Practical calculations with the GW approximation and Bethe-Salpeter equation in BerkeleyGW

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BerkeleyGW

octopus

NERSC

Benasque, Spain
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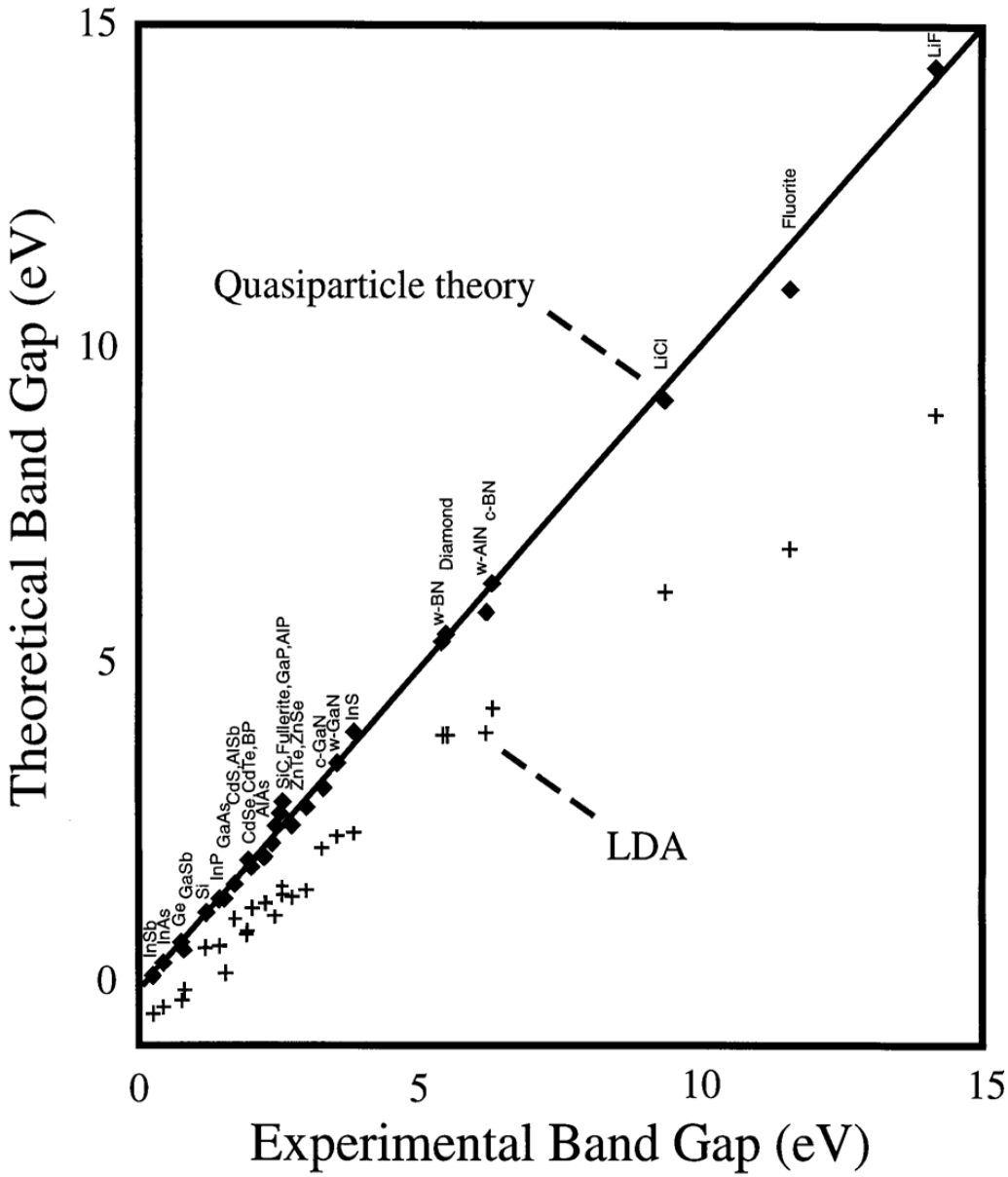
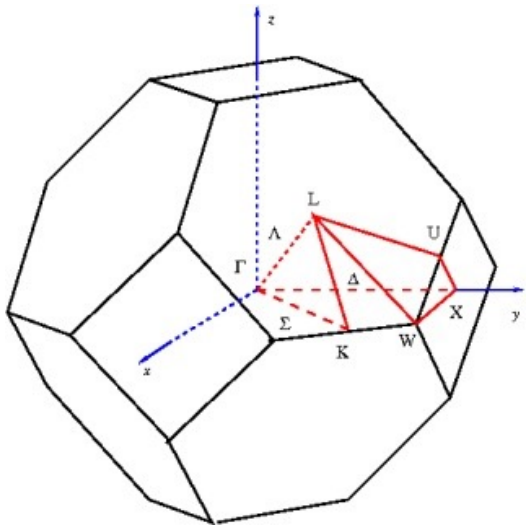
Band gaps: DFT-LDA and GW

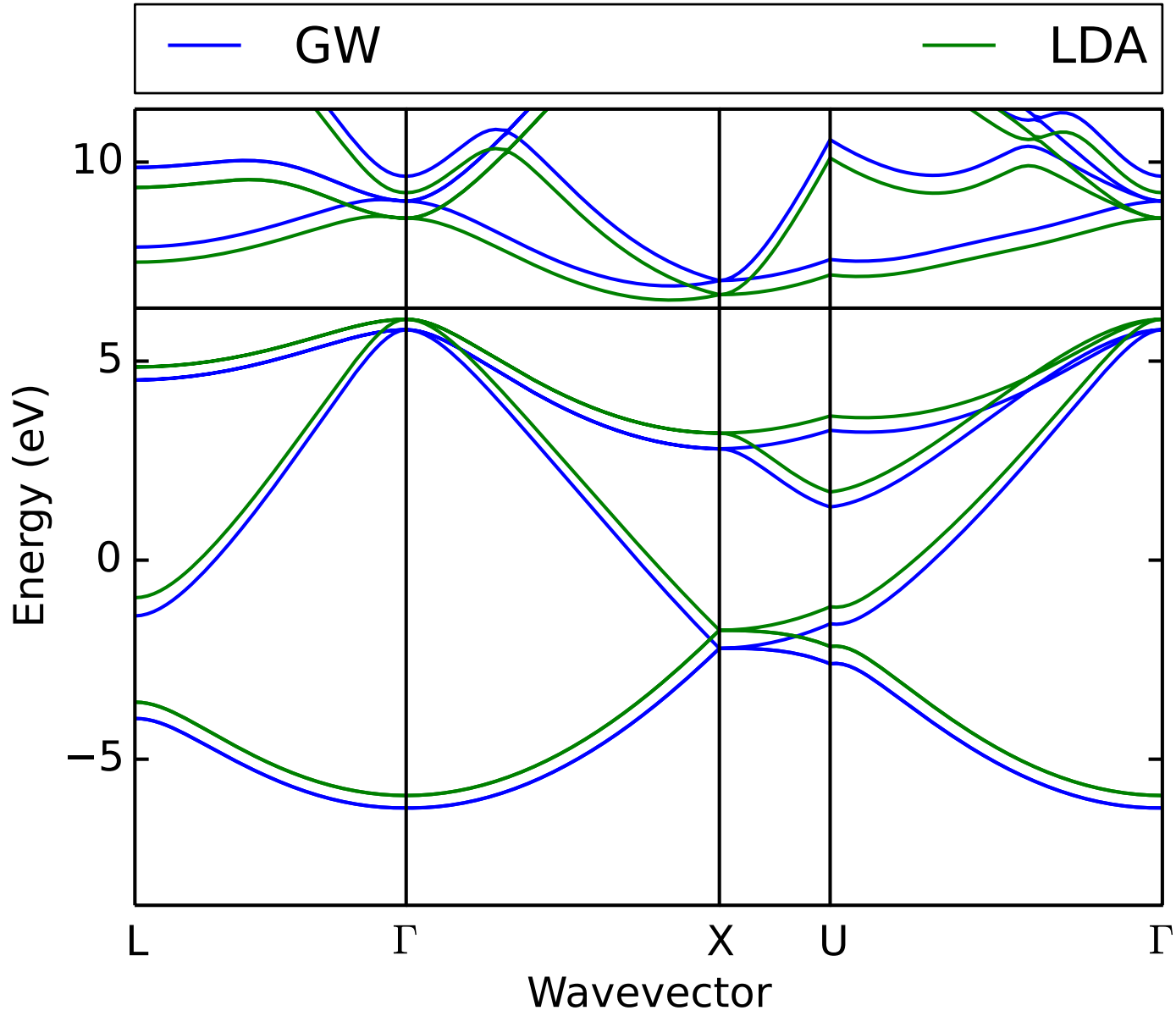
Materials:

InSb, InAs
Ge
GaSb
Si
InP
GaAs
CdS
AlSb, AlAs
CdSe, CdTe
BP
SiC
C_{60}
GaP
AlP
ZnTe, ZnSe
c-GaN, w-GaN
InS
w-BN, c-BN
diamond
w-AlN
LiCl
Fluorite
LiF



Silicon interpolated bandstructure

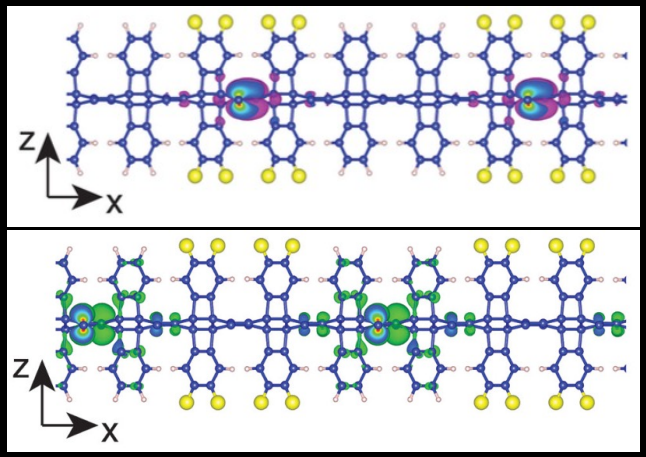


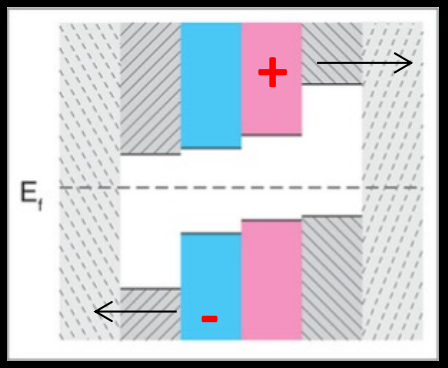


GW/Bethe-Salpeter for graphene-based PV

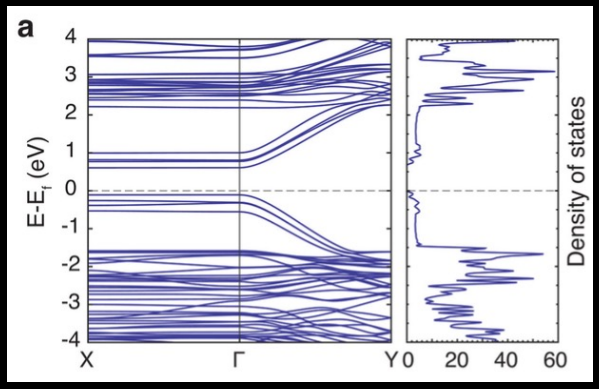
valence

conduction

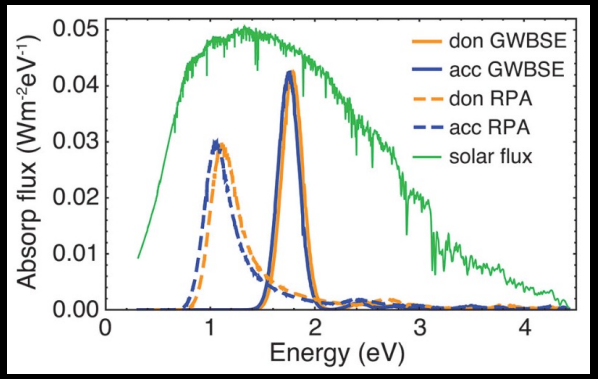


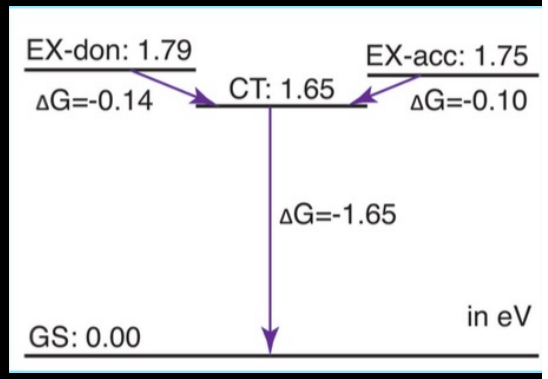


Band structure and density of states

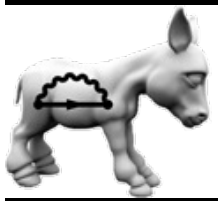


Excitons (electron-hole pairs) from Bethe-Salpeter equation





H. Li, D. A. Strubbe, and Jeffrey C. Grossman, *Adv. Funct. Mater.* **25**, 5199 (2015)



BerkeleyGW

Preview: GW approximation/Bethe-Salpeter eqn

Start with wavefunctions and energies from DFT as mean field

Add perturbation: difference between Vxc and true exchange-correlation

GW self-energy: single-electron energy levels (band structure)

$$\left[-\frac{1}{2}\nabla^2 + V_{\text{ion}} + V_{\text{H}} + \Sigma(E^{\text{QP}}_{n\mathbf{k}})\right]\psi^{\text{QP}}_{n\mathbf{k}} = E^{\text{QP}}_{n\mathbf{k}}\psi^{\text{QP}}_{n\mathbf{k}}$$

Bethe-Salpeter equation: electron-hole interaction for optical properties

$$\left(E^{\text{QP}}_{c\mathbf{k}} - E^{\text{QP}}_{v\mathbf{k}}\right)A^S_{vc\mathbf{k}} + \sum_{v'c'\mathbf{k}'}\left\langle vc\mathbf{k}\middle|K^{\text{eh}}\middle|v'c'\mathbf{k}'\right\rangle = \Omega^S A^S_{vc\mathbf{k}} \qquad \Psi(\mathbf{r}_e,\mathbf{r}_h) = \sum_{\mathbf{k},c,v} A^S_{vc\mathbf{k}}\psi_{\mathbf{k},c}(\mathbf{r}_e)\psi^*_{\mathbf{k},v}(\mathbf{r}_h)$$

BerkeleyGW

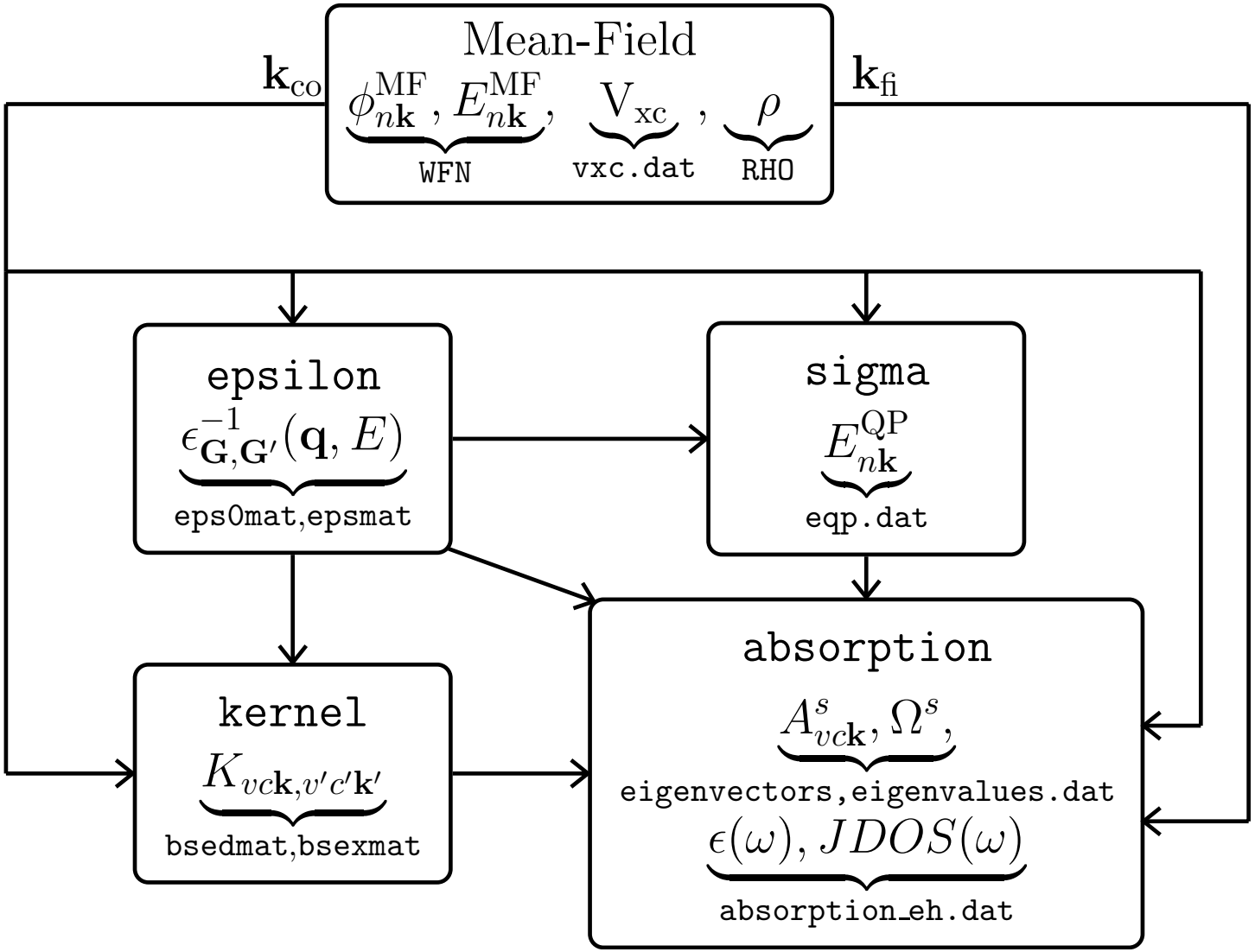
widely used massively parallel code
(~1000s of atoms)
www.berkeleygw.org

J. Deslippe, G. Samsonidze, D. A. Strubbe, M. Jain, M. L. Cohen, and S. G. Louie, *Comput. Phys. Comm.* **183**, 1269 (2012)

Why Use BerkeleyGW

- Supports a large set of Mean-Field codes: PARATEC, Quantum ESPRESSO, ABINIT, Octopus, PARSEC, SIESTA, EPM (TBPW)
- Supports 3D, 2D, 1D and Molecular Systems. Coulomb Truncation
- Support for Semiconductor, Metallic and Semi-Metallic Systems
- Efficient Algorithms and Use of Libraries. (BLAS, FFTW3, LAPACK, SCALAPACK, ELPA, OpenMP, HDF5)
- Massively Parallel. Scales to 100,000 CPUs, distributed Memory.
- Efficient accurate solution to BSE via k-point Interpolation
- Support for LDA/GGA/Hybrid/HF/COHSEX starting points as well as off-diagonal Σ calculations

GW Method


Mean-Field
$\mathbf{k}_{\mathrm{co}}$
$\phi^{\mathrm{MF}}_{n\mathbf{k}}, E^{\mathrm{MF}}_{n\mathbf{k}}$
WFN
V_{xc}
vxc.dat
ρ
RHO
$\mathbf{k}_{\mathrm{fi}}$
epsilon
$\epsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q}, E)$
eps0mat,epsmat
sigma
$E^{\mathrm{QP}}_{n\mathbf{k}}$
eqp.dat
kernel
$K_{vc\mathbf{k},v'c'\mathbf{k}'}$
bsedmat,bsexmat
absorption
$A^s_{vc\mathbf{k}}, \Omega^s,$
eigenvectors,eigenvalues.dat
$\epsilon(\omega), JDOS(\omega)$
absorption_eh.dat

Full-Frequency vs. Generalized Plasmon Pole (GPP)

$$\langle n\mathbf{k}|\,\Sigma_{\rm CH}(E)\,|n'\mathbf{k}\rangle = \frac{i}{2\pi}\sum_{n''}\sum_{\mathbf{q}\mathbf{G}\mathbf{G}'} M^*_{n''n}(\mathbf{k},-\mathbf{q},-\mathbf{G})M_{n''n'}(\mathbf{k},-\mathbf{q},-\mathbf{G}') \quad (20)$$

Full-Frequency

$$\times \int_0^\infty dE' \; \frac{\left[\epsilon^{\rm r}_{\mathbf{G}\mathbf{G}'}\right]^{-1}(\mathbf{q};E') - \left[\epsilon^{\rm a}_{\mathbf{G}\mathbf{G}'}\right]^{-1}(\mathbf{q};E')}{E - E_{n''\mathbf{k}-\mathbf{q}} - E' + i\delta} \; v(\mathbf{q}+\mathbf{G}')$$

$$\langle n\mathbf{k}|\,\Sigma_{\rm CH}(E)\,|n'\mathbf{k}\rangle = \frac{1}{2}\sum_{n''}\sum_{\mathbf{q}\mathbf{G}\mathbf{G}'} M^*_{n''n}(\mathbf{k},-\mathbf{q},-\mathbf{G})M_{n''n'}(\mathbf{k},-\mathbf{q},-\mathbf{G}') \quad (22)$$

GPP

$$\times \frac{\Omega^2_{\mathbf{G}\mathbf{G}'}(\mathbf{q})\,(1 - i\tan\phi_{\mathbf{G}\mathbf{G}'}(\mathbf{q}))}{\tilde{\omega}_{\mathbf{G}\mathbf{G}'}(\mathbf{q})\,(E - E_{n''\mathbf{k}-\mathbf{q}} - \tilde{\omega}_{\mathbf{G}\mathbf{G}'}(\mathbf{q}))} \; v(\mathbf{q}+\mathbf{G}')$$

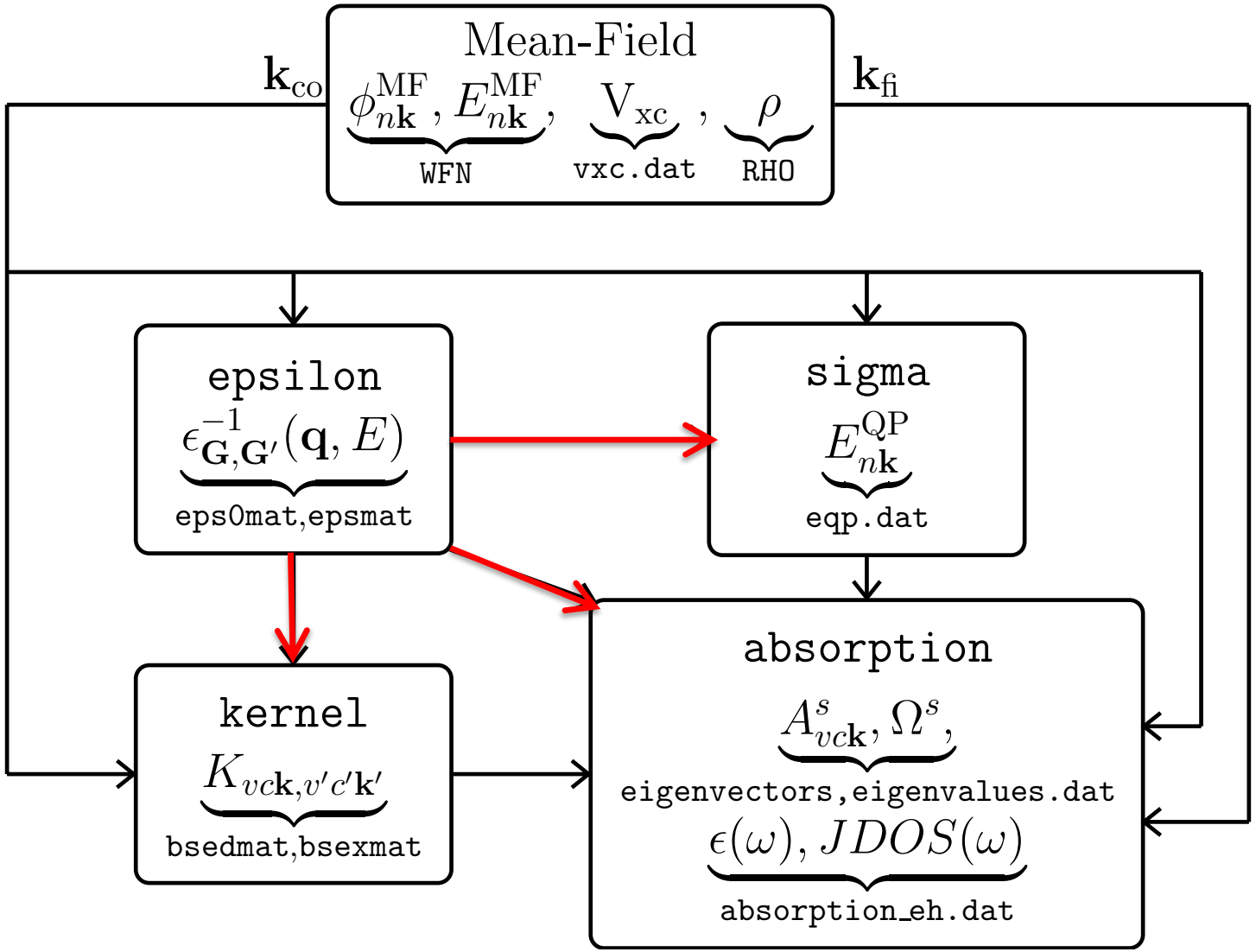
GPP is significantly faster. The integral over frequencies can be performed analytically if assume the dielectric response is dominated by a single plasmon pole.

BerkeleyGW supports both. With full-frequency you can compute spectral functions, lifetimes and weights. By contrast, GPP is (incorrectly) purely real.

Practical issues for *GW*

1. Screening models for Epsilon
2. Construction of **k**-grids
3. Symmetry and degeneracy
4. Real and complex version
5. Solving Dyson's equation
6. Convergence
7. Use of Octopus

Screening models: How do we use ε?



Screening models: How do we use ε?

Sigma integrates over **q** with $\varepsilon^{-1}(\mathbf{q})$

$$\langle n\mathbf{k}|\,\Sigma(E)\,|n'\mathbf{k}\rangle = \frac{i}{2\pi}\sum_{n''}\sum_{\mathbf{q}\mathbf{G}\mathbf{G}'} M^*_{n''n}(\mathbf{k},-\mathbf{q},-\mathbf{G})M_{n''n'}(\mathbf{k},-\mathbf{q},-\mathbf{G}') \times \int_{-\infty}^{\infty} dE' e^{-i\delta E'} \frac{\left[\epsilon_{\mathbf{G}\mathbf{G}'}\right]^{-1}(\mathbf{q};E')}{E - E_{n''\mathbf{k}-\mathbf{q}} - E' - i\delta_{n''\mathbf{k}-\mathbf{q}}} v(\mathbf{q}+\mathbf{G}')$$

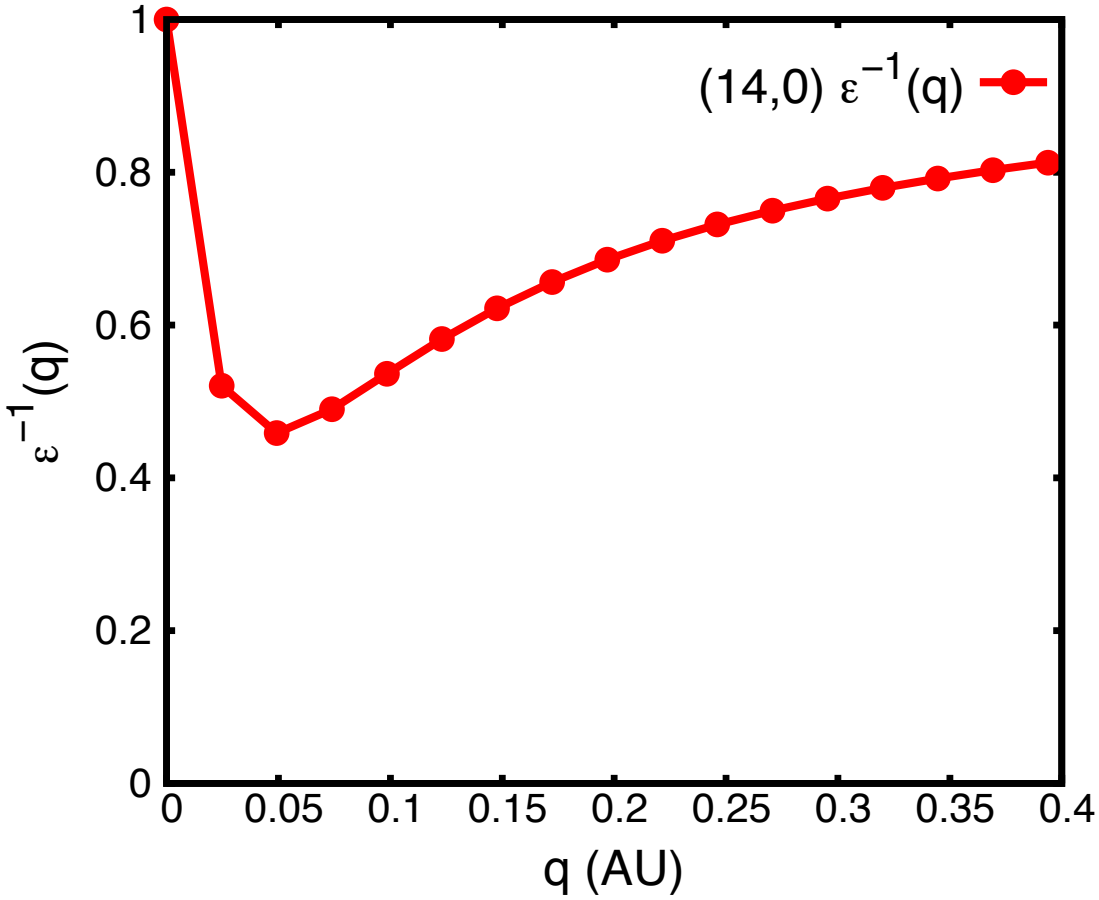
Absorption interpolates kernel over **q** with $W(\mathbf{q}) = \varepsilon^{-1}(\mathbf{q})\, v(\mathbf{q})$

$$\langle vc\mathbf{k}|K^{\mathrm{d}}|v'c'\mathbf{k}'\rangle = \sum_{\mathbf{G}\mathbf{G}'} M^*_{c'c}(\mathbf{k},\mathbf{q},\mathbf{G})W_{\mathbf{G}\mathbf{G}'}(\mathbf{q};0)M_{v'v}(\mathbf{k},\mathbf{q},\mathbf{G}')$$

Problem 1: Non-smooth behavior

(14, 0) carbon nanotube wire truncation

General for truncation: see BN tutorial



Problem 2: Divergent behavior

DOS inter/intra-band transitions gap

$$\chi_{\mathbf{GG'}}(\mathbf{q};0) = \sum_{n}^{\text{occ}} \sum_{n'}^{\text{emp}} \sum_{\mathbf{k}} M^{*}_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G}) M_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G'}) \frac{1}{E_{n\mathbf{k}+\mathbf{q}} - E_{n'\mathbf{k}}}.$$

Head: **G** = 0, **G'** = 0
Wing: **G** = 0, **G'** ≠ 0
Wing': **G** ≠ 0, **G'** = 0
Body: **G** ≠ 0, **G'** ≠ 0

Cannot calculate at **q** = 0!

q^2/q^2 diverges

$\epsilon^{-1}_{\mathbf{GG'}}$	head	wing	wing′	body
Semiconductor	const	$\mathbf{q}$	$\mathbf{q}/q^2$	const
Metal	q^2	q^2	const	const

$W_{\mathbf{GG'}}$	head	wing	wing′	body
Semiconductor	$1/q^2$	$\mathbf{q}/q^2$	$\mathbf{q}/q^2$	const
Metal	const	const	const	const

q^2/q^2

Solution: Screening models

Calculate at $\mathbf{q_0} \approx 0.001$ in periodic direction
use to parametrize screening model

Sigma: Integrate over region around $\mathbf{q} = 0$

Kernel:
Interpolate
in parts

head wing, wing' body

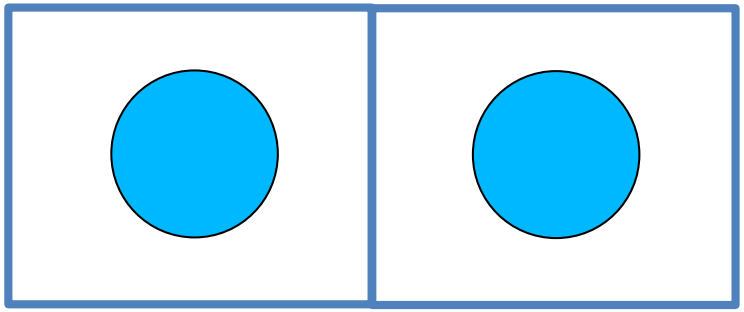
$$\langle vc\mathbf{k}\,|K|\,v'c'\mathbf{k}'\rangle = \frac{a_{vc\mathbf{k}v'c'\mathbf{k}'}}{A(\mathbf{q})} + \frac{b_{vc\mathbf{k}v'c'\mathbf{k}'}}{B(\mathbf{q})} + \frac{c_{vc\mathbf{k}v'c'\mathbf{k}'}}{C(\mathbf{q})}$$

$\epsilon^{-1}_{\mathbf{GG'}}$	head	wing	wing'	body
Semiconductor	const	$\mathbf{q}$	$\mathbf{q}/q^2$	const
Metal	q^2	q^2	const	const

$W_{\mathbf{GG'}}$	head	wing	wing'	body
Semiconductor	$1/q^2$	$\mathbf{q}/q^2$	$\mathbf{q}/q^2$	const
Metal	const	const	const	const

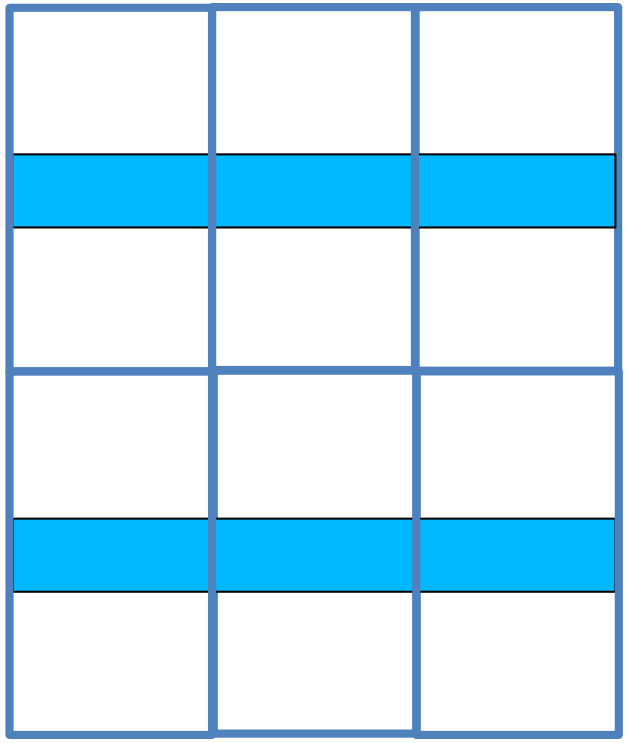
Truncation for non- or partially periodic systems

Periodicity in 0, 1, 2, or 3 dimensions. Eliminate spurious image interactions.



Cell (for molecule)

Wire (for nanotube or nanowire)



Slab (for graphene or surface)

Truncation of Coulomb potential

- GW and BSE utilize the Coulomb and screened Coulomb interaction

$$W = \varepsilon^{-1} V_c$$

- Long-range interactions make it computationally infeasible to increase lattice vectors until periodic images do not interact.
- Rule of thumb: non-periodic direction should include 99% of density

Truncation Schemes within BerkeleyGW

- Cell box: 0D
- Cell wire: 1D
- Cell slab: 2D
- Spherical: Define radius of truncation

$$v_t(\mathbf{r}) = \frac{\Theta(f(\mathbf{r}))}{r}$$

- **Cell truncation**: at half lattice vector length
  - Analytical form for Coulomb potential in k-space
- **Spherical truncation**: convenient, available in many packages

Regular **k**-grids

Epsilon

$$\chi_{\mathbf{G}\mathbf{G}'}(\mathbf{q};0) = \sum_{n}^{\text{occ}} \sum_{n'}^{\text{emp}} \sum_{\mathbf{k}} M^*_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G}) M_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G}') \frac{1}{E_{n\mathbf{k}+\mathbf{q}} - E_{n'\mathbf{k}}}.$$

where

$$M_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G}) = \langle n\mathbf{k}+\mathbf{q}| \, e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} \, |n'\mathbf{k}\rangle$$

Sigma

$$\langle n\mathbf{k}| \, \Sigma_{\text{SX}}(E) \, |n'\mathbf{k}\rangle = -\sum_{n''}^{\text{occ}} \sum_{\mathbf{q}\mathbf{G}\mathbf{G}'} M^*_{n''n}(\mathbf{k},-\mathbf{q},-\mathbf{G}) M_{n''n'}(\mathbf{k},-\mathbf{q},-\mathbf{G}')$$
$$\times \left[\epsilon_{\mathbf{G}\mathbf{G}'}\right]^{-1}(\mathbf{q}; E - E_{n''\mathbf{k}-\mathbf{q}}) v(\mathbf{q}+\mathbf{G}')$$

Kernel

$$\langle vc\mathbf{k}|K^{\text{d}}|v'c'\mathbf{k}'\rangle = \sum_{\mathbf{G}\mathbf{G}'} M^*_{c'c}(\mathbf{k},\mathbf{q},\mathbf{G}) W_{\mathbf{G}\mathbf{G}'}(\mathbf{q};0) M_{v'v}(\mathbf{k},\mathbf{q},\mathbf{G}')$$

$$\epsilon^{-1}(\mathbf{q}) \text{ for } \mathbf{q} = \mathbf{k} - \mathbf{k}'.$$

k-grids and bands

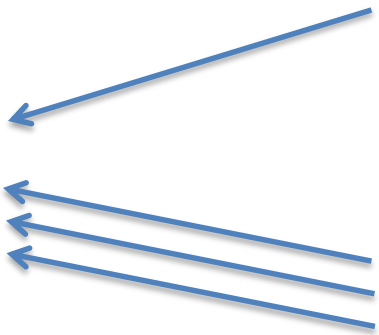
recommended approach

	k-grid	# bands	Comments
SCF	Uniform, 0.5 shift	occupied	as usual in DFT
WFN	Uniform, 0.5 shift	many	
WFNq	WFN + **q**-shift	occupied	
epsilon.inp **q**-points	WFN but no shift, $\mathbf{q}_0$	many	bands to sum over
WFN_inner	WFN but no shift	many	bands to sum over
sigma.inp **k**-points	subset of WFN_inner	few	can choose to calculate Sigma just for bands of interest
WFN_co	WFN_inner	few	
WFN_fi (absorption)	Uniform, random shift	few	
WFNq_fi	WFN_fi + **q**-shift	occupied	
WFN_fi (inteqp)	anything	few	whatever is of interest

epsilon.inp

Semiconductors

```
begin qpoints
   0.000000     0.000000     0.005000    1.0    1
   0.000000     0.000000     0.062500    1.0    0
   0.000000     0.000000     0.125000    1.0    0
   0.000000     0.000000     0.187500    1.0    0
  …
end
```



eps0mat:

$$\epsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q}_0)$$

epsmat:

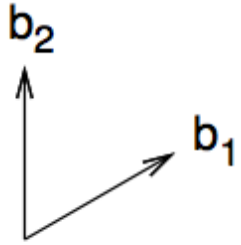
$$\epsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q} \neq \mathbf{q}_0)$$

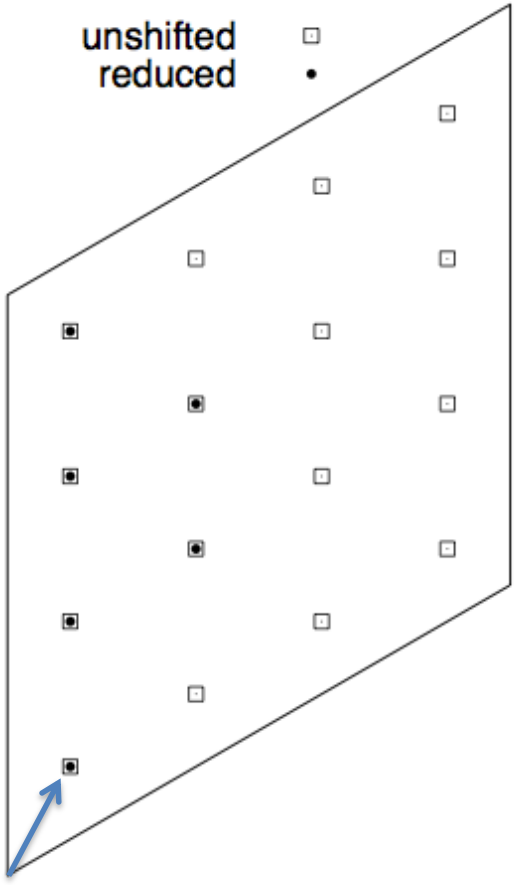
k-grid construction: 4×4 grid for graphene

(0.5, 0.5) Monkhorst-Pack shift

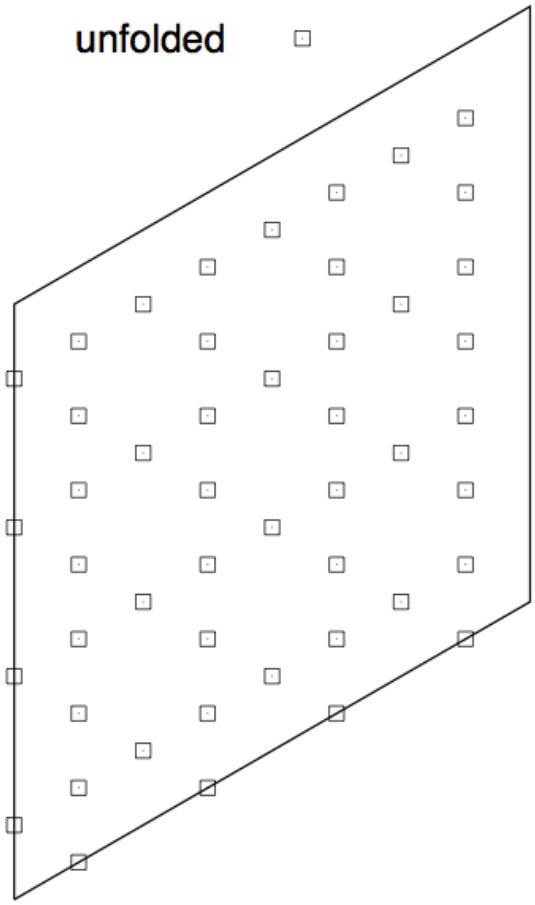
`kgrid.x`

Uniform -> unfold -> shift with **q** -> reduce





(0.5, 0.5)



Unfolding gives more points!

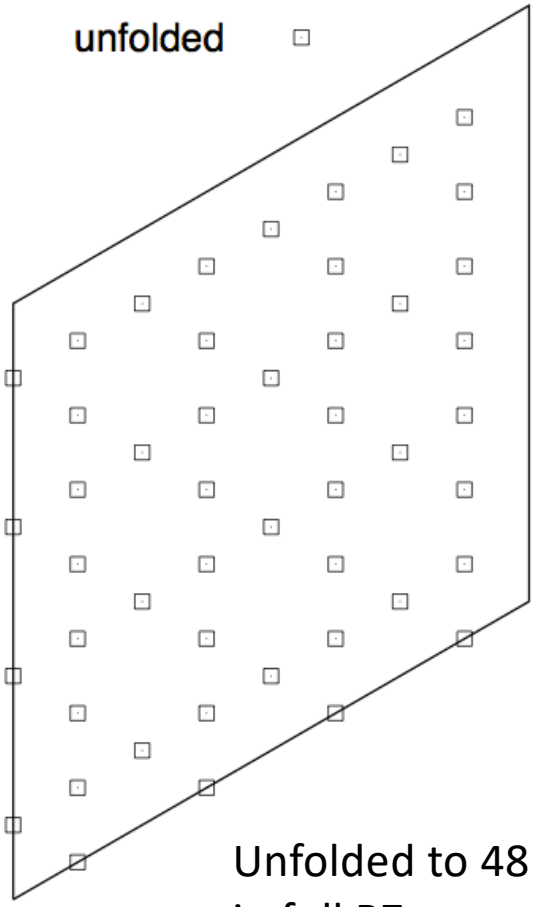
Main grid (WFN)
16 in full BZ
Reduced to 6

Unfolded to 48 in full BZ

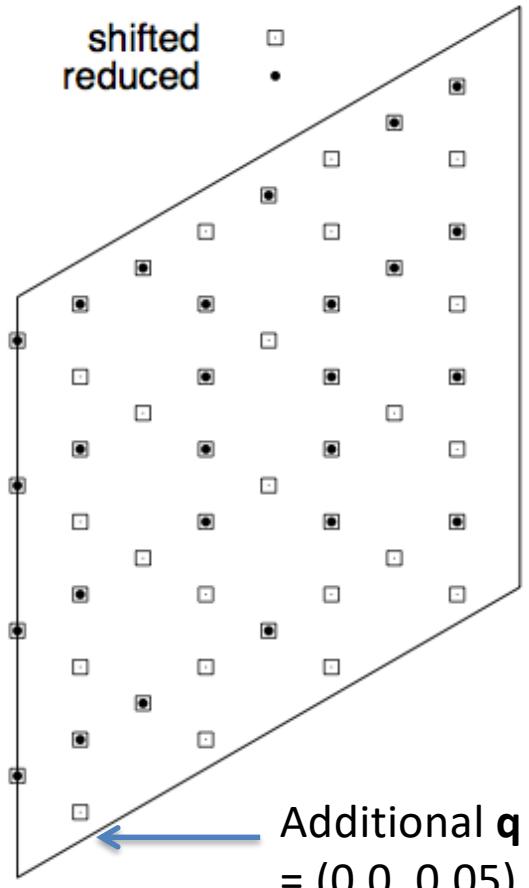
k-grid construction: 4×4 grid for graphene

`kgrid.x`

Uniform -> unfold ->
shift with **q** -> reduce



Unfolded to 48
in full BZ



Additional **q**
= (0.0, 0.05)

Shifted grid (WFNq)
48 in full BZ
Reduced to 26

Unfolding and breaking
symmetry gives more points!

Degeneracy

Epsilon, Sigma: symmetry of Hamiltonian

$$\langle n\mathbf{k}|\,\Sigma_{\mathrm{SX}}(E)\,|n'\mathbf{k}\rangle = -\sum_{n''}^{\mathrm{occ}}\sum_{\mathbf{q}\mathbf{G}\mathbf{G}'} M^{*}_{n''n}(\mathbf{k},-\mathbf{q},-\mathbf{G})M_{n''n'}(\mathbf{k},-\mathbf{q},-\mathbf{G}') \times \left[\epsilon_{\mathbf{G}\mathbf{G}'}\right]^{-1}(\mathbf{q};E-E_{n''\mathbf{k}-\mathbf{q}})v(\mathbf{q}+\mathbf{G}')$$

Absorption: symmetry of e-h basis

$$\left(E^{\mathrm{QP}}_{c\mathbf{k}}-E^{\mathrm{QP}}_{v\mathbf{k}}\right)A^{S}_{vc\mathbf{k}}+\sum_{v'c'\mathbf{k}'}\left\langle vc\mathbf{k}|K^{\mathrm{eh}}|v'c'\mathbf{k}'\right\rangle = \Omega^{S}A^{S}_{vc\mathbf{k}}$$

Summing over only some of a degenerate space will break symmetry.
Degeneracy in mean-field => broken in *GW*!
Results depends on arbitrary linear combinations in mean-field. Not reproducible!
Incorrect oscillator strengths in absorption!

Degeneracy check utility

```
$ degeneracy_check.x WFN

Reading eigenvalues from file WFN
Number of spins:                 1
Number of bands:                35
Number of k-points:              8

== Degeneracy-allowed numbers of bands (for epsilon and sigma) ==
             4
             8
            14
            18
            20
            32
Note: cannot assess whether or not highest band     35 is degenerate.
```

So, use `number_bands 32` in Epsilon.

Real or complex flavor?

e.g. bin/epsilon.real.x, bin/epsilon.cplx.x

Complex is general, but real is faster, uses less memory and disk space

Real: only with inversion symmetry about the origin $u(-\mathbf{r}) = au(\mathbf{r})$

and time-reversal symmetry $u^*(\mathbf{r}) = bu(\mathbf{r})$

a, b each equal to ± 1

What breaks time-reversal? Magnetic fields, spin-polarization, spinors
Plane-wave codes generally just use complex wavefunctions.
Conditions for reality depends on the basis! Real-space: *k* = 0, time-reversal.

Real output not implemented in Octopus yet.

Solving Dyson's equation in Sigma

$$E_{n\mathbf{k}}^{\mathrm{QP}} = E_{n\mathbf{k}}^{\mathrm{MF}} + \langle \psi_{n\mathbf{k}} | \Sigma(E_{n\mathbf{k}}^{\mathrm{QP}}) - \Sigma^{\mathrm{MF}} | \psi_{n\mathbf{k}} \rangle$$

How can we solve when we don't know E^{QP} yet?

(1) eqp0: evaluate at E^{MF}.

$$E_{n\mathbf{k}}^{\mathrm{QP0}} = E_{n\mathbf{k}}^{\mathrm{MF}} + \langle \psi_{n\mathbf{k}} | \Sigma(E_{n\mathbf{k}}^{\mathrm{MF}}) - \Sigma^{\mathrm{MF}} | \psi_{n\mathbf{k}} \rangle$$

(2) eqp1: solve linearized approximation (Newton's Method)

$$E_{n\mathbf{k}}^{\mathrm{QP1}} = E_{n\mathbf{k}}^{\mathrm{QP0}} + \frac{d\Sigma_{n\mathbf{k}}/dE}{1 - d\Sigma_{n\mathbf{k}}/dE} \left(E_{n\mathbf{k}}^{\mathrm{QP0}} - E_{n\mathbf{k}}^{\mathrm{MF}} \right)$$

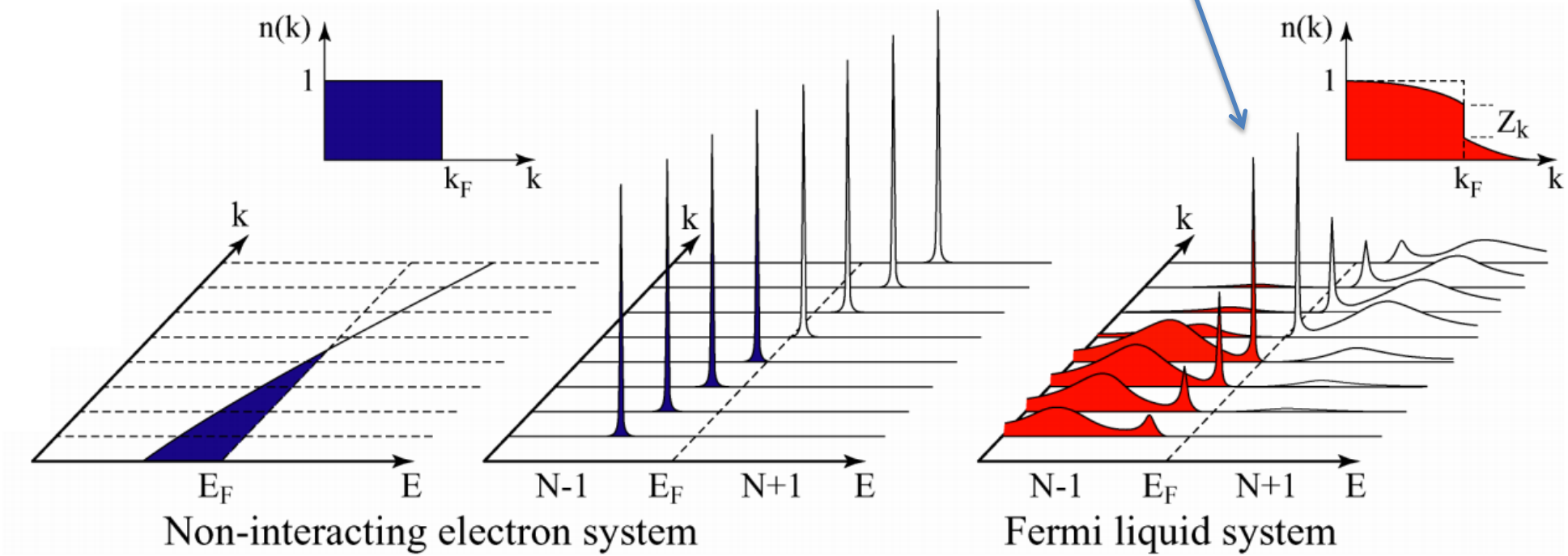
Available as columns in `sigma_hp.log`, and `eqp0.dat` and `eqp1.dat` files

Quasiparticle renormalization factor *Z*

$$E_{n\mathbf{k}}^{\mathrm{QP1}} = E_{n\mathbf{k}}^{\mathrm{QP0}} + (Z_{n\mathbf{k}} - 1)\left(E_{n\mathbf{k}}^{\mathrm{QP0}} - E_{n\mathbf{k}}^{\mathrm{MF}}\right)$$

$$Z_{n\mathbf{k}} = \frac{1}{1 - d\Sigma_{n\mathbf{k}}/dE}$$

Between 0 and 1
Weight in QP peak



A. Damascelli, Z. Hussain, Z.-X Shen, Rev. Mod. Phys. **75**, 473 (2003)

There are many convergence parameters in a GW calculations: convergence with each must be checked

Screened cutoff

Empty bands (dielectric matrix)

$$\chi_{\mathbf{GG'}}(\mathbf{q},0) = \sum_{n}^{\text{occ}} \sum_{n'}^{\text{emp}} \sum_{\mathbf{k}} M^*_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G}) M_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G'}) \frac{1}{E_{n\mathbf{k}+\mathbf{q}} - E_{n'\mathbf{k}}}$$

q-grid

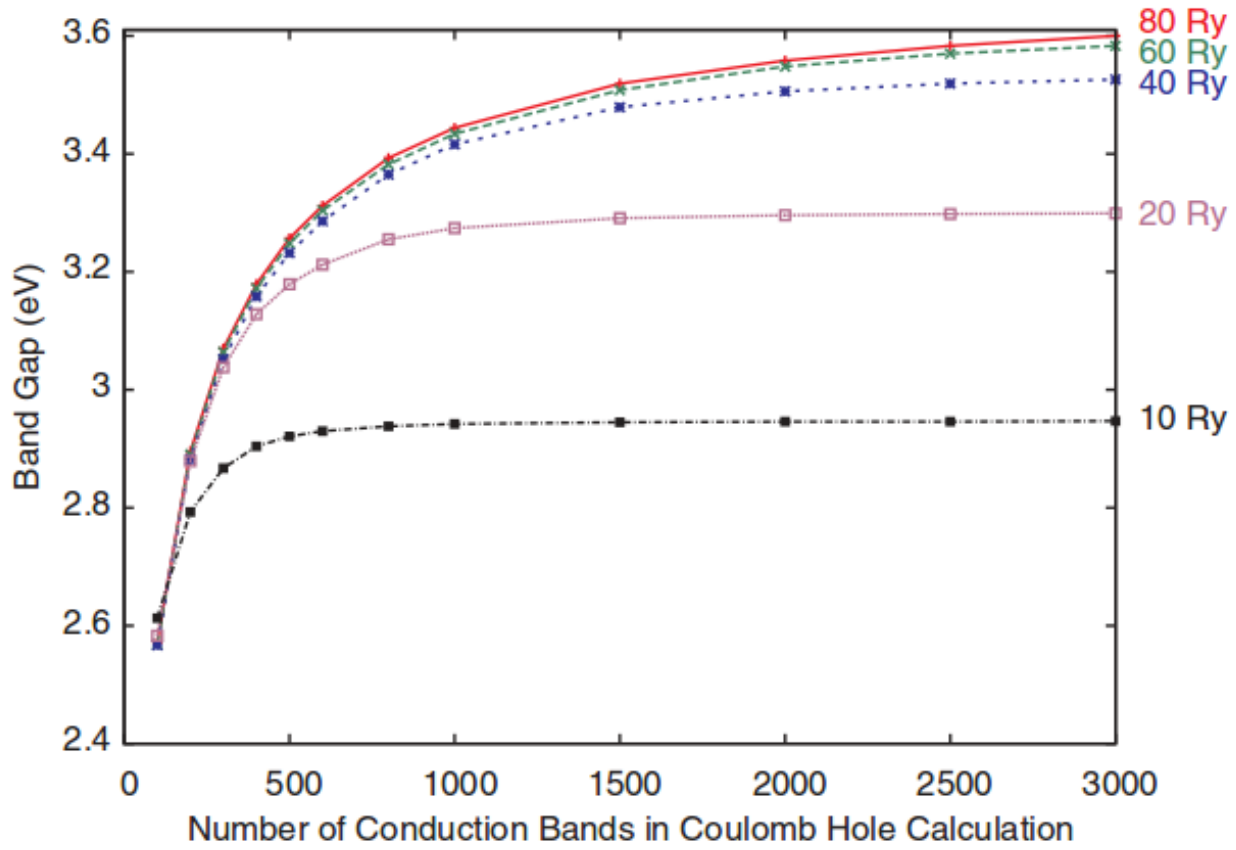
Bands in CH summation (sigma)

$$\langle n\mathbf{k}| \Sigma_{\text{CH}}(E) |n'\mathbf{k}\rangle = \frac{1}{2} \sum_{n''} \sum_{\mathbf{qGG'}} M^*_{n''n}(\mathbf{k},-\mathbf{q},-\mathbf{G}) M_{n''n'}(\mathbf{k},-\mathbf{q},-\mathbf{G'}) \times \frac{\Omega^2_{\mathbf{GG'}}(\mathbf{q})\,(1 - i\tan\phi_{\mathbf{GG'}}(\mathbf{q}))}{\tilde{\omega}_{\mathbf{GG'}}(\mathbf{q})\,(E - E_{n''\mathbf{k}-\mathbf{q}} - \tilde{\omega}_{\mathbf{GG'}}(\mathbf{q}))} v(\mathbf{q}+\mathbf{G'})$$

$$M_{nn'}(\mathbf{k},\mathbf{q},\mathbf{G}) = \langle n\mathbf{k}+\mathbf{q}| e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} |n'\mathbf{k}\rangle$$

Wavefunction cutoff (matrix elements)

Coupled convergence parameters



ZnO: B. Shih et al., *Phys. Rev. Lett.* 105, 146401 (2010)

See convergence and “When things go wrong” slides on BerkeleyGW 2022 tutorial page!

Octopus interface to BerkeleyGW

Real space transformed to plane-waves for GW.

Can only produce complex wavefunctions currently.

Good for:
- very large systems
- finite or perhaps partially periodic systems (molecules, nanowires, 2D sheets)
- charged systems
- model systems
- interfacing with special features of Octopus

Domain parallelization for real-space scales better than plane waves.

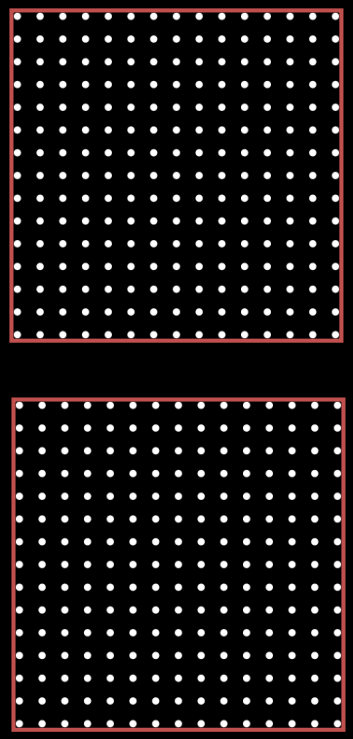
Application for spin-flip Bethe-Salpeter equation on molecules and defects:
B. A. Barker and D. A. Strubbe, https://arxiv.org/abs/2207.04549 (2022)

Fourier transform to plane-wave form

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \sum_{\mathbf{G}} u_{n\mathbf{k}}(\mathbf{G})$$

real space: cube for all quantities

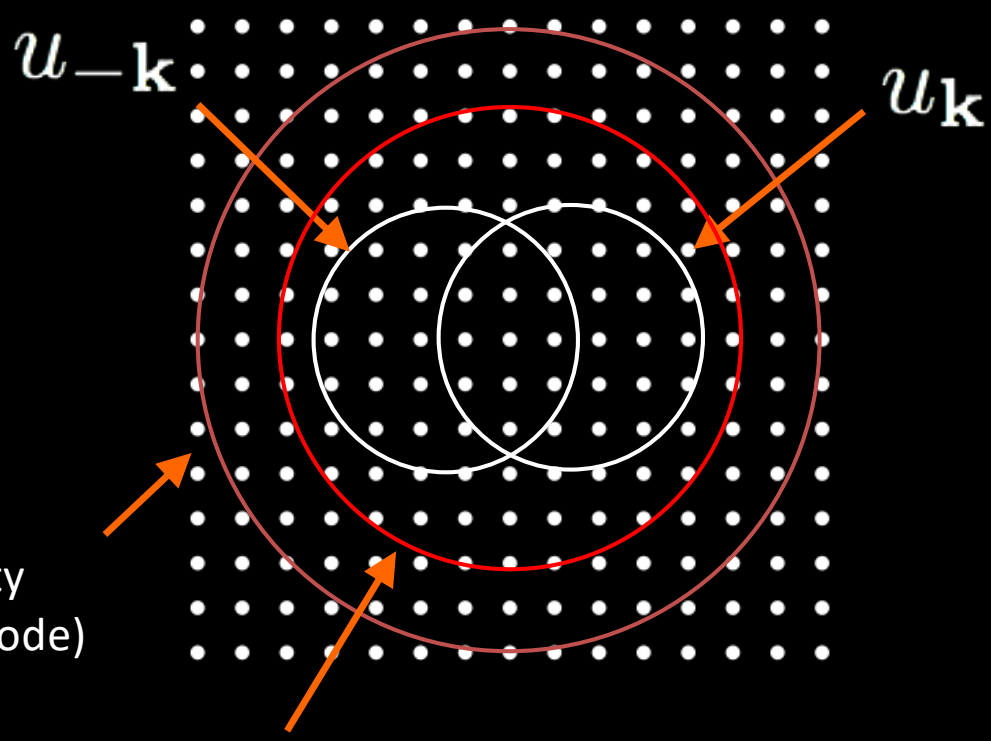
$$|\mathbf{k}+\mathbf{G}|^2 < E_{\text{cutoff}}$$



real space

FT

reciprocal space



density (PW code)

density (real-space code)

Must check norm, renormalize.

Finite *vs.* periodic boundary conditions for vacuum

Are plane waves more natural basis for unbound vacuum states?

"Particle in a box" spectrum

$$\psi_n(x) \sim e^{in\pi x/L}$$

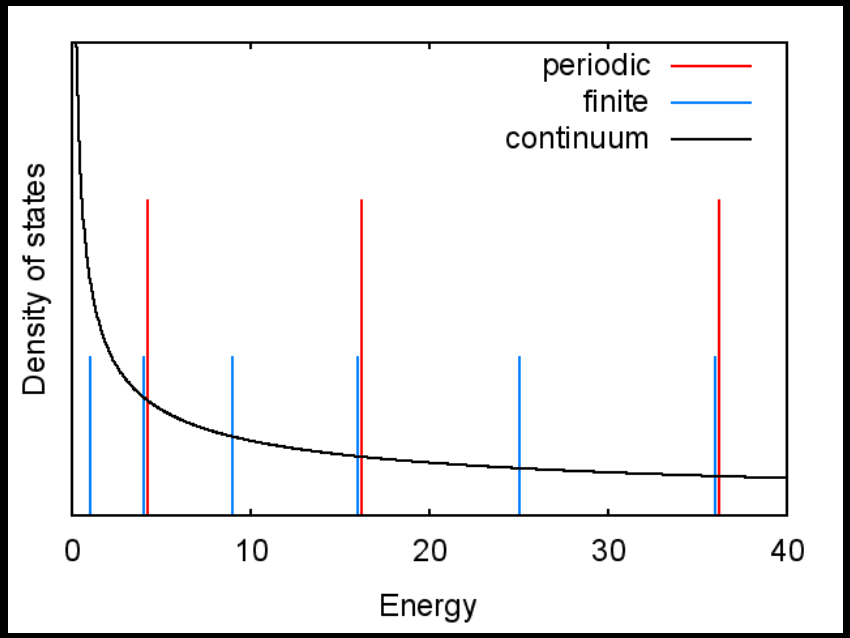
$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

periodic (plane waves) $\psi'(0) = \psi'(L) = 0$

$n = \pm 2, \pm 4, \pm 6, \ldots$

finite (real space) $\psi(0) = \psi(L) = 0$

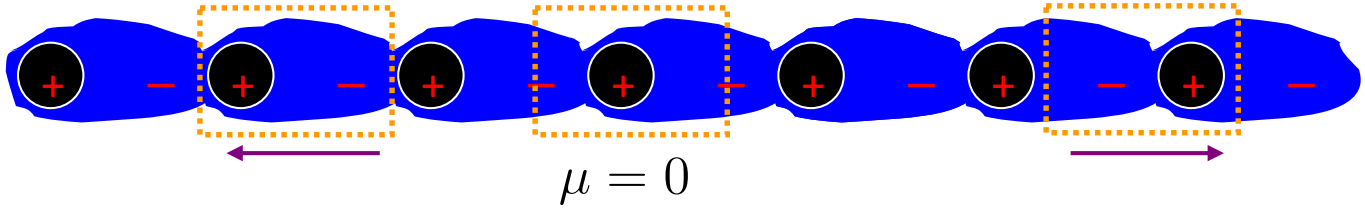
$n = 1, 2, 3, \ldots$



An opportunity: real-space dipole matrix elements

Bethe-Salpeter optical spectrum

velocity gauge $$\epsilon_2(\omega) = \frac{16\pi^2 e^2}{\omega^2} \sum_S \left|\mathbf{e}\cdot\langle 0|\mathbf{v}|S\rangle\right|^2 \delta\left(\omega - \Omega^S\right)$$



$$\mu = 0$$

Plane waves (inherently periodic) need the auxiliary shifted grid (WFNq_fi).

length gauge $$\langle v\mathbf{k}\,|\mathbf{r}|\,c\mathbf{k}\rangle = \lim_{\mathbf{q}\to 0} \frac{\langle v\mathbf{k}+\mathbf{q}\,|e^{i\mathbf{q}\cdot\mathbf{r}}-1|\,c\mathbf{k}\rangle}{iq}$$

$$= -i \lim_{\mathbf{q}\to 0} \frac{\langle v\mathbf{k}+\mathbf{q}\,|e^{i\mathbf{q}\cdot\mathbf{r}}|\,c\mathbf{k}\rangle}{q}$$

In finite direction, Octopus can calculate directly. Only one grid.
Simpler, less computation, no concern of finite differences or consistent phases

In principle, can use *k.p* perturbation theory for derivatives in periodic directions.

The tutorial

Three examples:

(1) benzene molecule, with Octopus

(2) silicon, with plane wave code Quantum ESPRESSO
(can be done in Octopus too in principle)

(3) LiCl exciton visualization