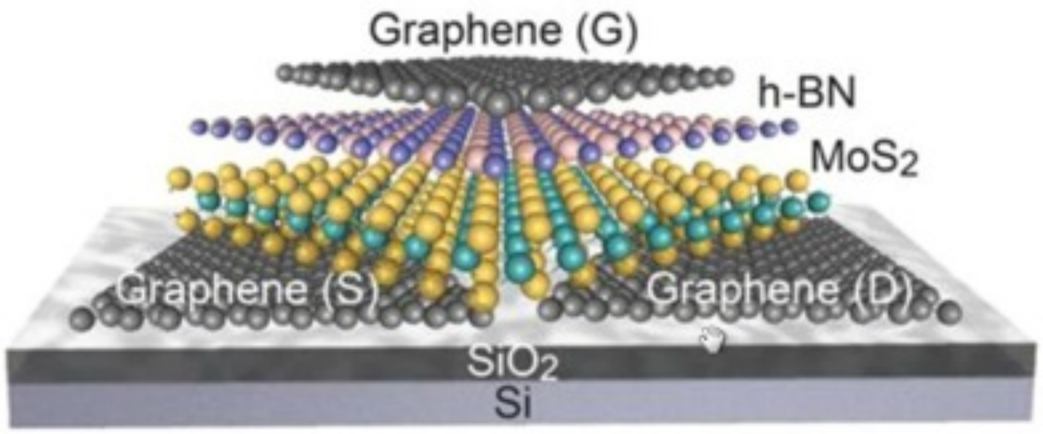
- design materials with better mobility for electronic applications
  - organic semiconductors
  - next generation CPUs
  - transparent conducting oxides (TCOs)
    better μ : both higher conductivity and transparency



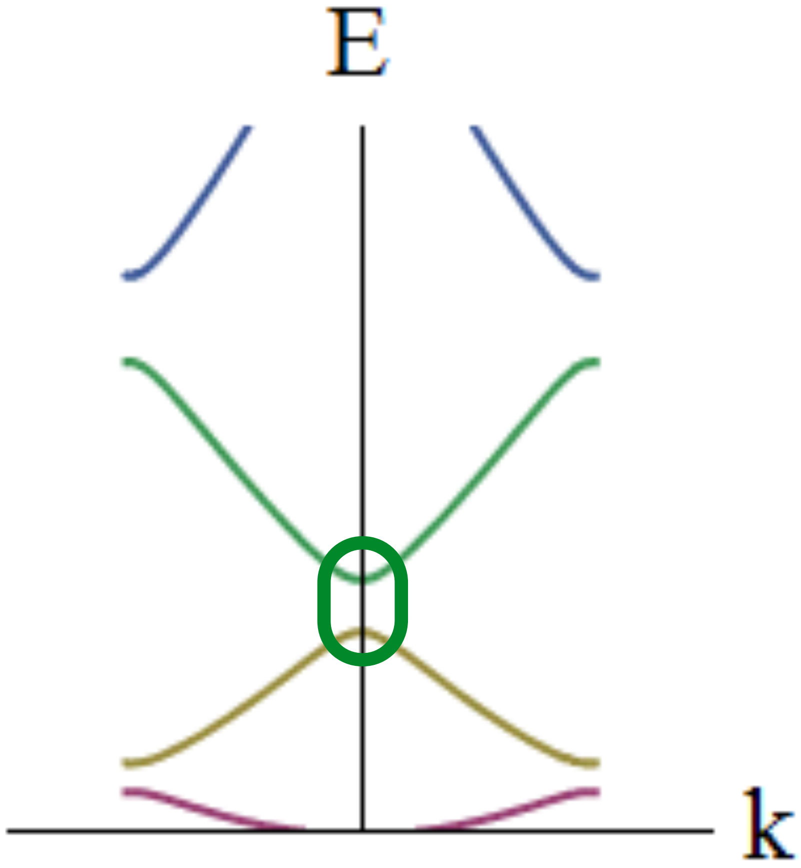


Effective masses

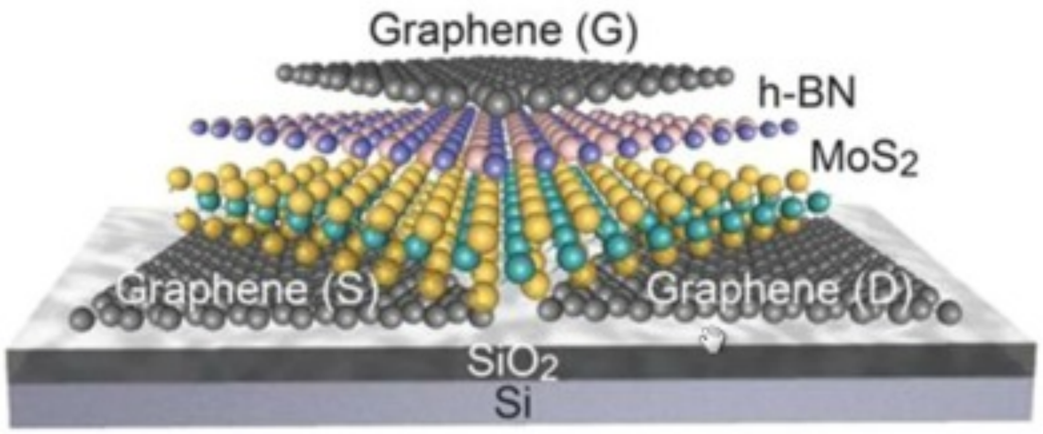
- design materials with better mobility for electronic applications
  - organic semiconductors
  - next generation CPUs
  - transparent conducting oxides (TCOs)
    better μ : both higher conductivity and transparency



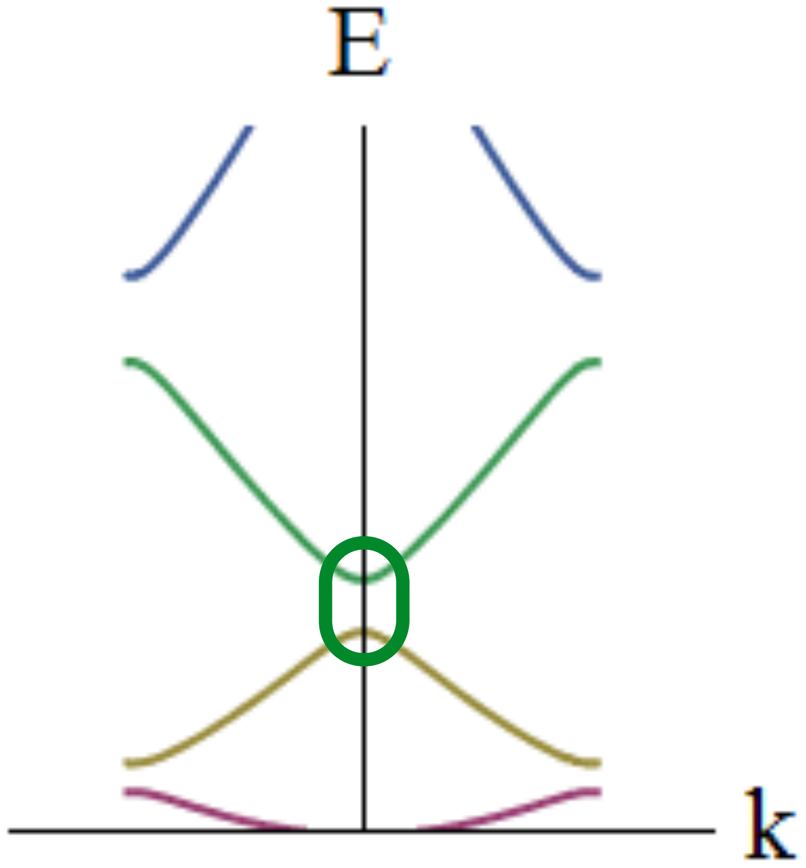
$$\varepsilon_{kn} \approx \varepsilon_{\Gamma n} + \frac{k^2}{2M}$$



- design materials with better mobility for electronic applications
  - organic semiconductors
  - next generation CPUs
  - transparent conducting oxides (TCOs)
    better μ : both higher conductivity and transparency

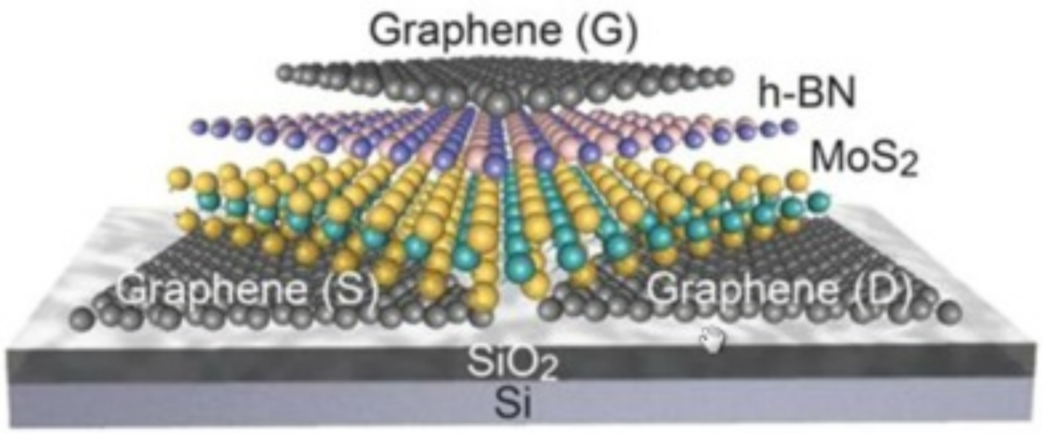


$$\varepsilon_{kn} \approx \varepsilon_{\Gamma n} + \frac{k^2}{2M} \qquad M \neq 1$$



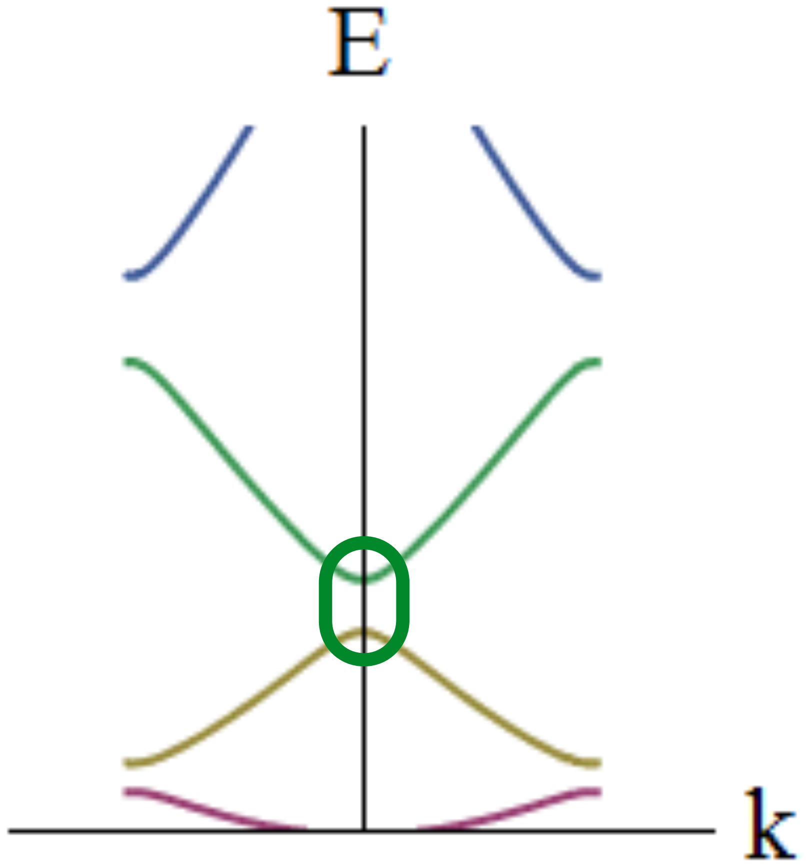
Effective masses

- design materials with better mobility for electronic applications
  - organic semiconductors
  - next generation CPUs
  - transparent conducting oxides (TCOs) better μ : both higher conductivity and transparency



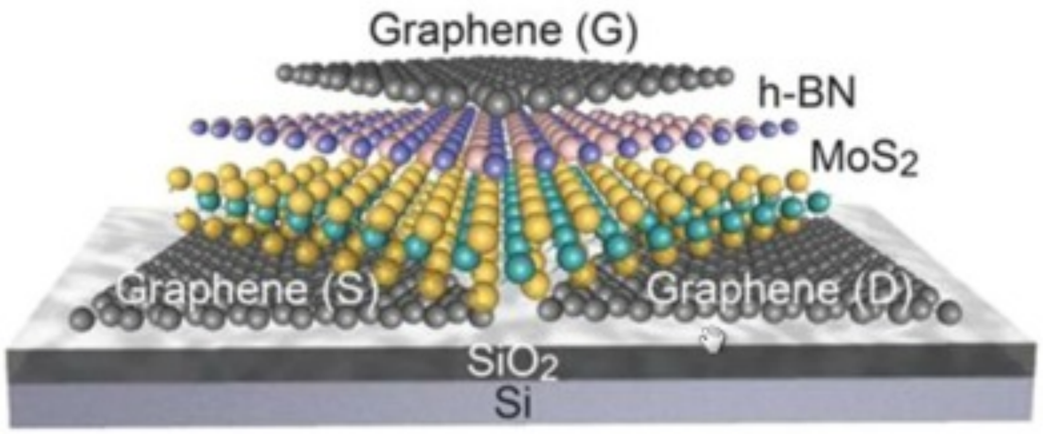
$$\varepsilon_{kn} \approx \varepsilon_{\Gamma n} + \frac{k^2}{2M} \qquad M \neq 1$$

$$\varepsilon_{\underline{k}n} \approx \varepsilon_{\Gamma n} + \tfrac{1}{2}\underline{k}^T \underline{\underline{M}}_{\Gamma n}^{-1} \underline{k} \quad \text{(3D)}$$



Effective masses

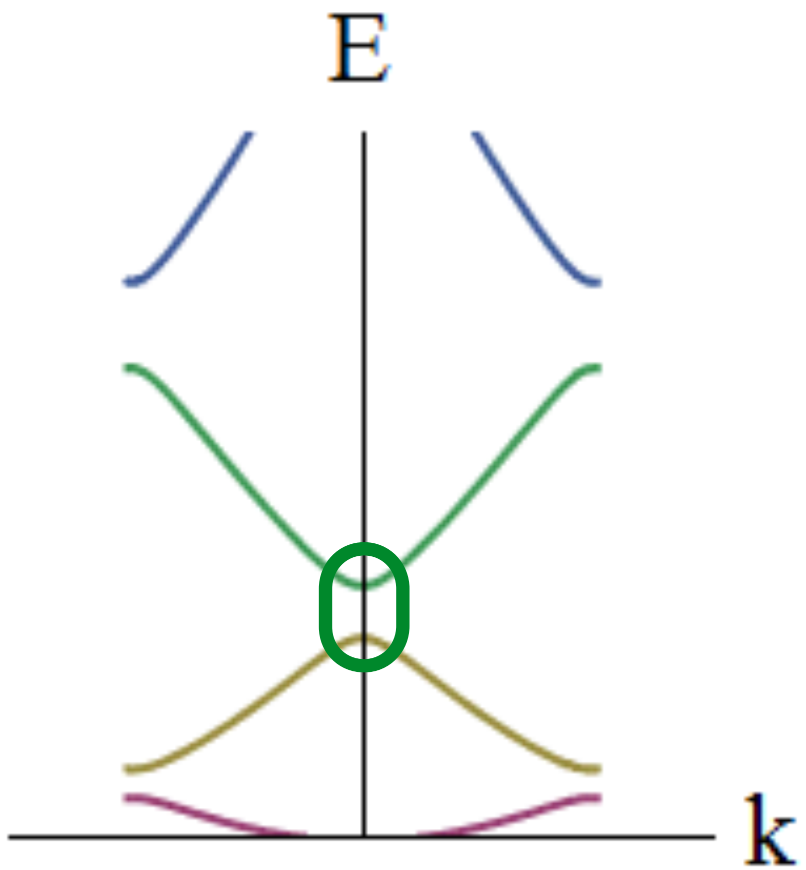
- design materials with better mobility for electronic applications
  - organic semiconductors
  - next generation CPUs
  - transparent conducting oxides (TCOs)
    better μ : both higher conductivity and transparency



$$\varepsilon_{kn} \approx \varepsilon_{\Gamma n} + \frac{k^2}{2M} \qquad M \neq 1$$

$$\varepsilon_{\underline{k}n} \approx \varepsilon_{\Gamma n} + \tfrac{1}{2}\underline{k}^T \underline{\underline{M}}_{\Gamma n}^{-1} \underline{k} \quad \text{(3D)}$$

$$\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \frac{\partial^2 \varepsilon_n}{\partial \underline{k}_\alpha \partial \underline{k}_\beta} \equiv \varepsilon_n^{\alpha\beta}$$



What's missing?

What's missing?

Effective masses calculation

What's missing?

Effective masses calculation

Traditional:

What's missing?

Effective masses calculation

Traditional:

- finite differences $$\varepsilon^{\alpha\beta}_{\underline{k},n} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{\left|\Delta\underline{k}\right|^2}$$

What's missing?

Effective masses calculation

Traditional:

- finite differences $$\varepsilon^{\alpha\beta}_{\underline{k},n} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{\left|\Delta\underline{k}\right|^2}$$
  - numerical noise

What's missing?

Effective masses calculation

Traditional:

- finite differences $$\varepsilon^{\alpha\beta}_{\underline{k},n} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{|\Delta\underline{k}|^2}$$
    - numerical noise
    - extra convergence

What's missing?

Effective masses calculation

Traditional:

- finite differences $$\varepsilon^{\alpha\beta}_{\underline{k},n} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{|\Delta\underline{k}|^2}$$
  - numerical noise
  - extra convergence

This project:

What's missing?

Effective masses calculation

Traditional:

- finite differences $\varepsilon_{\underline{k},n}^{\alpha\beta} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{\left|\Delta\underline{k}\right|^2}$
  - numerical noise
  - extra convergence

This project:

- density functional perturbation theory (DFPT)

What's missing?

Effective masses calculation

Traditional:

- finite differences $\varepsilon_{\underline{k},n}^{\alpha\beta} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{\left|\Delta\underline{k}\right|^2}$
  - numerical noise
  - extra convergence
- $\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \varepsilon_n^{\alpha\beta}$ when degenerate

This project:

- density functional perturbation theory (DFPT)

What's missing?

Effective masses calculation

Traditional:

- finite differences $\varepsilon^{\alpha\beta}_{\underline{k},n} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{|\Delta\underline{k}|^2}$
  - numerical noise
  - extra convergence
- $\left(\underline{\underline{M}}^{-1}_n\right)^{\alpha\beta} = \varepsilon^{\alpha\beta}_n$ when degenerate

This project:

- density functional perturbation theory (DFPT)
- accurate calculation of $\underline{\underline{M}}^{-1}_n$

What's missing?

Effective masses calculation

Traditional:

- finite differences $\varepsilon_{\underline{k},n}^{\alpha\beta} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{\left|\Delta\underline{k}\right|^2}$
  - numerical noise
  - extra convergence
- $\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \varepsilon_n^{\alpha\beta}$ when degenerate
- density functional theory

This project:

- density functional perturbation theory (DFPT)
- accurate calculation of $\underline{\underline{M}}_n^{-1}$

What's missing?

Effective masses calculation

Traditional:

- finite differences $\varepsilon_{\underline{k},n}^{\alpha\beta} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{\left|\Delta\underline{k}\right|^2}$
  - numerical noise
  - extra convergence
- $\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \varepsilon_n^{\alpha\beta}$ when degenerate
- density functional theory
  - poorly assessed accuracy

This project:

- density functional perturbation theory (DFPT)
- accurate calculation of $\underline{\underline{M}}_n^{-1}$

What's missing?

Effective masses calculation

Traditional:

- finite differences $$\varepsilon_{\underline{k},n}^{\alpha\beta} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{\left|\Delta\underline{k}\right|^2}$$
  - numerical noise
  - extra convergence
- $\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \varepsilon_n^{\alpha\beta}$ when degenerate
- density functional theory
  - poorly assessed accuracy

This project:

- density functional perturbation theory (DFPT)
- accurate calculation of $\underline{\underline{M}}_n^{-1}$
- include interactions:

What's missing?

Effective masses calculation

Traditional:

- finite differences $\varepsilon_{\underline{k},n}^{\alpha\beta} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{\left|\Delta\underline{k}\right|^2}$
  - numerical noise
  - extra convergence
- $\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \varepsilon_n^{\alpha\beta}$ when degenerate
- density functional theory
  - poorly assessed accuracy

This project:

- density functional perturbation theory (DFPT)
- accurate calculation of $\underline{\underline{M}}_n^{-1}$
- include interactions:
  - electron-electron (GW)

What's missing?

Effective masses calculation

Traditional:

- finite differences $\varepsilon^{\alpha\beta}_{\underline{k},n} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{|\Delta\underline{k}|^2}$
    - numerical noise
    - extra convergence
- $\left(\underline{\underline{M}}^{-1}_n\right)^{\alpha\beta} = \varepsilon^{\alpha\beta}_n$ when degenerate
- density functional theory
    - poorly assessed accuracy

This project:

- density functional perturbation theory (DFPT)
- accurate calculation of $\underline{\underline{M}}^{-1}_n$
- include interactions:
    - electron-electron (GW)
    - electron-phonon

DFPT

DFPT

Direct calculation of effective masses:

Direct calculation of effective masses:

$$\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \frac{\partial^2 \varepsilon_n}{\partial \underline{k}_\alpha \, \partial \underline{k}_\beta} \equiv \varepsilon_n^{\alpha\beta}$$

$$\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$$

DFPT

Direct calculation of effective masses:

$$\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \frac{\partial^2 \varepsilon_n}{\partial \underline{k}_\alpha \, \partial \underline{k}_\beta} \equiv \varepsilon_n^{\alpha\beta} \qquad \alpha\beta = \{xx, yy, zz, xy, yz, xz\}$$

$$= \langle \psi_n | \hat{H} | \psi_n \rangle^{\alpha\beta}$$

DFPT

Direct calculation of effective masses:

$$\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \frac{\partial^2 \varepsilon_n}{\partial \underline{k}_\alpha \, \partial \underline{k}_\beta} \equiv \varepsilon_n^{\alpha\beta}$$

$$\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$$

$$= \langle \psi_n | \hat{H} | \psi_n \rangle^{\alpha\beta}$$

$$= \langle \psi_n | \hat{H}^{\alpha\beta} | \psi_n \rangle$$

$$+ \left(\langle \psi_n^\alpha | \hat{H}^\beta | \psi_n \rangle + \alpha \leftrightarrow \beta \right) + cc.$$

$$+ \langle \psi_n^\alpha | \hat{H} - \varepsilon_n | \psi_n^\beta \rangle + cc.$$

Direct calculation of effective masses:

$$\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \frac{\partial^2 \varepsilon_n}{\partial \underline{k}_\alpha \partial \underline{k}_\beta} \equiv \varepsilon_n^{\alpha\beta} \qquad \alpha\beta = \{xx, yy, zz, xy, yz, xz\}$$

$$= \langle \psi_n | \hat{H} | \psi_n \rangle^{\alpha\beta}$$

$$= \langle \psi_n | \hat{H}^{\alpha\beta} | \psi_n \rangle$$

$$+ \left(\langle \psi_n^\alpha | \hat{H}^\beta | \psi_n \rangle + \alpha \leftrightarrow \beta \right) + cc.$$

$$+ \langle \psi_n^\alpha | \hat{H} - \varepsilon_n | \psi_n^\beta \rangle + cc.$$

DFPT

Direct calculation of effective masses:

$$\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \frac{\partial^2 \varepsilon_n}{\partial \underline{k}_\alpha \, \partial \underline{k}_\beta} \equiv \varepsilon_n^{\alpha\beta} \qquad \alpha\beta = \{xx, yy, zz, xy, yz, xz\}$$

$$= \langle \psi_n | \hat{H} | \psi_n \rangle^{\alpha\beta}$$

$$= \langle \psi_n | \hat{H}^{\alpha\beta} | \psi_n \rangle$$

$$+ \left(\langle \psi_n^\alpha | \hat{H}^\beta | \psi_n \rangle + \alpha \leftrightarrow \beta \right) + cc.$$

$$+ \langle \psi_n^\alpha | \hat{H} - \varepsilon_n | \psi_n^\beta \rangle + cc.$$

Direct calculation of effective masses:

$$\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \frac{\partial^2 \varepsilon_n}{\partial \underline{k}_\alpha \, \partial \underline{k}_\beta} \equiv \varepsilon_n^{\alpha\beta} \qquad \alpha\beta = \{xx, yy, zz, xy, yz, xz\}$$

$$= \left\langle \psi_n \middle| \hat{H} \middle| \psi_n \right\rangle^{\alpha\beta}$$

$$= \left\langle \psi_n \middle| \hat{H}^{\alpha\beta} \middle| \psi_n \right\rangle$$

$$+ \left(\left\langle \psi_n^{\alpha} \middle| \hat{H}^{\beta} \middle| \psi_n \right\rangle + \alpha \leftrightarrow \beta \right) + cc.$$

$$+ \left\langle \psi_n^{\alpha} \middle| \hat{H} - \varepsilon_n \middle| \psi_n^{\beta} \right\rangle + cc.$$

$$\left(\hat{H} - \varepsilon_n \right) \left| \psi_n^{\alpha} \right\rangle = \left(\hat{H}^{\alpha} - \varepsilon_n^{\alpha} \right) \left| \psi_n \right\rangle$$

DFPT

Direct calculation of effective masses:

$$\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \frac{\partial^2 \varepsilon_n}{\partial \underline{k}_\alpha \partial \underline{k}_\beta} \equiv \varepsilon_n^{\alpha\beta} \qquad \alpha\beta = \{xx, yy, zz, xy, yz, xz\}$$

$$= \langle \psi_n | \hat{H} | \psi_n \rangle^{\alpha\beta}$$

$$= \langle \psi_n | \hat{H}^{\alpha\beta} | \psi_n \rangle$$

$$+ \left(\langle \psi_n^\alpha | \hat{H}^\beta | \psi_n \rangle + \alpha \leftrightarrow \beta \right) + cc.$$

$$+ \langle \psi_n^\alpha | \hat{H} - \varepsilon_n | \psi_n^\beta \rangle + cc.$$

$$\left(\hat{H} - \varepsilon_n\right) |\psi_n^\alpha\rangle = \left(\hat{H}^\alpha - \varepsilon_n^\alpha\right) |\psi_n\rangle$$

Direct calculation of effective masses:

$$\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \frac{\partial^2 \varepsilon_n}{\partial \underline{k}_\alpha \partial \underline{k}_\beta} \equiv \varepsilon_n^{\alpha\beta} \qquad \alpha\beta = \{xx, yy, zz, xy, yz, xz\}$$

$$= \langle \psi_n | \hat{H} | \psi_n \rangle^{\alpha\beta}$$

$$= \langle \psi_n | \hat{H}^{\alpha\beta} | \psi_n \rangle$$

$$+ \left(\langle \psi_n^\alpha | \hat{H}^\beta | \psi_n \rangle + \alpha \leftrightarrow \beta \right) + cc.$$

$$+ \langle \psi_n^\alpha | \hat{H} - \varepsilon_n | \psi_n^\beta \rangle + cc.$$

$$\left(\hat{H} - \varepsilon_n\right) |\psi_n^\alpha\rangle = \left(\hat{H}^\alpha - \varepsilon_n^\alpha\right) |\psi_n\rangle$$

DFPT

Direct calculation of effective masses:

$$\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \frac{\partial^2 \varepsilon_n}{\partial \underline{k}_\alpha \, \partial \underline{k}_\beta} \equiv \varepsilon_n^{\alpha\beta} \qquad \alpha\beta = \{xx, yy, zz, xy, yz, xz\}$$

$$= \langle \psi_n | \hat{H} | \psi_n \rangle^{\alpha\beta}$$

$$= \langle \psi_n | \hat{H}^{\alpha\beta} | \psi_n \rangle$$

$$+ \left(\langle \psi_n^\alpha | \hat{H}^\beta | \psi_n \rangle + \alpha \leftrightarrow \beta \right) + cc.$$

$$+ \langle \psi_n^\alpha | \hat{H} - \varepsilon_n | \psi_n^\beta \rangle + cc.$$

$$\left(\hat{H} - \varepsilon_n \right) | \psi_n^\alpha \rangle = \left(\hat{H}^\alpha - \varepsilon_n^\alpha \right) | \psi_n \rangle$$

DFPT

Direct calculation of effective masses:

$$\left(\underline{\underline{M}}_n^{-1}\right)^{\alpha\beta} = \frac{\partial^2 \varepsilon_n}{\partial \underline{k}_\alpha \, \partial \underline{k}_\beta} \equiv \varepsilon_n^{\alpha\beta} \qquad \alpha\beta = \{xx, yy, zz, xy, yz, xz\}$$

$$= \langle \psi_n | \hat{H} | \psi_n \rangle^{\alpha\beta}$$

$$= \langle \psi_n | \hat{H}^{\alpha\beta} | \psi_n \rangle$$

$$+ \left(\langle \psi_n^\alpha | \hat{H}^\beta | \psi_n \rangle + \alpha \leftrightarrow \beta \right) + cc.$$

$$+ \langle \psi_n^\alpha | \hat{H} - \varepsilon_n | \psi_n^\beta \rangle + cc.$$

$$\left(\hat{H} - \varepsilon_n \right) | \psi_n^\alpha \rangle = \left(\hat{H}^\alpha - \varepsilon_n^\alpha \right) | \psi_n \rangle$$

Derivatives of $\hat{H}$ up to 2nd order

DFPT

DFPT

Derivatives of $\hat{H}$

Derivatives of $\hat{H}$

$$\langle \underline{G} | \hat{H}_{\underline{k}} | \underline{G}' \rangle = \frac{\left(\underline{k} + \underline{G}\right)^2}{2} \delta_{\underline{G}\underline{G}'} + V_{\underline{G}-\underline{G}'} + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}$$

DFPT

Derivatives of $\hat{H}$

$$\langle \underline{G} | \hat{H}_{\underline{k}} | \underline{G}' \rangle = \frac{(\underline{k} + \underline{G})^2}{2} \delta_{\underline{G}\underline{G}'} + V_{\underline{G}-\underline{G}'} + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}$$

DFT: $\langle \underline{r} | \hat{V} | \underline{r}' \rangle = V(\underline{r}) \delta(\underline{r} - \underline{r}')$

Derivatives of $\hat{H}$

$$\langle \underline{G} | \hat{H}_{\underline{k}} | \underline{G}' \rangle = \frac{(\underline{k}+\underline{G})^2}{2} \delta_{\underline{G}\underline{G}'} + V_{\underline{G}-\underline{G}'} + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}$$

DFT: $\langle \underline{r} | \hat{V} | \underline{r}' \rangle = V(\underline{r}) \delta(\underline{r} - \underline{r}')$

pseudo: $\langle \underline{r} | \hat{\tilde{V}} | \underline{r}' \rangle = \tilde{V}(\underline{r}, \underline{r}')$

Derivatives of $\hat{H}$

$$\langle \underline{G} | \hat{H}_{\underline{k}} | \underline{G}' \rangle = \frac{(\underline{k}+\underline{G})^2}{2} \delta_{\underline{G}\underline{G}'} + V_{\underline{G}-\underline{G}'} + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}$$

DFT: $\langle \underline{r} | \hat{V} | \underline{r}' \rangle = V(\underline{r}) \delta(\underline{r}-\underline{r}')$

pseudo: $\langle \underline{r} | \hat{\tilde{V}} | \underline{r}' \rangle = \tilde{V}(\underline{r},\underline{r}')$

$$\langle \underline{G} | \hat{H}^{\alpha}_{\underline{k}} | \underline{G}' \rangle = (\underline{k}+\underline{G})_{\alpha} \delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}^{\alpha}_{\underline{k},\underline{G}\underline{G}'}$$

DFPT

Derivatives of $\hat{H}$

$$\langle \underline{G} | \hat{H}_{\underline{k}} | \underline{G}' \rangle = \frac{(\underline{k}+\underline{G})^2}{2} \delta_{\underline{G}\underline{G}'} + V_{\underline{G}-\underline{G}'} + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}$$

DFT: $\langle \underline{r} | \hat{V} | \underline{r}' \rangle = V(\underline{r})\delta(\underline{r}-\underline{r}')$

pseudo: $\langle \underline{r} | \hat{\tilde{V}} | \underline{r}' \rangle = \tilde{V}(\underline{r},\underline{r}')$

$$\langle \underline{G} | \hat{H}_{\underline{k}}^{\alpha} | \underline{G}' \rangle = (\underline{k}+\underline{G})_{\alpha} \delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}^{\alpha}$$

$$\langle \underline{G} | \hat{H}_{\underline{k}}^{\alpha\beta} | \underline{G}' \rangle = \delta_{\alpha\beta}\delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}^{\alpha\beta}$$

DFPT

Derivatives of $\hat{H}$

$$\langle \underline{G} | \hat{H}_{\underline{k}} | \underline{G}' \rangle = \frac{(\underline{k}+\underline{G})^2}{2} \delta_{\underline{G}\underline{G}'} + V_{\underline{G}-\underline{G}'} + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}$$

DFT: $\langle \underline{r} | \hat{V} | \underline{r}' \rangle = V(\underline{r}) \delta(\underline{r}-\underline{r}')$

pseudo: $\langle \underline{r} | \hat{\tilde{V}} | \underline{r}' \rangle = \tilde{V}(\underline{r},\underline{r}')$

$$\langle \underline{G} | \hat{H}_{\underline{k}}^{\alpha} | \underline{G}' \rangle = (\underline{k}+\underline{G})_{\alpha} \delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}^{\alpha}_{\underline{k},\underline{G}\underline{G}'}$$

$$\langle \underline{G} | \hat{H}_{\underline{k}}^{\alpha\beta} | \underline{G}' \rangle = \delta_{\alpha\beta} \delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}^{\alpha\beta}_{\underline{k},\underline{G}\underline{G}'}$$

$$\langle \underline{G} | \hat{\tilde{V}}_{\underline{k}} | \underline{G}' \rangle = \sum_{ij} \langle \underline{k}+\underline{G} | p_i \rangle D_{ij} \langle p_j | \underline{k}+\underline{G}' \rangle$$

DFPT

Derivatives of $\hat{H}$

$$\langle \underline{G} | \hat{H}_{\underline{k}} | \underline{G}' \rangle = \frac{(\underline{k}+\underline{G})^2}{2} \delta_{\underline{G}\underline{G}'} + V_{\underline{G}-\underline{G}'} + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}$$

DFT: $\langle \underline{r} | \hat{V} | \underline{r}' \rangle = V(\underline{r}) \delta(\underline{r} - \underline{r}')$

pseudo: $\langle \underline{r} | \hat{\tilde{V}} | \underline{r}' \rangle = \tilde{V}(\underline{r}, \underline{r}')$

$$\langle \underline{G} | \hat{H}_{\underline{k}}^{\alpha} | \underline{G}' \rangle = (\underline{k}+\underline{G})_{\alpha} \delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}^{\alpha}$$

$$\langle \underline{G} | \hat{H}_{\underline{k}}^{\alpha\beta} | \underline{G}' \rangle = \delta_{\alpha\beta} \delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}^{\alpha\beta}$$

$$\langle \underline{G} | \hat{\tilde{V}}_{\underline{k}} | \underline{G}' \rangle = \sum_{ij} \langle \underline{k}+\underline{G} | p_i \rangle D_{ij} \langle p_j | \underline{k}+\underline{G}' \rangle$$

$$\langle \underline{k}+\underline{G} | p_i \rangle \propto e^{i(\underline{k}+\underline{G})\cdot r} Y_{l_i m_i}\left(\frac{\underline{k}+\underline{G}}{|\underline{k}+\underline{G}|} \right) \int_0^{r_c} dr\, p_i(r)\, j_{l_i}\left(|\underline{k}+\underline{G}| r \right)$$

DFPT

Derivatives of $\hat{H}$

$$\langle \underline{G} | \hat{H}_{\underline{k}} | \underline{G}' \rangle = \frac{(\underline{k}+\underline{G})^2}{2} \delta_{\underline{G}\underline{G}'} + V_{\underline{G}-\underline{G}'} + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}$$

DFT: $\langle \underline{r} | \hat{V} | \underline{r}' \rangle = V(\underline{r}) \delta(\underline{r} - \underline{r}')$

pseudo: $\langle \underline{r} | \hat{\tilde{V}} | \underline{r}' \rangle = \tilde{V}(\underline{r}, \underline{r}')$

$$\langle \underline{G} | \hat{H}^{\alpha}_{\underline{k}} | \underline{G}' \rangle = (\underline{k}+\underline{G})_{\alpha} \delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}^{\alpha}_{\underline{k},\underline{G}\underline{G}'}$$

$$\langle \underline{G} | \hat{H}^{\alpha\beta}_{\underline{k}} | \underline{G}' \rangle = \delta_{\alpha\beta} \delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}^{\alpha\beta}_{\underline{k},\underline{G}\underline{G}'}$$

$$\langle \underline{G} | \hat{\tilde{V}}_{\underline{k}} | \underline{G}' \rangle = \sum_{ij} \langle \underline{k}+\underline{G} | p_i \rangle D_{ij} \langle p_j | \underline{k}+\underline{G}' \rangle$$

$$\langle \underline{k}+\underline{G} | p_i \rangle \propto e^{i(\underline{k}+\underline{G})\cdot \underline{r}} Y_{l_i m_i}\left(\frac{\underline{k}+\underline{G}}{|\underline{k}+\underline{G}|} \right) \int_0^{r_c} dr\, p_i(r)\, j_{l_i}(|\underline{k}+\underline{G}| r)$$

DFPT

Derivatives of $\hat{H}$

$$\langle \underline{G} | \hat{H}_{\underline{k}} | \underline{G}' \rangle = \frac{(\underline{k}+\underline{G})^2}{2} \delta_{\underline{G}\underline{G}'} + V_{\underline{G}-\underline{G}'} + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}$$

DFT: $\langle \underline{r} | \hat{V} | \underline{r}' \rangle = V(\underline{r}) \delta(\underline{r}-\underline{r}')$

pseudo: $\langle \underline{r} | \hat{\tilde{V}} | \underline{r}' \rangle = \tilde{V}(\underline{r},\underline{r}')$

$$\langle \underline{G} | \hat{H}^{\alpha}_{\underline{k}} | \underline{G}' \rangle = (\underline{k}+\underline{G})_{\alpha} \delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}^{\alpha}_{\underline{k},\underline{G}\underline{G}'}$$

$$\langle \underline{G} | \hat{H}^{\alpha\beta}_{\underline{k}} | \underline{G}' \rangle = \delta_{\alpha\beta} \delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}^{\alpha\beta}_{\underline{k},\underline{G}\underline{G}'}$$

$$\langle \underline{G} | \hat{\tilde{V}}_{\underline{k}} | \underline{G}' \rangle = \sum_{ij} \langle \underline{k}+\underline{G} | p_i \rangle D_{ij} \langle p_j | \underline{k}+\underline{G}' \rangle$$

$$\langle \underline{k}+\underline{G} | p_i \rangle \propto e^{i(\underline{k}+\underline{G})\cdot \underline{r}} Y_{l_i m_i}\left(\frac{\underline{k}+\underline{G}}{|\underline{k}+\underline{G}|} \right) \int_0^{r_c} dr\, p_i(r)\, j_{l_i}(|\underline{k}+\underline{G}| r)$$

DFPT

Derivatives of $\hat{H}$

$$\langle \underline{G} | \hat{H}_{\underline{k}} | \underline{G}' \rangle = \frac{(\underline{k}+\underline{G})^2}{2} \delta_{\underline{G}\underline{G}'} + V_{\underline{G}-\underline{G}'} + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}$$

DFT: $\langle \underline{r} | \hat{V} | \underline{r}' \rangle = V(\underline{r}) \delta(\underline{r} - \underline{r}')$

pseudo: $\langle \underline{r} | \hat{\tilde{V}} | \underline{r}' \rangle = \tilde{V}(\underline{r}, \underline{r}')$

$$\langle \underline{G} | \hat{H}_{\underline{k}}^{\alpha} | \underline{G}' \rangle = (\underline{k}+\underline{G})_{\alpha} \delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}^{\alpha}$$

$$\langle \underline{G} | \hat{H}_{\underline{k}}^{\alpha\beta} | \underline{G}' \rangle = \delta_{\alpha\beta} \delta_{\underline{G}\underline{G}'} + 0 + \tilde{V}_{\underline{k},\underline{G}\underline{G}'}^{\alpha\beta}$$

$$\langle \underline{G} | \hat{\tilde{V}}_{\underline{k}} | \underline{G}' \rangle = \sum_{ij} \langle \underline{k}+\underline{G} | p_i \rangle D_{ij} \langle p_j | \underline{k}+\underline{G}' \rangle$$

$$\langle \underline{k}+\underline{G} | p_i \rangle \propto e^{i(\underline{k}+\underline{G})\cdot \underline{r}} Y_{l_i m_i}\left(\frac{\underline{k}+\underline{G}}{|\underline{k}+\underline{G}|} \right) \int_0^{r_c} dr\, p_i(r) j_{l_i}(|\underline{k}+\underline{G}| r)$$

Degenerescences?

Degenerescences?

- Degenerate perturbation theory:

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0$$

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \quad \Rightarrow \quad \underline{\underline{M}}_{n}^{-1} \rightarrow \underline{\underline{M}}_{nn'}^{-1}$$

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \Rightarrow \underline{\underline{M}}_n^{-1} \rightarrow \underline{\underline{M}}_{nn'}^{-1}$ Luttinger and Kohn, *Phys Rev* **97** 869 (1955)

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \;\Rightarrow\; \underline{\underline{M}}_n^{-1} \rightarrow \underline{\underline{M}}_{nn'}^{-1}$ Luttinger and Kohn, *Phys Rev* **97** 869 (1955)

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \;\Rightarrow\; \underline{\underline{M}}_n^{-1} \rightarrow \underline{\underline{M}}_{nn'}^{-1}$ Luttinger and Kohn, *Phys Rev* **97** 869 (1955)

- Around band extrema

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \quad \Rightarrow \quad \underline{\underline{M}}_n^{-1} \rightarrow \underline{\underline{M}}_{nn'}^{-1}$ Luttinger and Kohn, *Phys Rev* **97** 869 (1955)

- Around band extrema

$$\varepsilon_{nn'}(\underline{k}) \approx \frac{1}{2} \underline{k}^T \underline{\underline{M}}_{nn'}^{-1} \underline{k}$$

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \;\Rightarrow\; \underline{\underline{M}}_n^{-1} \rightarrow \underline{\underline{M}}_{nn'}^{-1}$ Luttinger and Kohn, *Phys Rev* **97** 869 (1955)

- Around band extrema

$$\varepsilon_{nn'}(\underline{k}) \approx \frac{1}{2}\underline{k}^T \underline{\underline{M}}_{nn'}^{-1}\underline{k} = \frac{k^2}{2}\hat{k}(\theta,\phi)^T \underline{\underline{M}}_{nn'}^{-1}\hat{k}(\theta,\phi) = \frac{k^2}{2}M_{nn'}^{-1}(\theta,\phi)$$

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \quad \Rightarrow \quad \underline{\underline{M}}_n^{-1} \rightarrow \underline{\underline{M}}_{nn'}^{-1}$$

Luttinger and Kohn, *Phys Rev* **97** 869 (1955)

- Around band extrema

$$\varepsilon_{nn'}(\underline{k}) \approx \frac{1}{2} \underline{k}^T \underline{\underline{M}}_{nn'}^{-1} \underline{k} = \frac{k^2}{2} \hat{k}(\theta,\phi)^T \underline{\underline{M}}_{nn'}^{-1} \hat{k}(\theta,\phi) = \frac{k^2}{2} M_{nn'}^{-1}(\theta,\phi)$$

$$\varepsilon_n(k,\theta,\phi) \approx \frac{k^2}{2} M_n^{-1}(\theta,\phi)$$

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \quad \Rightarrow \quad \underline{\underline{M}}_n^{-1} \rightarrow \underline{\underline{M}}_{nn'}^{-1}$ Luttinger and Kohn, *Phys Rev* **97** 869 (1955)

- Around band extrema

$$\varepsilon_{nn'}(\underline{k}) \approx \frac{1}{2} \underline{k}^T \underline{\underline{M}}_{nn'}^{-1} \underline{k} = \frac{k^2}{2} \hat{k}(\theta,\phi)^T \underline{\underline{M}}_{nn'}^{-1} \hat{k}(\theta,\phi) = \frac{k^2}{2} M_{nn'}^{-1}(\theta,\phi)$$

$$\varepsilon_n(k,\theta,\phi) \approx \frac{k^2}{2} M_n^{-1}(\theta,\phi)$$

- $M_n(\theta,\phi)$ not convenient for transport properties calculation

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \quad \Rightarrow \quad \underline{\underline{M}}_n^{-1} \rightarrow \underline{\underline{M}}_{nn'}^{-1}$ Luttinger and Kohn, *Phys Rev* **97** 869 (1955)

- Around band extrema

$$\varepsilon_{nn'}(\underline{k}) \approx \frac{1}{2} \underline{k}^T \underline{\underline{M}}_{nn'}^{-1} \underline{k} = \frac{k^2}{2} \hat{k}(\theta,\phi)^T \underline{\underline{M}}_{nn'}^{-1} \hat{k}(\theta,\phi) = \frac{k^2}{2} M_{nn'}^{-1}(\theta,\phi)$$

$$\varepsilon_n(k,\theta,\phi) \approx \frac{k^2}{2} M_n^{-1}(\theta,\phi)$$

- $M_n(\theta,\phi)$ not convenient for transport properties calculation

Mecholsky *et al.*, PRB **89** 155131 (2014)

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \;\Rightarrow\; \underline{\underline{M}}_n^{-1} \to \underline{\underline{M}}_{nn'}^{-1}$ Luttinger and Kohn, *Phys Rev* **97** 869 (1955)

- Around band extrema

$$\varepsilon_{nn'}(\underline{k}) \approx \frac{1}{2} \underline{k}^T \underline{\underline{M}}_{nn'}^{-1} \underline{k} = \frac{k^2}{2} \hat{k}(\theta,\phi)^T \underline{\underline{M}}_{nn'}^{-1} \hat{k}(\theta,\phi) = \frac{k^2}{2} M_{nn'}^{-1}(\theta,\phi)$$

$$\varepsilon_n(k,\theta,\phi) \approx \frac{k^2}{2} M_n^{-1}(\theta,\phi)$$

- $M_n(\theta,\phi)$ not convenient for transport properties calculation

$M_n(\theta,\phi)$ Mecholsky *et al.*, PRB **89** 155131 (2014)

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \quad \Rightarrow \quad \underline{\underline{M}}_n^{-1} \rightarrow \underline{\underline{M}}_{nn'}^{-1}$ Luttinger and Kohn, *Phys Rev* **97** 869 (1955)

- Around band extrema

$$\varepsilon_{nn'}(\underline{k}) \approx \frac{1}{2} \underline{k}^T \underline{\underline{M}}_{nn'}^{-1} \underline{k} = \frac{k^2}{2} \hat{k}(\theta,\phi)^T \underline{\underline{M}}_{nn'}^{-1} \hat{k}(\theta,\phi) = \frac{k^2}{2} M_{nn'}^{-1}(\theta,\phi)$$

$$\varepsilon_n(k,\theta,\phi) \approx \frac{k^2}{2} M_n^{-1}(\theta,\phi)$$

- $M_n(\theta,\phi)$ not convenient for transport properties calculation

$M_n(\theta,\phi) \rightarrow \underline{\underline{\sigma}}_n$ Mecholsky *et al.*, PRB **89** 155131 (2014)

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \quad \Rightarrow \quad \underline{\underline{M}}_n^{-1} \rightarrow \underline{\underline{M}}_{nn'}^{-1}$ Luttinger and Kohn, *Phys Rev* **97** 869 (1955)

- Around band extrema

$$\varepsilon_{nn'}(\underline{k}) \approx \frac{1}{2} \underline{k}^T \underline{\underline{M}}_{nn'}^{-1} \underline{k} = \frac{k^2}{2} \hat{k}(\theta,\phi)^T \underline{\underline{M}}_{nn'}^{-1} \hat{k}(\theta,\phi) = \frac{k^2}{2} M_{nn'}^{-1}(\theta,\phi)$$

$$\varepsilon_n(k,\theta,\phi) \approx \frac{k^2}{2} M_n^{-1}(\theta,\phi)$$

- $M_n(\theta,\phi)$ not convenient for transport properties calculation

$M_n(\theta,\phi) \rightarrow \underline{\underline{\sigma}}_n \rightarrow \underline{\underline{M}}_n^{\text{eqv}}$ Mecholsky *et al.*, PRB **89** 155131 (2014)

Degenerescences?

- Degenerate perturbation theory:
  - in degenerate subspace, diagonalize $\hat{H}^{\alpha\beta}$
- But cannot diag. w/r to 6 perturbations! $\alpha\beta = \{xx, yy, zz, xy, yz, xz\}$

$\langle n | \hat{H}^{\alpha\beta} | n' \rangle \neq 0 \;\; \Rightarrow \;\; \underline{\underline{M}}_n^{-1} \rightarrow \underline{\underline{M}}_{nn'}^{-1}$ Luttinger and Kohn, *Phys Rev* **97** 869 (1955)

- Around band extrema

$$\varepsilon_{nn'}(\underline{k}) \approx \frac{1}{2} \underline{k}^T \underline{\underline{M}}_{nn'}^{-1} \underline{k} = \frac{k^2}{2} \hat{k}(\theta,\phi)^T \underline{\underline{M}}_{nn'}^{-1} \hat{k}(\theta,\phi) = \frac{k^2}{2} M_{nn'}^{-1}(\theta,\phi)$$

$$\varepsilon_n(k,\theta,\phi) \approx \frac{k^2}{2} M_n^{-1}(\theta,\phi)$$

- $M_n(\theta,\phi)$ not convenient for transport properties calculation

$M_n(\theta,\phi) \rightarrow \underline{\underline{\sigma}}_n \rightarrow \underline{\underline{M}}_n^{\text{eqv}}$ Mecholsky *et al.*, PRB **89** 155131 (2014)

Results

Results

- Degenerescence support under implementation

Results

- Degenerescence support under implementation

Si, 1^{st} band, Γ

Results

- Degenerescence support under implementation

Si, 1st band, Γ

Finite

1.161	0.000	0.000
0.000	1.161	-0.000
0.000	-0.000	1.161

DFPT

1.161	0.000	0.000
0.000	1.161	0.000
0.000	0.000	1.161

Results

- Degenerescence support under implementation

Si, 1^{st} band, Γ

Finite

1.161	0.000	0.000
0.000	1.161	-0.000
0.000	-0.000	1.161

DFPT

1.161	0.000	0.000
0.000	1.161	0.000
0.000	0.000	1.161

Δ

3E-09	1E-07	7E-08
1E-07	9E-08	1E-11
7E-08	1E-11	2E-07

Results

- Degenerescence support under implementation

Si, 1st band, Γ

Finite

1.161	0.000	0.000
0.000	1.161	-0.000
0.000	-0.000	1.161

DFPT

1.161	0.000	0.000
0.000	1.161	0.000
0.000	0.000	1.161

Δ

3E-09	1E-07	7E-08
1E-07	9E-08	1E-11
7E-08	1E-11	2E-07

Si, 1st band, $\left(\frac{1}{4},0,0\right)$

Results

- Degenerescence support under implementation

Si, 1st band, Γ

Finite

1.161	0.000	0.000
0.000	1.161	-0.000
0.000	-0.000	1.161

DFPT

1.161	0.000	0.000
0.000	1.161	0.000
0.000	0.000	1.161

Δ

3E-09	1E-07	7E-08
1E-07	9E-08	1E-11
7E-08	1E-11	2E-07

Si, 1st band, $(1/4, 0, 0)$

Ge, 1st band

Results

- Degenerescence support under implementation

Si, 1st band, Γ

Finite

1.161	0.000	0.000
0.000	1.161	-0.000
0.000	-0.000	1.161

DFPT

1.161	0.000	0.000
0.000	1.161	0.000
0.000	0.000	1.161

Δ

3E-09	1E-07	7E-08
1E-07	9E-08	1E-11
7E-08	1E-11	2E-07

Si, 1st band, $\left(\frac{1}{4},0,0\right)$

Ge, 1st band

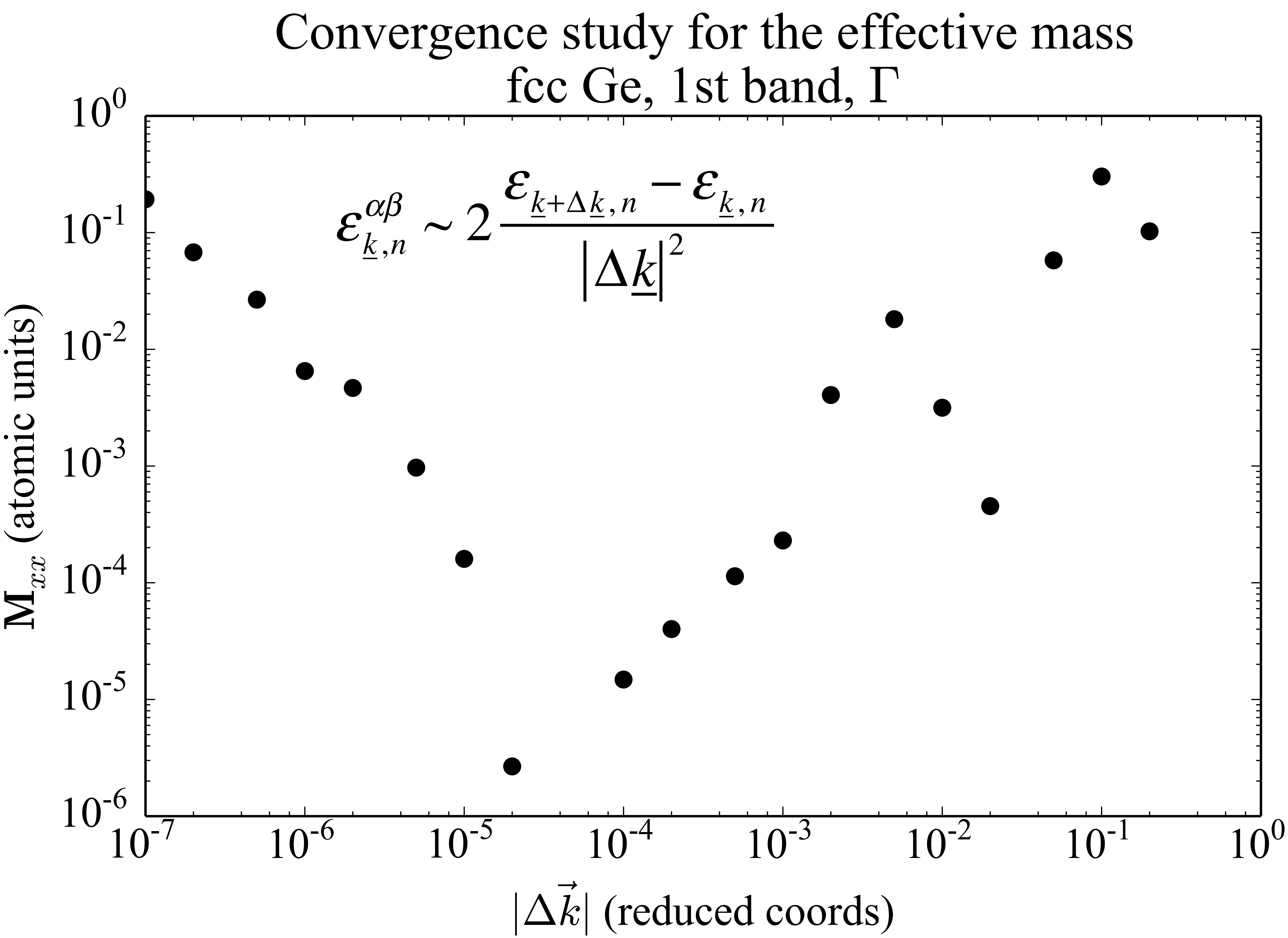
$$\bar{\Delta} = 10^{-4}$$

Numerical noise : finite differences

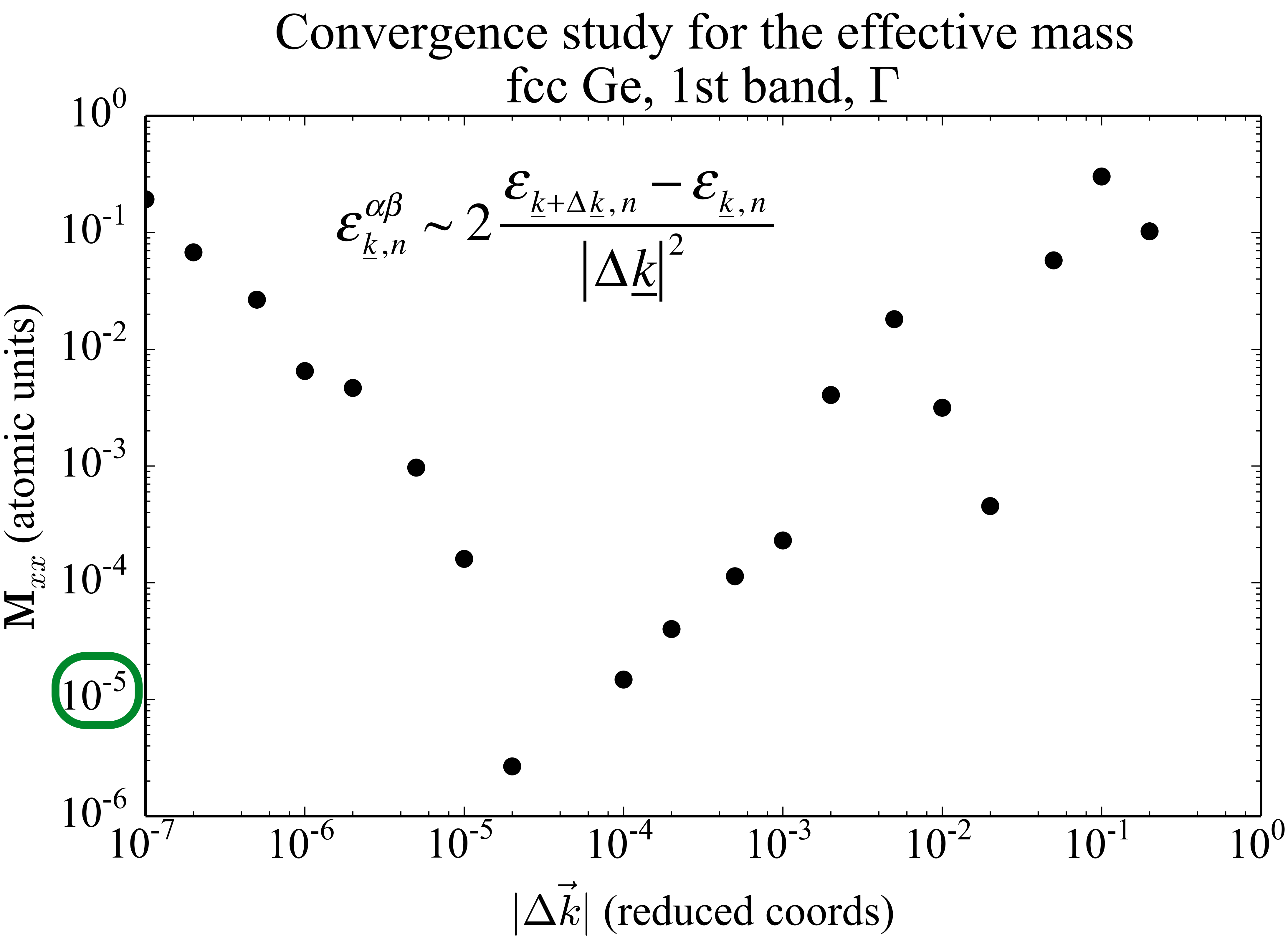
Numerical noise : finite differences

$$\varepsilon_{\underline{k},n}^{\alpha\beta} \sim 2\frac{\varepsilon_{\underline{k}+\Delta\underline{k},n} - \varepsilon_{\underline{k},n}}{\left|\Delta\underline{k}\right|^2}$$

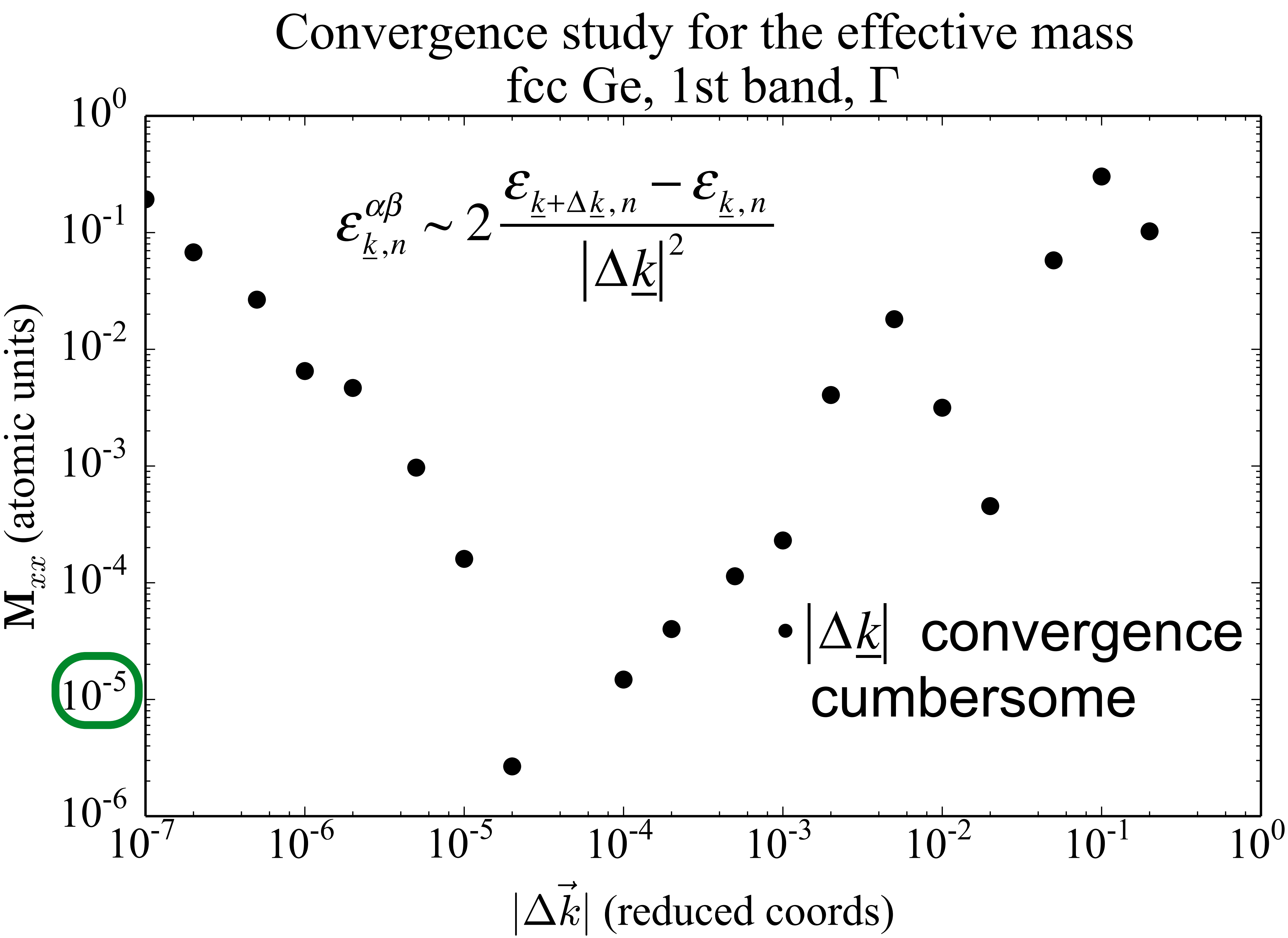
Numerical noise : finite differences



Numerical noise : finite differences



Numerical noise : finite differences



- $|\Delta \underline{k}|$ convergence cumbersome

Conclusion

Conclusion

- Effective masses important for material design

Conclusion

- Effective masses important for material design
- Not much effort to ➚ precision

Conclusion

- Effective masses important for material design
- Not much effort to ↗ precision
- Here

Conclusion

- Effective masses important for material design
- Not much effort to ↗ precision
- Here
  - DFPT implemented

Conclusion

- Effective masses important for material design
- Not much effort to ↗ precision
- Here
  - DFPT implemented
    - One less convergence to do

Conclusion

- Effective masses important for material design
- Not much effort to ↗ precision
- Here
  - DFPT implemented
    - One less convergence to do
    - Better numerical precision

Conclusion

- Effective masses important for material design
- Not much effort to ➚ precision
- Here
  - DFPT implemented
    - One less convergence to do
    - Better numerical precision
  - Degenerate bands: accurate treatment,

Conclusion

- Effective masses important for material design
- Not much effort to ➚ precision
- Here
  - DFPT implemented
    - One less convergence to do
    - Better numerical precision
  - Degenerate bands: accurate treatment, $\underline{\underline{M}}_{nn'}^{-1} \rightarrow M_n(\theta,\phi) \rightarrow \underline{\underline{\sigma}}_n \rightarrow \underline{\underline{M}}_n^{\mathrm{eqv}}$

Conclusion

- Effective masses important for material design
- Not much effort to ↗ precision
- Here
  - DFPT implemented
    - One less convergence to do
    - Better numerical precision
  - Degenerate bands: accurate treatment, $\underline{\underline{M}}_{nn'}^{-1} \rightarrow M_n(\theta,\phi) \rightarrow \underline{\underline{\sigma}}_n \rightarrow \underline{\underline{M}}_n^{\mathrm{eqv}}$
  - Future directions

Conclusion

- Effective masses important for material design
- Not much effort to ↗ precision
- Here
  - DFPT implemented
    - One less convergence to do
    - Better numerical precision
  - Degenerate bands: accurate treatment, $\underline{\underline{M}}_{nn'}^{-1} \rightarrow M_n(\theta,\phi) \rightarrow \underline{\underline{\sigma}}_n \rightarrow \underline{\underline{M}}_n^{\mathrm{eqv}}$
  - Future directions
    - electron-electron interactions

Conclusion

- Effective masses important for material design
- Not much effort to ➚ precision
- Here
  - DFPT implemented
    - One less convergence to do
    - Better numerical precision
  - Degenerate bands: accurate treatment, $\underline{\underline{M}}_{nn'}^{-1} \rightarrow M_n(\theta,\phi) \rightarrow \underline{\underline{\sigma}}_n \rightarrow \underline{\underline{M}}_n^{\mathrm{eqv}}$
  - Future directions
    - electron-electron interactions
    - electron-phonon interactions

Acknowledgments

Xavier Gonze's group

Samuel Poncé
Yannick Gillet
Michiel van Setten
Matteo Giantomassi
Yongchao Jia

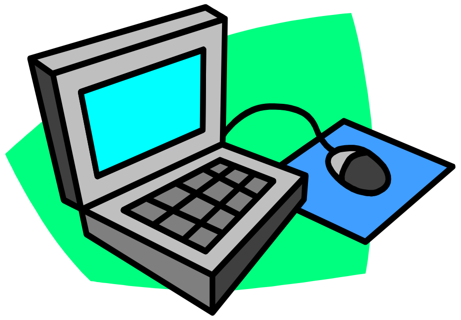
UCL
Université catholique de Louvain

Acknowledgments

Xavier Gonze's group

Samuel Poncé
Yannick Gillet
Michiel van Setten
Matteo Giantomassi
Yongchao Jia

UCL
Université catholique de Louvain



CISM

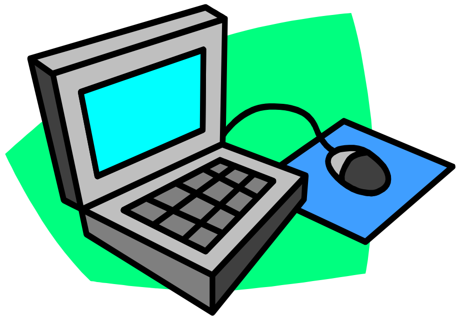
C.E.C.I

Acknowledgments

Xavier Gonze's group

Samuel Poncé
Yannick Gillet
Michiel van Setten
Matteo Giantomassi
Yongchao Jia

UCL
Université catholique de Louvain



CISM

C.E.C.I

Fonds de recherche sur la nature et les technologies
Québec

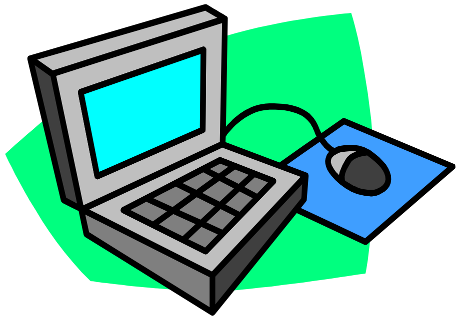
fnrs
FREEDOM TO RESEARCH

ETSF

Acknowledgments

Xavier Gonze's group

Thank you!



Samuel Poncé
Yannick Gillet
Michiel van Setten
Matteo Giantomassi
Yongchao Jia

CISM

Fonds de recherche sur la nature et les technologies Québec

fnrs FREEDOM TO RESEARCH

UCL Université catholique de Louvain

C.E.C.I

ETSF

Future directions

Future directions

- Correction factor for e-e interactions

Future directions

- Correction factor for e-e interactions

$$\frac{M^{\mathrm{G_0W_0}}}{M^{\mathrm{DFT}}} = \frac{\partial^2 \varepsilon^{\mathrm{DFT}} / \partial k^2}{\partial^2 \varepsilon^{\mathrm{G_0W_0}} / \partial k^2} = \frac{\partial \varepsilon^{\mathrm{DFT}}}{\partial \varepsilon^{\mathrm{G_0W_0}}}$$

Future directions

- Correction factor for e-e interactions

$$\frac{M^{\mathrm{G_0W_0}}}{M^{\mathrm{DFT}}} = \frac{\partial^2 \varepsilon^{\mathrm{DFT}} \big/ \partial k^2}{\partial^2 \varepsilon^{\mathrm{G_0W_0}} \big/ \partial k^2} = \frac{\partial \varepsilon^{\mathrm{DFT}}}{\partial \varepsilon^{\mathrm{G_0W_0}}}$$

$$\partial \varepsilon^{\mathrm{G_0W_0}} = \partial \varepsilon^{\mathrm{DFT}} + \frac{\partial \left\langle \hat{\Sigma}(\omega) \right\rangle}{\partial k} \delta k + \frac{\partial \left\langle \hat{\Sigma}(\omega) \right\rangle}{\partial \omega} \delta \varepsilon^{\mathrm{G_0W_0}}$$

Future directions

- Correction factor for e-e interactions

$$\frac{M^{\mathrm{G_0W_0}}}{M^{\mathrm{DFT}}} = \frac{\partial^2 \varepsilon^{\mathrm{DFT}} \Big/ \partial k^2}{\partial^2 \varepsilon^{\mathrm{G_0W_0}} \Big/ \partial k^2} = \frac{\partial \varepsilon^{\mathrm{DFT}}}{\partial \varepsilon^{\mathrm{G_0W_0}}}$$

Oshikiri et al. PRB **66** 125204 (2002)

$$\partial \varepsilon^{\mathrm{G_0W_0}} = \partial \varepsilon^{\mathrm{DFT}} + \frac{\partial \left\langle \hat{\Sigma}(\omega) \right\rangle}{\partial k} \delta k + \frac{\partial \left\langle \hat{\Sigma}(\omega) \right\rangle}{\partial \omega} \delta \varepsilon^{\mathrm{G_0W_0}}$$

Future directions

- Correction factor for e-e interactions

$$\frac{M^{\mathrm{G_0W_0}}}{M^{\mathrm{DFT}}} = \frac{\partial^2 \varepsilon^{\mathrm{DFT}} / \partial k^2}{\partial^2 \varepsilon^{\mathrm{G_0W_0}} / \partial k^2} = \frac{\partial \varepsilon^{\mathrm{DFT}}}{\partial \varepsilon^{\mathrm{G_0W_0}}}$$

Oshikiri et al. PRB **66** 125204 (2002)

$$\partial \varepsilon^{\mathrm{G_0W_0}} = \partial \varepsilon^{\mathrm{DFT}} + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial k} \delta k + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial \omega} \delta \varepsilon^{\mathrm{G_0W_0}}$$

Future directions

- Correction factor for e-e interactions

$$\frac{M^{G_0W_0}}{M^{DFT}} = \frac{\partial^2 \varepsilon^{DFT} / \partial k^2}{\partial^2 \varepsilon^{G_0W_0} / \partial k^2} = \frac{\partial \varepsilon^{DFT}}{\partial \varepsilon^{G_0W_0}}$$

Oshikiri et al. PRB **66** 125204 (2002)

$$\partial \varepsilon^{G_0W_0} = \partial \varepsilon^{DFT} + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial k} \delta k + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial \omega} \delta \varepsilon^{G_0W_0}$$

Future directions

- Correction factor for e-e interactions

$$\frac{M^{\mathrm{G_0W_0}}}{M^{\mathrm{DFT}}} = \frac{\partial^2 \varepsilon^{\mathrm{DFT}} / \partial k^2}{\partial^2 \varepsilon^{\mathrm{G_0W_0}} / \partial k^2} = \frac{\partial \varepsilon^{\mathrm{DFT}}}{\partial \varepsilon^{\mathrm{G_0W_0}}}$$

<0.02% M in AlAs

Oshikiri et al. PRB **66** 125204 (2002)

$$\partial \varepsilon^{\mathrm{G_0W_0}} = \partial \varepsilon^{\mathrm{DFT}} + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial k} \delta k + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial \omega} \delta \varepsilon^{\mathrm{G_0W_0}}$$

Future directions

- Correction factor for e-e interactions

$$\frac{M^{\mathrm{G_0W_0}}}{M^{\mathrm{DFT}}} = \frac{\partial^2 \varepsilon^{\mathrm{DFT}} / \partial k^2}{\partial^2 \varepsilon^{\mathrm{G_0W_0}} / \partial k^2} = \frac{\partial \varepsilon^{\mathrm{DFT}}}{\partial \varepsilon^{\mathrm{G_0W_0}}}$$

<0.02% M in AlAs

Oshikiri et al. PRB **66** 125204 (2002)

$$\partial \varepsilon^{\mathrm{G_0W_0}} = \partial \varepsilon^{\mathrm{DFT}} + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial k} \delta k + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial \omega} \delta \varepsilon^{\mathrm{G_0W_0}}$$

~16% M in AlAs

Future directions

- Correction factor for e-e interactions

$$\frac{M^{G_0W_0}}{M^{DFT}} = \frac{\partial^2 \varepsilon^{DFT} / \partial k^2}{\partial^2 \varepsilon^{G_0W_0} / \partial k^2} = \frac{\partial \varepsilon^{DFT}}{\partial \varepsilon^{G_0W_0}}$$

<0.02% M in AlAs

Oshikiri et al. PRB **66** 125204 (2002)

$$\partial \varepsilon^{G_0W_0} = \partial \varepsilon^{DFT} + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial k} \delta k + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial \omega} \delta \varepsilon^{G_0W_0}$$

~16% M in AlAs

$$\frac{\partial \varepsilon^{DFT}}{\partial \varepsilon^{G_0W_0}} = 1 - \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial \omega} = \frac{1}{Z}$$

Future directions

- Correction factor for e-e interactions

$$\frac{M^{\mathrm{G_0W_0}}}{M^{\mathrm{DFT}}} = \frac{\partial^2 \varepsilon^{\mathrm{DFT}} \big/ \partial k^2}{\partial^2 \varepsilon^{\mathrm{G_0W_0}} \big/ \partial k^2} = \frac{\partial \varepsilon^{\mathrm{DFT}}}{\partial \varepsilon^{\mathrm{G_0W_0}}}$$

<0.02% M in AlAs

Oshikiri et al. PRB **66** 125204 (2002)

$$\partial \varepsilon^{\mathrm{G_0W_0}} = \partial \varepsilon^{\mathrm{DFT}} + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial k} \delta k + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial \omega} \delta \varepsilon^{\mathrm{G_0W_0}}$$

~16% M in AlAs

$$\frac{\partial \varepsilon^{\mathrm{DFT}}}{\partial \varepsilon^{\mathrm{G_0W_0}}} = 1 - \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial \omega} = \frac{1}{Z} = \frac{M^{\mathrm{G_0W_0}}}{M^{\mathrm{DFT}}}$$

Future directions

- Correction factor for e-e interactions

$$\frac{M^{G_0W_0}}{M^{DFT}} = \frac{\partial^2 \varepsilon^{DFT} / \partial k^2}{\partial^2 \varepsilon^{G_0W_0} / \partial k^2} = \frac{\partial \varepsilon^{DFT}}{\partial \varepsilon^{G_0W_0}}$$

<0.02% M in AlAs

Oshikiri et al. PRB **66** 125204 (2002)

$$\partial \varepsilon^{G_0W_0} = \partial \varepsilon^{DFT} + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial k} \delta k + \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial \omega} \delta \varepsilon^{G_0W_0}$$

~16% M in AlAs

$$\frac{\partial \varepsilon^{DFT}}{\partial \varepsilon^{G_0W_0}} = 1 - \frac{\partial \langle \hat{\Sigma}(\omega) \rangle}{\partial \omega} = \frac{1}{Z} = \frac{M^{G_0W_0}}{M^{DFT}}$$

- How general is this apprx?