Challenges, problems and achievements in response functions calculations

Francesco Sottile

École Polytechnique, CNRS, CEA and
European Theoretical Spectroscopy Facility

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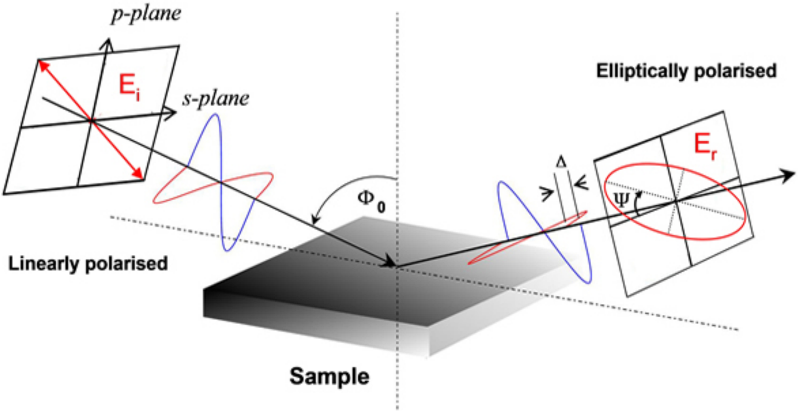
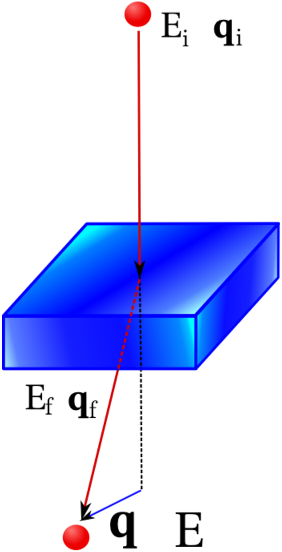
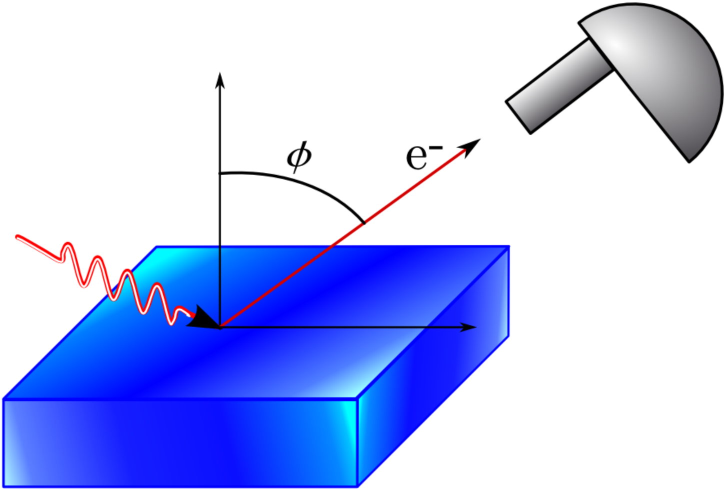
Response Functions :: Why ?



Response Functions :: Why ?



Response Functions :: Why ?



Fundamental quantity :: the dielectric function

$$\varepsilon^{-1}(\mathbf{r}, \mathbf{r}', \omega)$$

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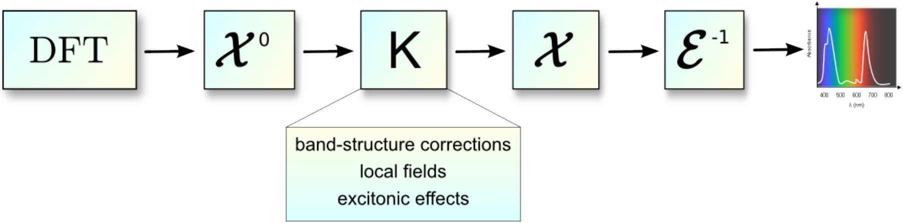
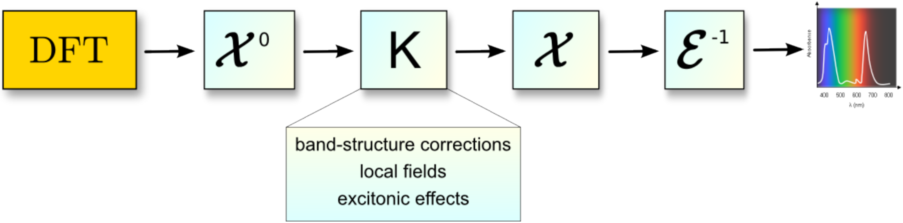
$$\varepsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q}, \omega)$$



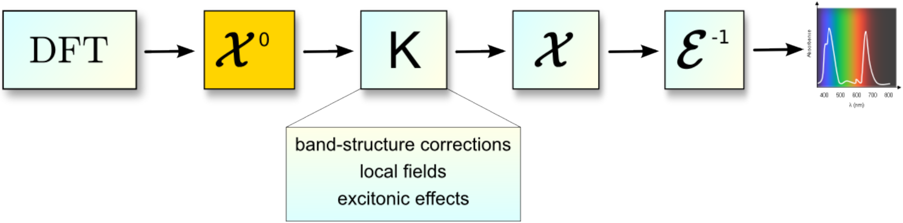
- DP :: TDDFT linear response plane waves (`www.dp-code.org`)
- EXC :: BSE linear response transition space (`bethe-salpeter.org`)



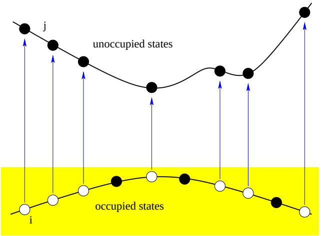
- DFT with plane waves basis $\psi(\mathbf{r}) = \sum_{\mathbf{G}} c_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}$
- Cutoff energy $E_{\mathrm{cutoff}} = \frac{|\mathbf{G}_{\mathrm{max}}|^2}{2}$ as a unique convergence parameter
- pseudopotential (norm-conserving)
- LDA, GGA exchange-correlation potential

Results :: Eigenvalues (and eigenvectors)

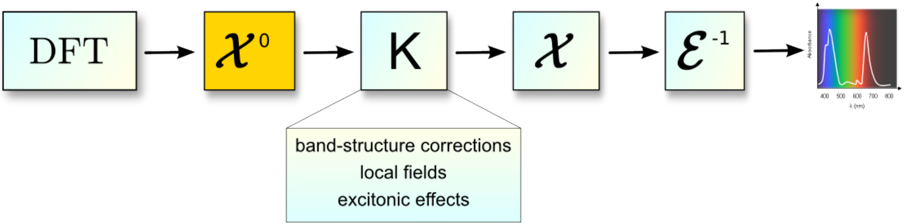
$$\psi_{nk}, \epsilon_{nk}, f_{nk}$$



$$\chi^0_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \sum_{ij} (f_i - f_j) \frac{< \psi_i | e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}} | \psi_j >< \psi_i | e^{-i(\mathbf{q}+\mathbf{G}')\mathbf{r}'} | \psi_j >}{\omega - (\epsilon_i - \epsilon_j)}$$



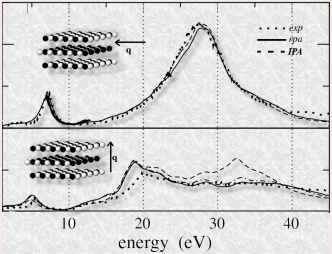
Towards the spectrum :: schematic view of the DP/EXC code

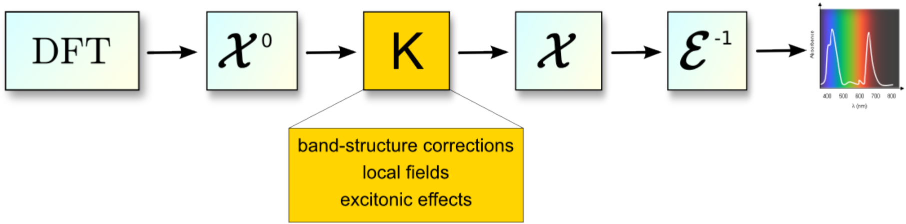


ELS at the DFT level

$$\varepsilon(\mathbf{q},\omega) = 1 - v_{\mathbf{q}}\chi^0(\mathbf{q},\omega)$$

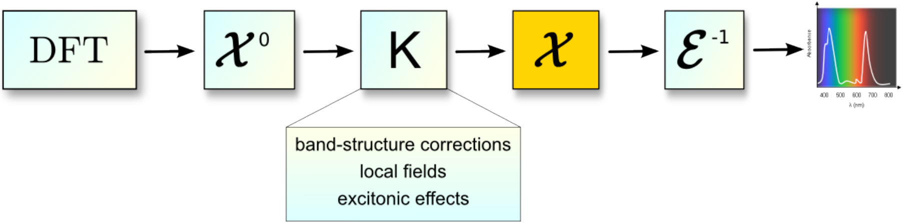
$$\mathrm{ELS} = \mathrm{Im}\left\{\frac{1}{\varepsilon(\mathbf{q},\omega)}\right\}$$



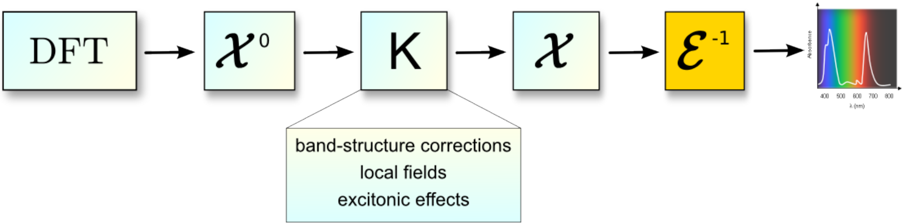


using TDDFT $\begin{cases} v & \text{local fields} \\ f_{xc} & \text{exchange-correlation kernel} \end{cases}$

using Many-Body $\begin{cases} v & \text{local fields} \\ E_i & \text{correct band-structure} \\ W = \varepsilon^{-1} v & \text{electron-hole} \end{cases}$



$$\chi = \left(1 - K\chi^0\right)^{-1}\chi^0$$



$$\varepsilon^{-1} = 1 + v\chi$$

{{Absorption spectrum, Loss Spectrum, refraction index, inelastic X-ray scattering, surface spectroscopies, photoemission}}

The challenge :: IP polarizability

$$\chi^0_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \sum_{ij}(f_i - f_j)\frac{<\psi_i|e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}}|\psi_j><\psi_i|e^{-i(\mathbf{q}+\mathbf{G}')\mathbf{r}'}|\psi_j>}{\omega - (\epsilon_i - \epsilon_j)}$$

The challenge :: IP polarizability

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- not (too) big in memory $N_{\mathbf{G}}^2 N\omega < 1\text{Gb}$
- expensive calculation (many transitions) :: N_{at}^4

The challenge :: IP polarizability

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- not (too) big in memory $N^2_{\mathbf{G}} N\omega < 1\text{Gb}$
- expensive calculation (many transitions) :: N^4_{at}
- DP :: naïve MPI parallelization over ij $\Rightarrow$ 4000procs

Towards massively parallel calculations :: challenges and problems

- I\O data (in particular input)
- What about 10000-100000 procs ?
- What about new paradigm (GPU, Xeon PHI) ?

Towards massively parallel calculations :: challenges and problems

- I\O data (in particular input) towards NetCDF 4 implementation
- What about 10000-100000 procs ?
- What about new paradigm (GPU, Xeon PHI) ? PRACE project

In collaboration with the Maison de la Simulation

MAISON DE LA SIMULATION

DP over GPUs :: a PRACE project

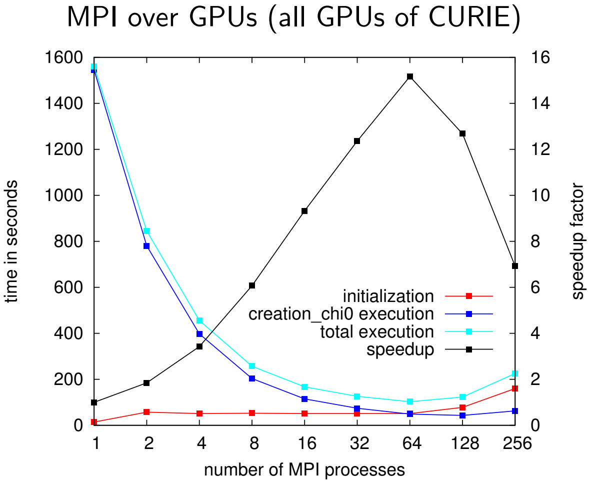
- identify parts of the code to run over GPU (operation-wise)
- check the possibility of data transfer (memory-wise)
- try several strategies

DP step	S1 : Strategy 1	S2 : Strategy 2
Create χ^0	DO nbTransitions ↳ DO nbAlpha ↳ CGERC (BLAS) CPU ⇄ GPU	CPU → GPU DO nbTransitions ↳ DO nbAlpha ↳ CGERC (BLAS) CPU ← GPU
Create ε	DO nbAlpha ↳ CGINV (LAPACK)	DO nbAlpha ↳ CGINV (LAPACK)

- S1 :: simple implementation, lots of data transfer
- S2 :: heavier implementation, 2 data transfers

DP over GPUs :: a PRACE project

- S2 strategy better than S1
- Speedup $\frac{\text{GPU (NvidiaM2090 T20A)}}{\text{CPU (Intel Westmere 2.66 GHz)}} \sim 16 \div 30$


MPI over GPUs (all GPUs of CURIE)
time in seconds
speedup factor
number of MPI processes
1600
1400
1200
1000
800
600
400
200
0
16
14
12
10
8
6
4
2
0
1
2
4
8
16
32
64
128
256
initialization
creation_chi0 execution
total execution
speedup

DP over GPUs :: a PRACE project

DP successfully ported over GPUs

but

difficult implementation and use

performances not comparable to simple OpenMP

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disadvantageous policies on the national computing centers

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Towards massively parallel calculations :: challenges and problems

- I\O data (in particular input) towards NetCDF 4 implementation
- What about 10000-100000 procs ?
- What about new paradigm (GPU, Xeon PHI) ? Ile-de-France grant for Xeon PHI

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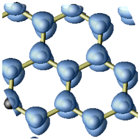
MAISON DE LA SIMULATION

IP polarizability :: Why ?

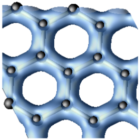
$$\chi^0_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega) = \sum_{ij}(f_i - f_j)\frac{< \psi_i|e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}}|\psi_j >< \psi_i|e^{-i(\mathbf{q}+\mathbf{G}')\mathbf{r}'}|\psi_j >}{\omega - (\epsilon_i - \epsilon_j)}$$

- Bad scaling but very small prefactor !
- Full non-diagonal polarizability $\chi_{\mathbf{G},\mathbf{G}'}$ useful in other situation:
  - non diagonal response in Inelastic x-ray scattering
  - screening ingredient for GW calculation ($W = \varepsilon^{-1}v$)
  - plasmon visualization $\delta\rho(\mathbf{r},\omega) = \int d\mathbf{r} e^{i\mathbf{G}\mathbf{r}} \sum_{\mathbf{G}'} \chi_{\mathbf{G}\mathbf{G}'}(\omega) V_{ext}(\mathbf{G}',\omega)$

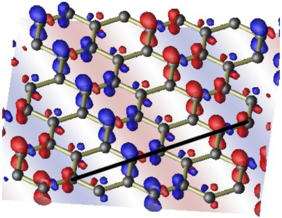
Plasmon visualization of graphite



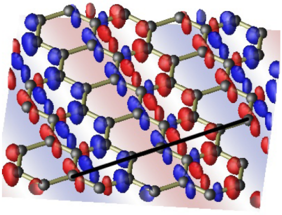
p_z



sp_2



E=9eV



E=30eV

$$\delta\rho(\mathbf{r},t) = \int d\mathbf{r}\, e^{i\mathbf{G}\mathbf{r}} \sum_{\mathbf{G}'} \chi_{\mathbf{G}\mathbf{G}'} e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}-i\omega t}$$