BERKELEYGW: OVERVIEW & PRACTICAL ISSUES

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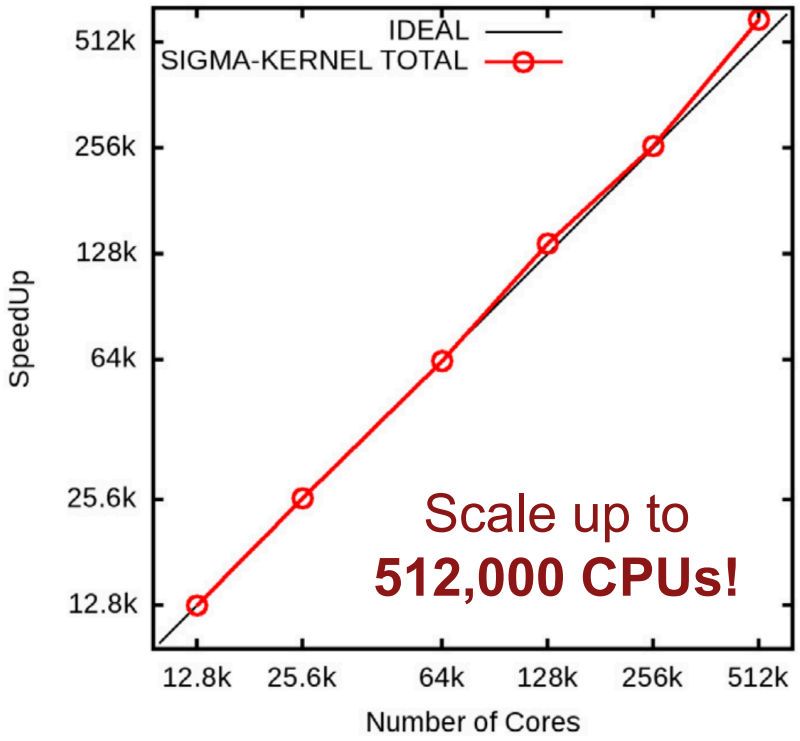
Why BerkeleyGW?

Our SW engineer:
M. Del Ben, LBL

- **Versatile**: supports **3D**, **2D**, **1D** and molecular systems, with **Coulomb truncation** and **efficient k-point sampling** algorithms.
- **Agnostic**: supports a **large set of mean-field codes**: Quantum ESPRESSO, ABINIT, PARATEC, Octopus, PARSEC, SIESTA, JDFTx, RMGDFT, EPM.
- **General**: support for **semiconductor**, **metallic** and **semi-metallic** systems.
- **Massively parallel**: scales to **512,000 CPU cores**, supports distributed memory and hybrid architectures. High-performance GPU support to be released. Can handle large systems containing **thousands of atoms**.
- **Free & open source.**

Del Ben, Jornada, Deslippe, Louie,
CPC 235, 187 (2018).



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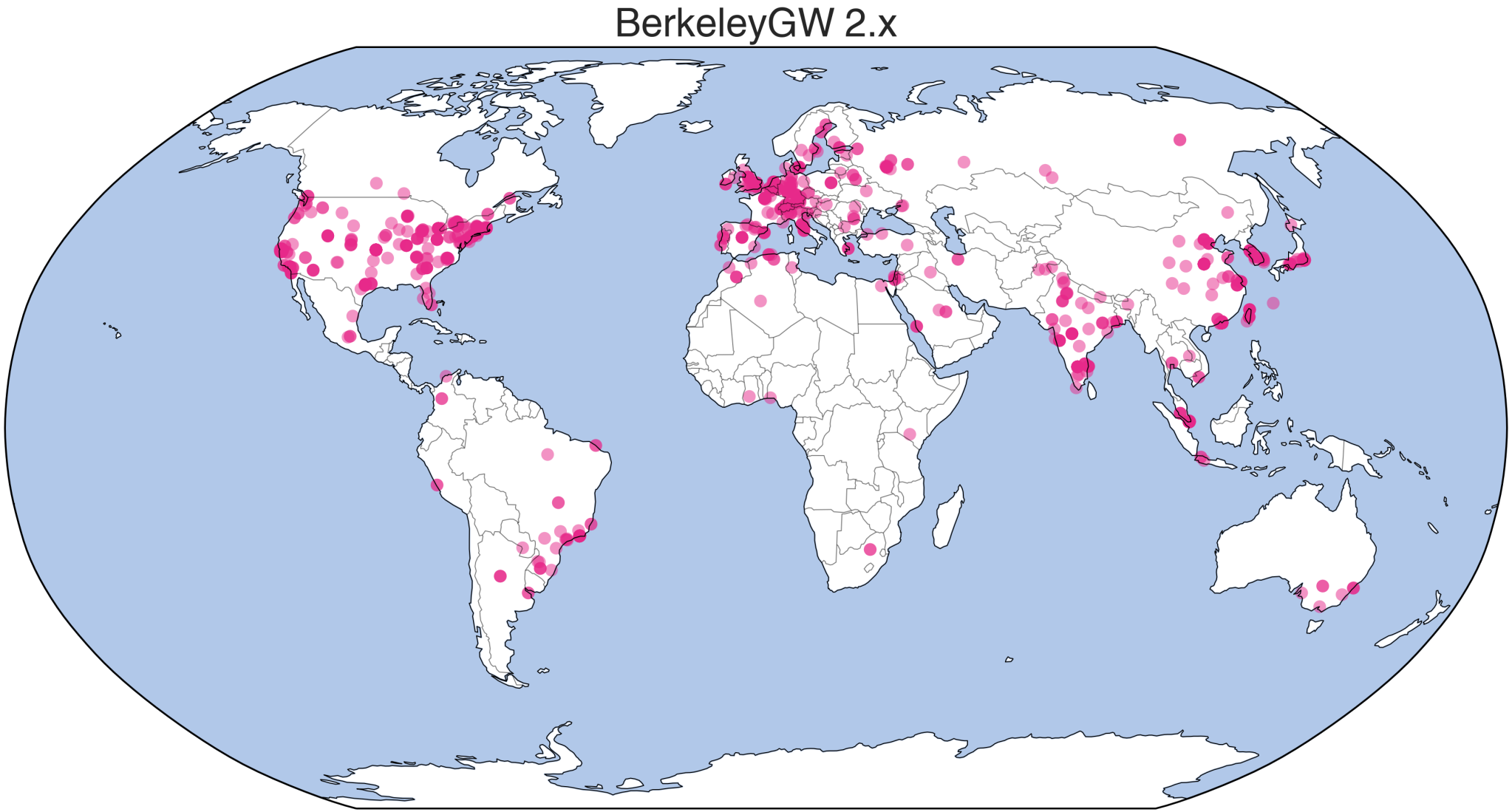
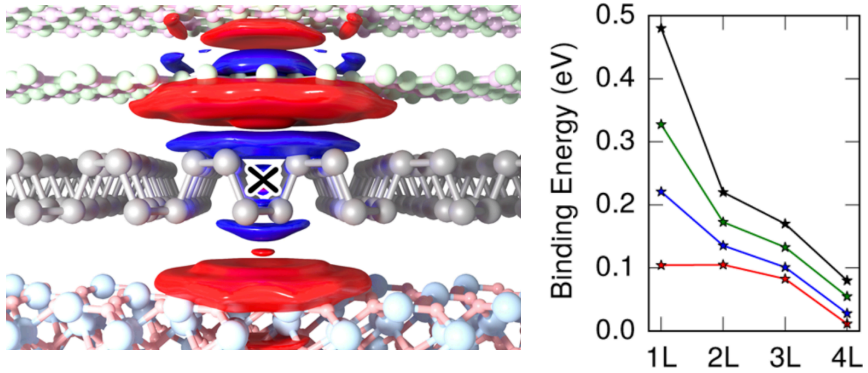
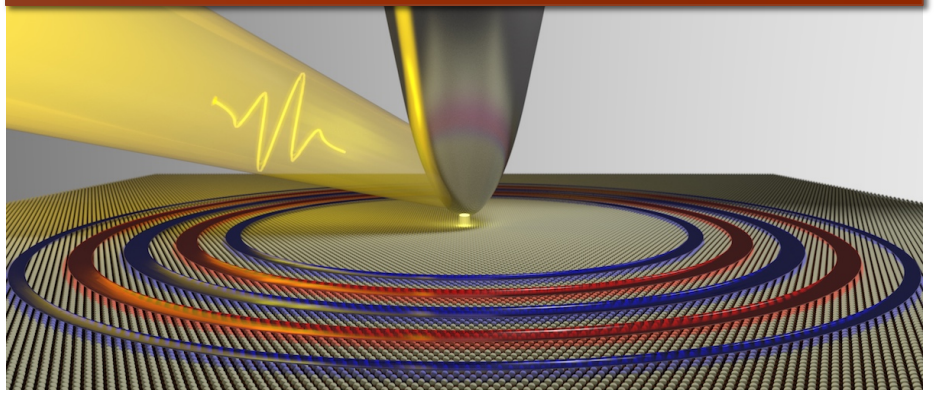


Substrate renormalization of the self-energy and excitonic effects



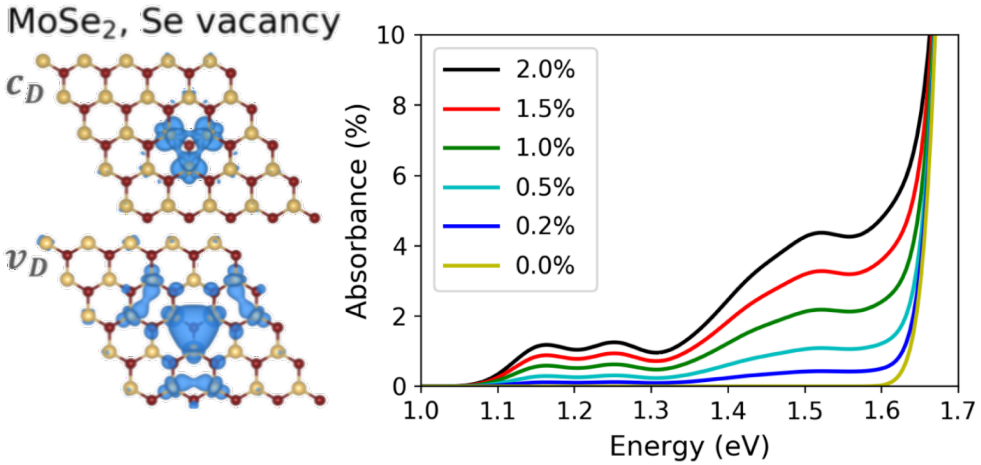
Qiu, Jornada, Louie, Nano Lett., 17, 4706 (2017).

Long-lived dispersionless plasmons in quasi-2D metals



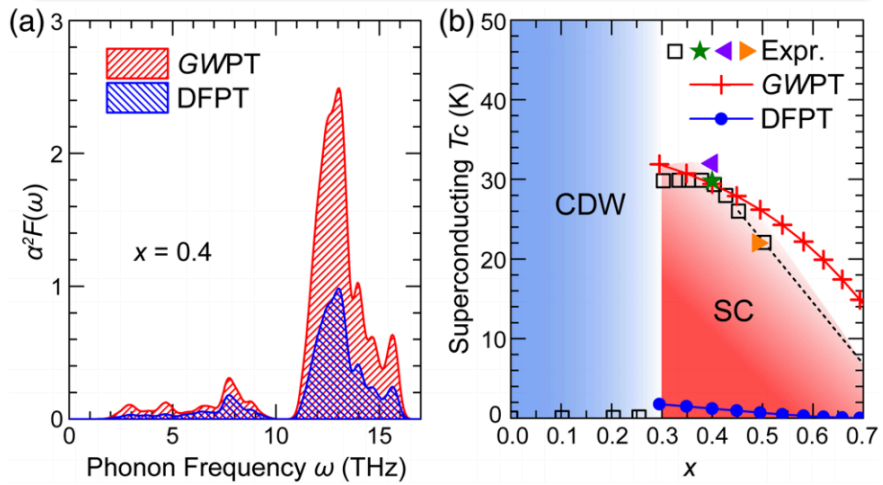
Jornada, Xian, Rubio, Louie, Nat. Comm 11, 1013 (2020).

Defects in monolayer TMDs



Refaely-Abramson, Qiu, Louie, Neaton, PRL 121, 167402 (2018)

Correlation-enhanced e-ph superconductivity in $Ba_{1-x}K_xBiO_3$



Li, Antonius, Wu, Jornada, Louie, PRL 122, 186402 (2019).

BerkeleyGW philosophy

- What we strive for:
  - Code correctness
  - Supporting a diversity of mean-field codes (Quantum ESPRESSO, Abinit, Paratec, JDFTx, RMGDFT, PARSETC etc.)
  - Implementing scalable codes & algorithms
  - Supporting new physics / features

- What we do not focus on:
  - Black-box design

Outline

1. Introduction
2. K-point vs. Q-point grids
3. Screening models for $\varepsilon(\mathbf{q})$
4. Frequency dependence of $\varepsilon(\omega)$
5. Symmetry and degeneracy
6. Solving Dyson's equation
7. Real and complex versions

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1. Introduction: GW calculations – Theory

Electronic self-energy Σ within the GW approximation: 2

$$\Sigma(\mathbf{r},\mathbf{r}';t) \approx iG_0(\mathbf{r},\mathbf{r}';t)W_0(\mathbf{r},\mathbf{r}';t)$$

Screened Coulomb interaction W:

$$W^0_{\mathbf{GG}'}(\mathbf{q};\omega) \equiv \varepsilon^{-1}_{\mathbf{GG}'}(\mathbf{q};\omega)v(\mathbf{q}+\mathbf{G}')$$

Sum over wavevectors **q**!

RPA dielectric matrix: 1

$$\varepsilon_{\mathbf{GG}'}(\mathbf{q},\omega) = \delta_{\mathbf{GG}'} - v(\mathbf{q}+\mathbf{G})\chi^0_{\mathbf{GG}'}(\mathbf{q},\omega)$$

Noninteracting polarizability matrix:

$$\chi^0(\mathbf{r},\mathbf{r}';t) = G_0(\mathbf{r},\mathbf{r}';t)G_0(\mathbf{r}',\mathbf{r};-t)$$

Noninteracting Green's function (spectral representation) 0

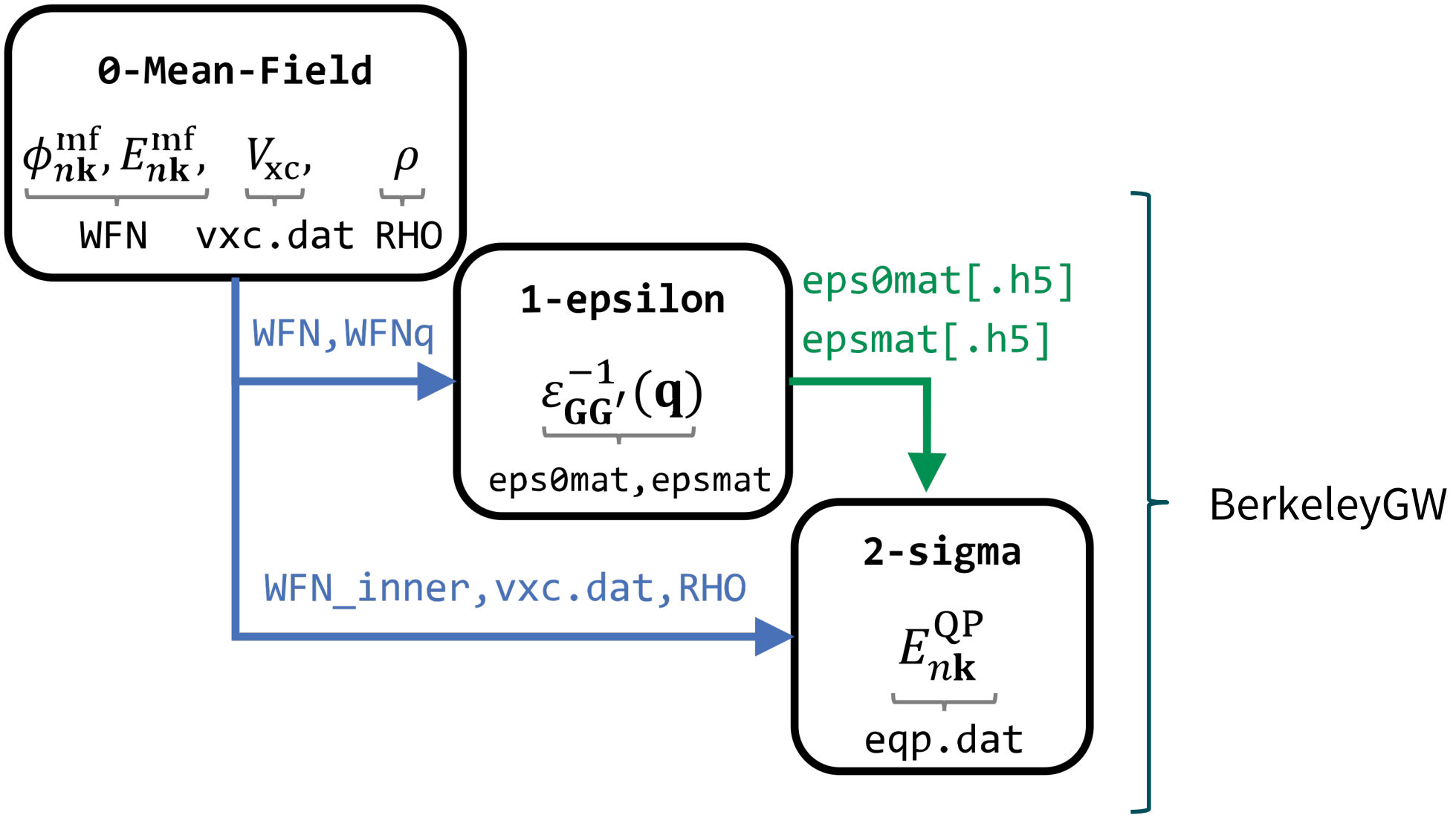
$$G_0(\mathbf{r},\mathbf{r}';\omega) = \sum_{n\mathbf{k}} \frac{\phi_{n\mathbf{k}}(\mathbf{r})\phi^*_{n\mathbf{k}}(\mathbf{r}')}{\omega - E^{\mathrm{mf}}_{n\mathbf{k}} \pm i\eta}$$

Sum over all occupied and unoccupied states *n*!

1. Introduction: GW calculations – Practice

DFT codes:

- Quantum Espresso
- Abinit
- Paratec
- Octopus
- Parsec
- RMGDFT
- JDFTx



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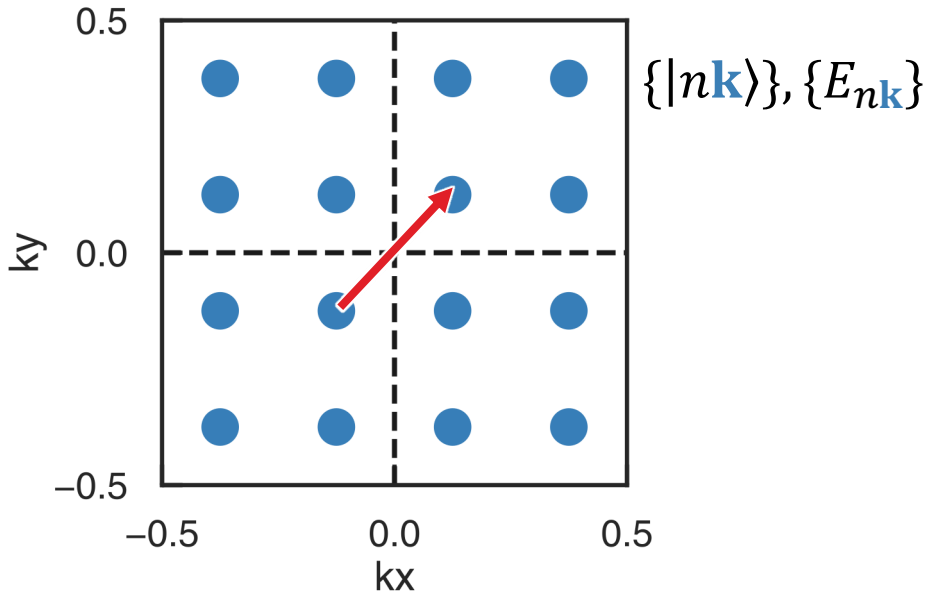
2. **k**-grids and **q**-grids

$$\chi^0_{\mathbf{GG}'}(\mathbf{q},\omega=0) \sim \sum_{v\,c\,\mathbf{k}} \frac{M^*_{v\mathbf{k}+\mathbf{q},c\mathbf{k}}(\mathbf{G})\, M_{v\mathbf{k}+\mathbf{q},c\mathbf{k}}(\mathbf{G}')}{E_{v\mathbf{k}+\mathbf{q}} - E_{c\mathbf{k}}}$$

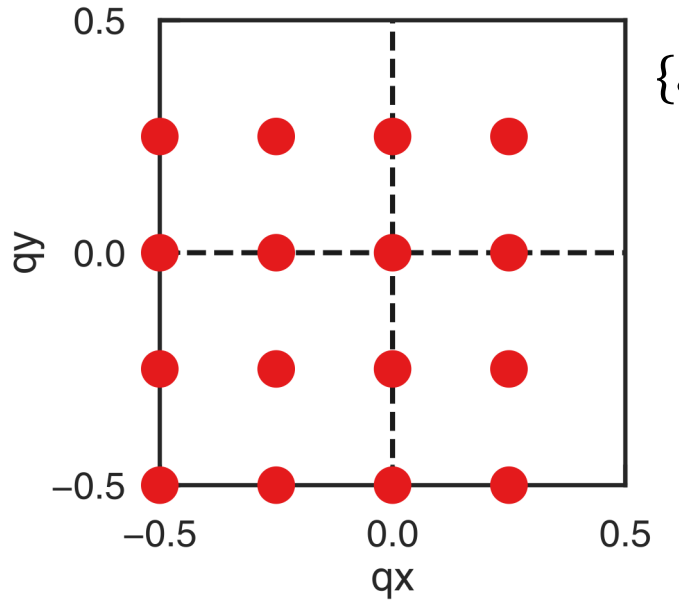
$$M_{v\mathbf{k}+\mathbf{q},c\mathbf{k}}(\mathbf{G}) \equiv \left\langle v\mathbf{k}+\mathbf{q}\middle| e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}\middle| c\mathbf{k}\right\rangle$$

- Mean-field quantities: computed in any regular **k**-point grid (does not need to be Γ centered)



$\{|n\mathbf{k}\rangle\}, \{E_{n\mathbf{k}}\}$

- Polarizability & dielectric matrices: computed in a regular, Γ-centered **q**-point grid, with $\mathbf{q} = \mathbf{k}' - \mathbf{k}$



$\{\varepsilon^{-1}(\mathbf{q})\}$

In practice: often use the **same Γ-centered grid** for both k and q points (esp. bulk systems)

2. **k**-grids and **q**-grids: **q**=0 point

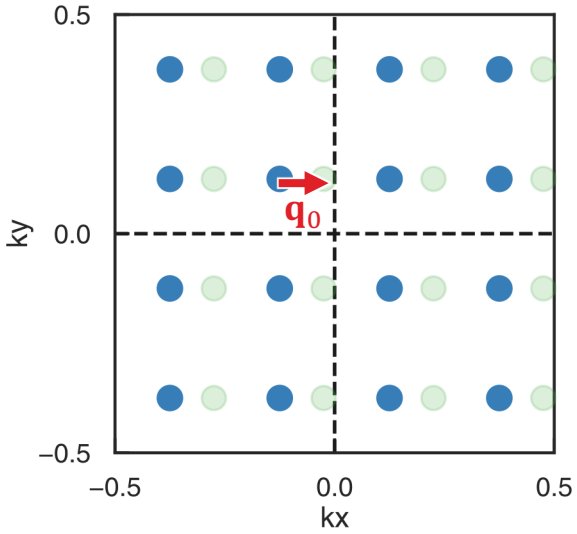
- Take $\mathbf{G} = \mathbf{G}' = 0$ and $\omega = 0$:

$$\varepsilon_{\mathbf{00}}(\mathbf{q}, 0) = 1 - \frac{4\pi e^2}{|\mathbf{q}|^2} \chi^0_{\mathbf{00}}(\mathbf{q}, 0)$$

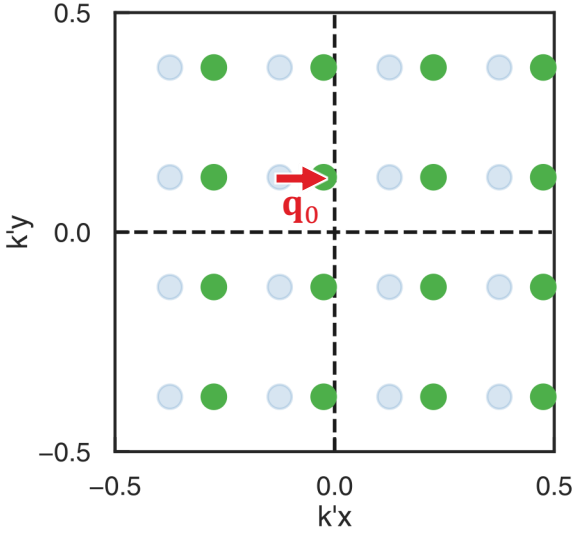
- Cannot directly compute $\varepsilon(\mathbf{q} = \mathbf{0})$!
- For gapped systems:
  - Compute $\varepsilon(\mathbf{q_0})$ at a small but finite $\mathbf{q_0} \sim 0.001$.
  - Use two sets of **k**-point grids and wave functions for valence/conduction states.

- **WFN**: provides **conduction states** for $\varepsilon(\mathbf{q} = \mathbf{q_0})$ + **all states** for $\mathbf{q} \neq \mathbf{q_0}$.
- **WFNq**: provides **valence states** for $\varepsilon(\mathbf{q} = \mathbf{q_0})$.

k-point grid (**WFN**)

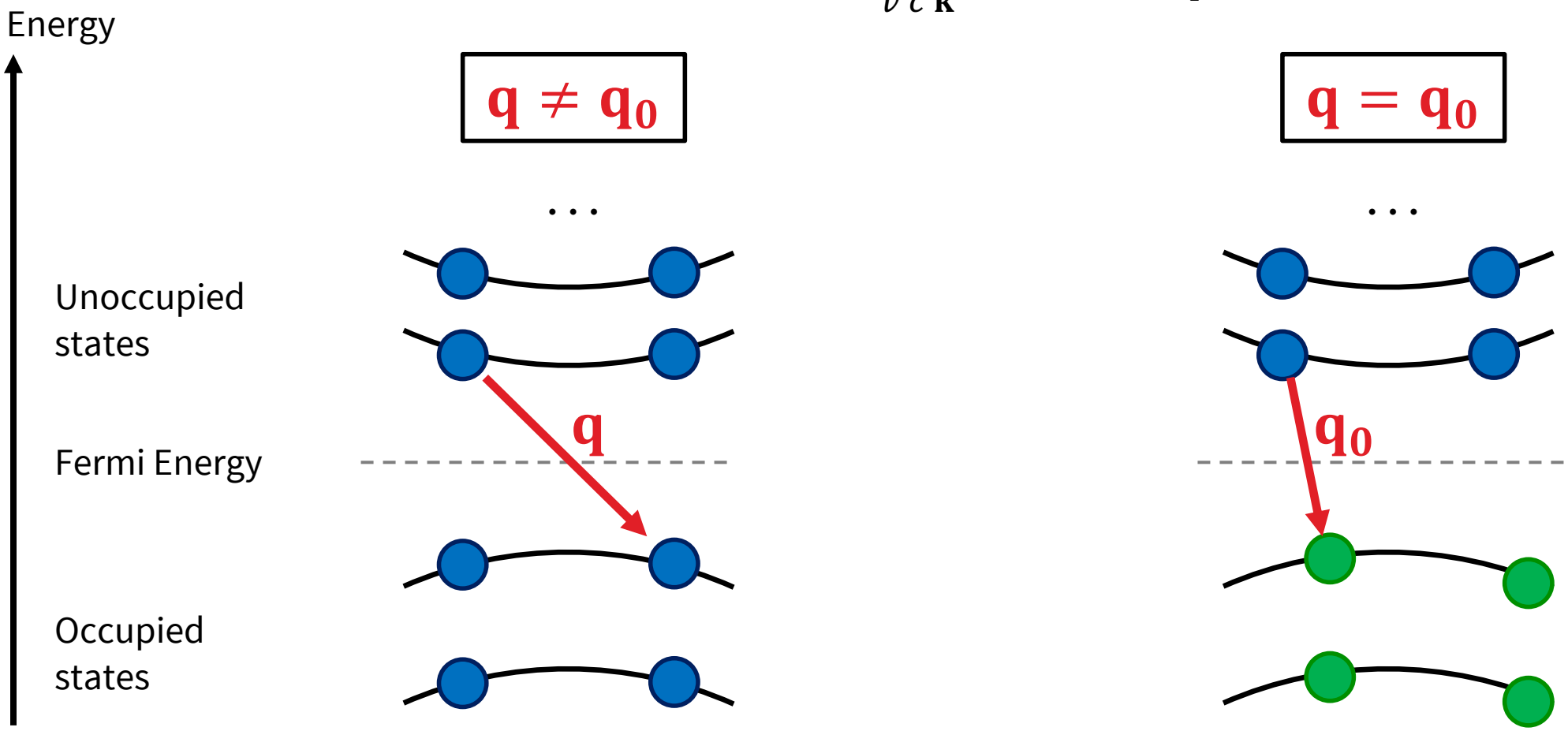


$\mathbf{q_0}$-shifted $\mathbf{k}'$-point grid (**WFNq**)



2. **k**-grids and **q**-grids

$$\chi^0_{\mathbf{GG'}}(\mathbf{q}, \omega = 0) \sim \sum_{v\, c\, \mathbf{k}} \frac{M^*_{v\mathbf{k+q},c\mathbf{k}}(\mathbf{G})\, M_{v\mathbf{k+q},c\mathbf{k}}(\mathbf{G'})}{E_{v\mathbf{k+q}} - E_{c\mathbf{k}}}$$



Files:

- WFN
- WFNq

2. Specification of **q**-points in epsilon.inp

- Semiconductors (**epsilon.inp**)

```
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.h5: $\epsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q}_0)$

epsmat.h5: $\epsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q} \neq \mathbf{q}_0)$

- Metals
  - Screening depends critically on sampling DOS at Fermi surface for intraband transitions. **Cannot use shifted grid**! See manual / 2019 BerkeleyGW Workshop

- Sigma, Kernel, Absorption use **q**-grid defined by eps0mat.h5 / epsmat.h5

2. Example **k**-grid construction: 4 × 4 grid for graphene

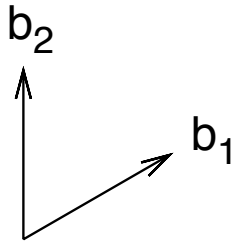
How to construct k-point grid (**WFN**) and q-shifted k-point grids (**WFNq**)?

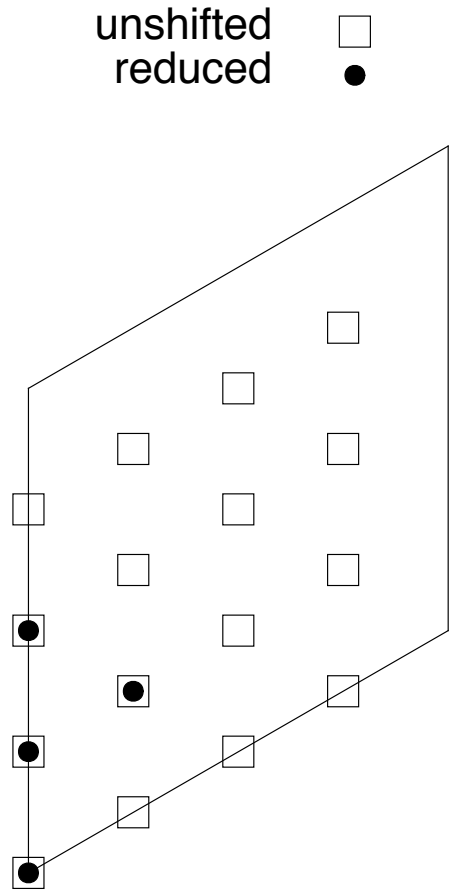
➢ **`kgrid.x`** utility!

Example on the right:

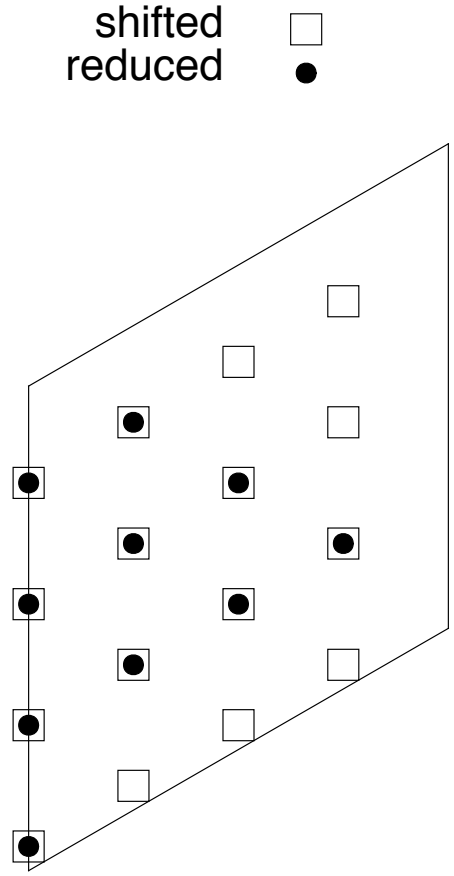
- Graphene
- 4x4x1 Monkhorst-Pack grid
- $\mathbf{q}_0$= (0.0,0.05,0.0)

$\mathbf{q}_0$ shift breaks symmetry and gives more points.





Main grid (**WFN**)
16 in full BZ
Reduced to 4



Shifted grid (**WFNq**)
16 in full BZ
Reduced to 10

2. **k**-, **q**-grids and bands

For reference: simplified approach for tutorial

	k-grid	# bands	Comments
SCF	uniform, no shift	occupied	
WFN	uniform, no shift	many	
WFNq	WFN + **q**-shift	occupied	
epsilon.inp **q**-points	WFN but $\mathbf{q}_0$ instead of 0	many	bands to sum over
WFN_inner	WFN	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

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3. Divergent behavior of $W_{\mathbf{G},\mathbf{G}'}$ for $\mathbf{q} = 0$

Head: $\mathbf{G} = 0, \mathbf{G}' = 0$
Wing: $\mathbf{G} = 0, \mathbf{G}' \neq 0$
Wing′: $\mathbf{G} \neq 0, \mathbf{G}' = 0$
Body: $\mathbf{G} \neq 0, \mathbf{G}' \neq 0$

v(**q**) DOS inter/intra-band transitions

$$\varepsilon_{\mathbf{GG}'}(\mathbf{q}, \omega = 0) \sim \frac{1}{|\mathbf{q}+\mathbf{G}|^2} \sum_{v\,c\,\mathbf{k}} \frac{M^*_{v\mathbf{k}+\mathbf{q},c\mathbf{k}}(\mathbf{G})\, M_{v\mathbf{k}+\mathbf{q},c\mathbf{k}}(\mathbf{G}')}{E_{v\mathbf{k}+\mathbf{q}} - E_{c\mathbf{k}}}$$

gap

$$W_{\mathbf{G},\mathbf{G}'}(\mathbf{q};\omega) = \varepsilon^{-1}_{\mathbf{GG}'}(\mathbf{q};\omega)\, v(\mathbf{q}+\mathbf{G})$$

$W_{\mathbf{G},\mathbf{G}'}(\mathbf{q};0)$ for $\mathbf{q} \to 0$:

- Diverges for semiconductors
- Is finite for metals

Note: integral of $W_{\mathbf{G},\mathbf{G}'}(\mathbf{q})$ over $\mathbf{q}$ is finite

q^2/q^2

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

See BerkeleyGW paper: arXiv:1111.4429.

3. Solution: screening models

Use calculation of $\varepsilon(\mathbf{q}_0 \sim 0.001)$ along the periodic direction to **parametrize screening model** for **q** ≈ 0.

📌 The calculation is still *ab initio*! The screening model is just a "hint" the the user give to BerkeleyGW to improve w.r.t. k-point sampling!

Input file `epsilon.inp`:

```
screening_semiconductor
#screening_graphene
#screening_metal
```

See BerkeleyGW paper arXiv:1111.4429 and manual.

Sigma: Use model to perform Monte Carlo integration $\int d^3\mathrm{q}\, M(\mathbf{q}) W_{\mathbf{G},\mathbf{G}'}(\mathbf{q})$ over region around **q** = 0

Absorption: interpolate kernel

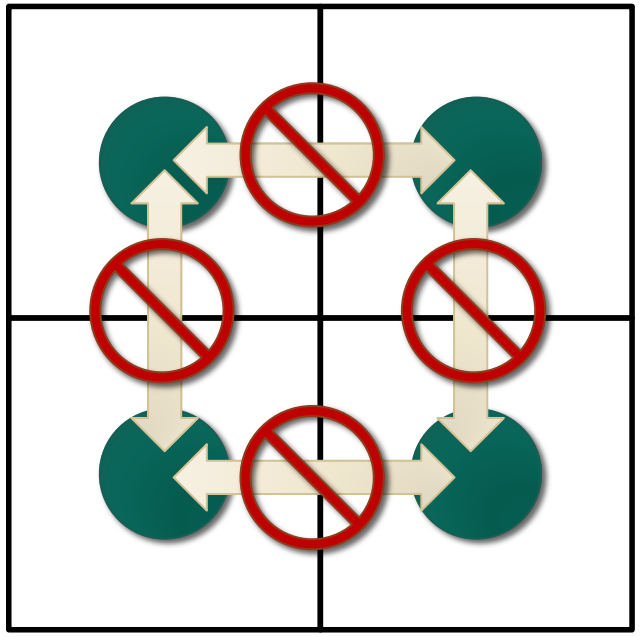
$$\langle vc\mathbf{k}\,|K|\,v'c'\mathbf{k}'\rangle = \underbrace{\frac{a_{vc\mathbf{k}v'c'\mathbf{k}'}}{A(\mathbf{q})}}_{\text{head}} + \underbrace{\frac{b_{vc\mathbf{k}v'c'\mathbf{k}'}}{B(\mathbf{q})}}_{\text{wing, wing'}} + \underbrace{\frac{c_{vc\mathbf{k}v'c'\mathbf{k}'}}{C(\mathbf{q})}}_{\text{body}}$$

Note: anisotropic materials need to use direction such that $\epsilon^{-1}(\mathbf{q}_0) = \langle \epsilon^{-1}(\mathbf{q}) \rangle$

3. Coulomb truncation: different screening models

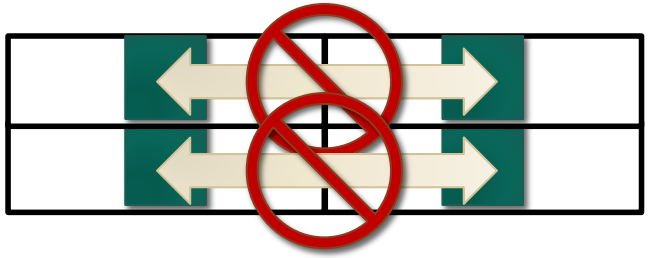
$$v_{\mathrm{t}} = \frac{\Theta\left(f\left(\mathbf{r}\right)\right)}{r}$$

0D (e.g.: molecule)
fully confined

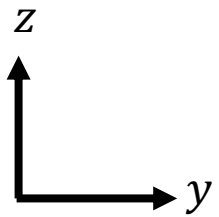


cell_box_truncation

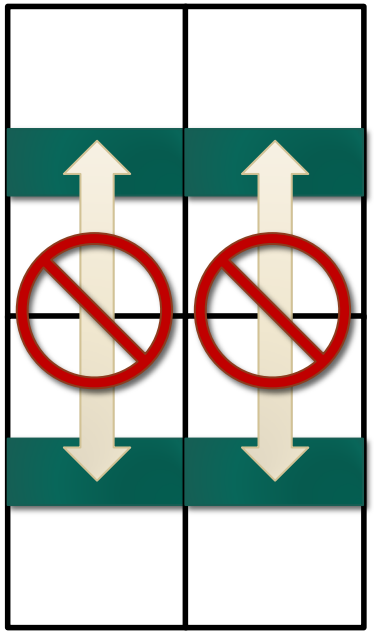
1D (e.g.: nanotube)
periodic along z



cell_wire_truncation



2D (e.g.: graphene)
periodic along x,y



cell_slab_truncation

See BerkeleyGW paper arXiv:1111.4429 and manual.

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4. Frequency dependence of ε(ω)

Computationally expensive part of the calculation: correlation contribution to Σ:

$$\Sigma^{\mathrm{Cor}}(\mathbf{r},\mathbf{r}';\omega) = -\frac{1}{\pi}\sum_n \psi_n(\mathbf{x})\psi_n^*(\mathbf{x}') \int_0^\infty \mathrm{d}\omega'\, W_{\mathrm{aH}}(\mathbf{x},\mathbf{x}';\omega') \times \frac{1}{\omega - \epsilon_n - (\omega' - i\eta)\,\mathrm{sgn}(\epsilon_n - \epsilon_{\mathrm{F}})}$$

$W_{\mathrm{aH}} \sim \varepsilon^{-1}(\omega')v$

- Computationally expensive: need $\varepsilon(\omega)$ for all frequencies
- Extra convergence parameters

Simplification: plasmon-pole model (PPM)

- Compute $\varepsilon(\omega = 0)$, use physical models & constraints to obtain $\varepsilon(\omega \neq 0)$: charge density **RHO**.
- PPM is the default option (and a good idea for a first calculation).

"**full-frequency**" vs. "**plasmon-pole**"

Input file `epsilon.inp`:

```
#frequency_dependence 0
```

See BerkeleyGW paper arXiv:1111.4429 and manual.

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5. Degeneracy check utility

- Choice of bands can break symmetry of degenerate states and lead to arbitrary results:

  ERROR: Selected number of bands breaks degenerate subspace.

- Use **degeneracy_check.x** utility to find number of bands that does not break degeneracies.

```
$ 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, could use **number_bands 32** in Epsilon.

- Can also turn off degeneracy enforcement (**degeneracy_check_override** flag).
  - Ok if include many unoccupied bands (error from breaking deg. subspace vanishes)

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6. 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

📌 Note: for full frequency calculations, **`eqp1`** reports the full numerical solution of Dyson's equation.

6. Mean-field exchange-correlation functional

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

If we start from KS DFT, $\Sigma - \Sigma^{\mathrm{MF}} = \Sigma^{GW} - V_{XC}$

BerkeleyGW accepts two forms of V_{XC} :

- **VXC**: Binary file containing the operator in G space: $V_{XC}(\mathbf{r}) \rightarrow V_{XC}(\mathbf{G})$
  - BerkeleyGW can compute arbitrary matrix elements given the operator.

- **`vxc.dat`**: ASCII file containing the matrix elements in a KS orbitals: $\langle n\mathbf{k}|V_{XC}|n'\mathbf{k}\rangle$.
  - DFT code must compute all matrix elements for the relevant states.

📌 BerkeleyGW also natively supports some hybrid functionals even if the DFT wrapper cannot write $\langle n\mathbf{k}|\Sigma_x|n'\mathbf{k}\rangle$. See flag **`bare_exchange_fraction`** for the `Sigma` code.

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7. Real or complex flavor?

e.g. `epsilon.real.x, epsilon.cplx.x`

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

Real: only with inversion symmetry about the origin **and** time-reversal symmetry

$$u(-\mathbf{r}) = au(\mathbf{r})$$
$$u^*(\mathbf{r}) = bu(\mathbf{r})$$

a, b each equal to ± 1

Plane-wave expansion:

$$u(\mathbf{r}) = \sum_{\mathbf{G}} u_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} \longrightarrow u_{\mathbf{G}} = cu^*_{\mathbf{G}}$$

➢ Can choose $c = 1$ for real coefficients

Same for density and V_{xc}, except no need for time-reversal $\rho(\mathbf{r}) = \rho^*(\mathbf{r})$

- What breaks time-reversal? Fractional translations, 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.

Questions?

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7. Real and complex versions

Homework: try installing code on your own cluster!

Extra slides: discussion of half-shifted grids, calculations for metals

k-, **q**-grids and bands

recommended approach (using half-shifted grids)

	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

5. Choice of bands can break symmetry in GW/BSE

Symmetry operations are only defined for non-degenerate states!

Example:

- 2D system with mirror symmetry $\hat{\sigma}_x$ about the x=0 plane.
- Consider two degenerate KS states of $|p_x\rangle$ and $|p_y\rangle$ characters:
  - $\hat{\sigma}_x|p_x\rangle = -|p_x\rangle$
  - $\hat{\sigma}_x|p_y\rangle = |p_y\rangle$
- If $|p_x\rangle$ and $|p_y\rangle$ degenerate, the DFT code generates arbitrary linear combination, e.g. $|p_x\rangle \pm i|p_y\rangle$, which are not an eigenstate of $\hat{\sigma}_x$.

➢ Including only some of a degenerate space will break symmetry.

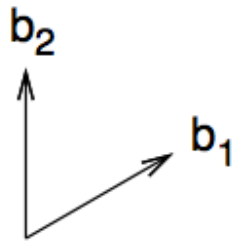
➢ Results depends on arbitrary linear combinations in mean-field. Not reproducible!

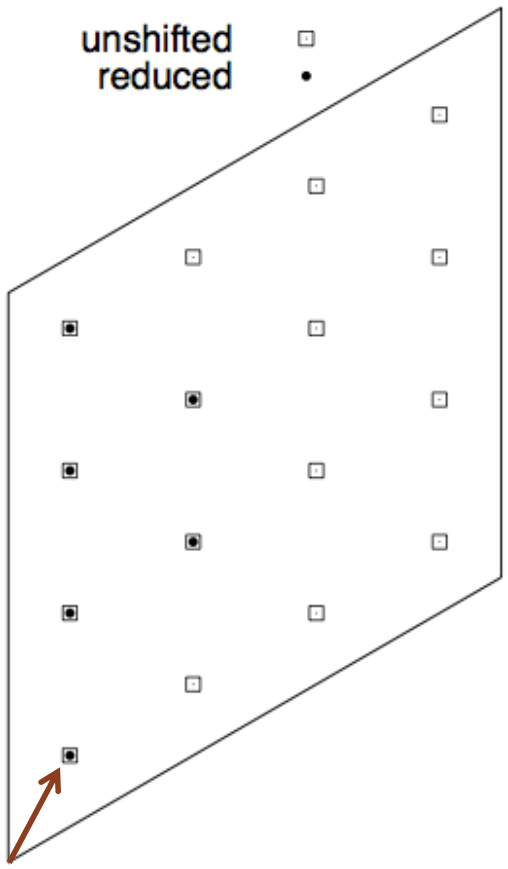
k-grid construction: 4 × 4 shifted grid for graphene

(0.5, 0.5) Monkhorst-Pack shift

`kgrid.x`

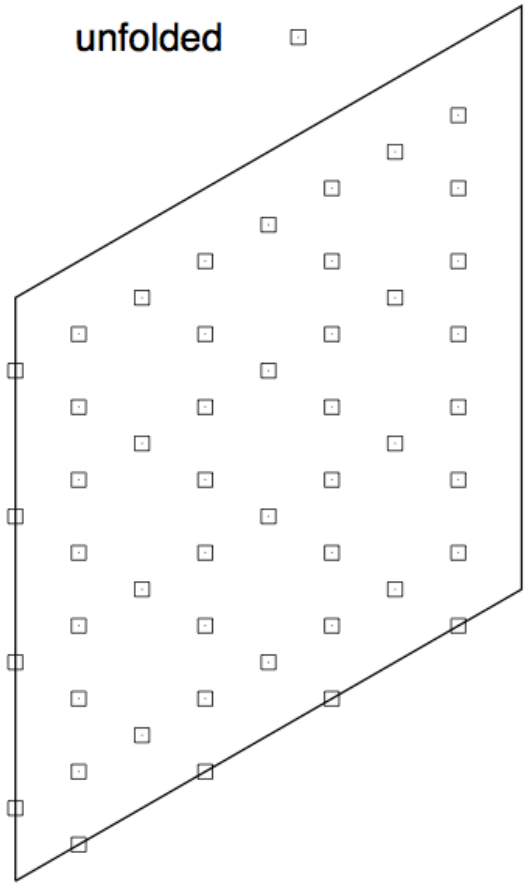
Uniform -> unfold -> shift with **q** -> reduce





(0.5, 0.5)

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



0.05)

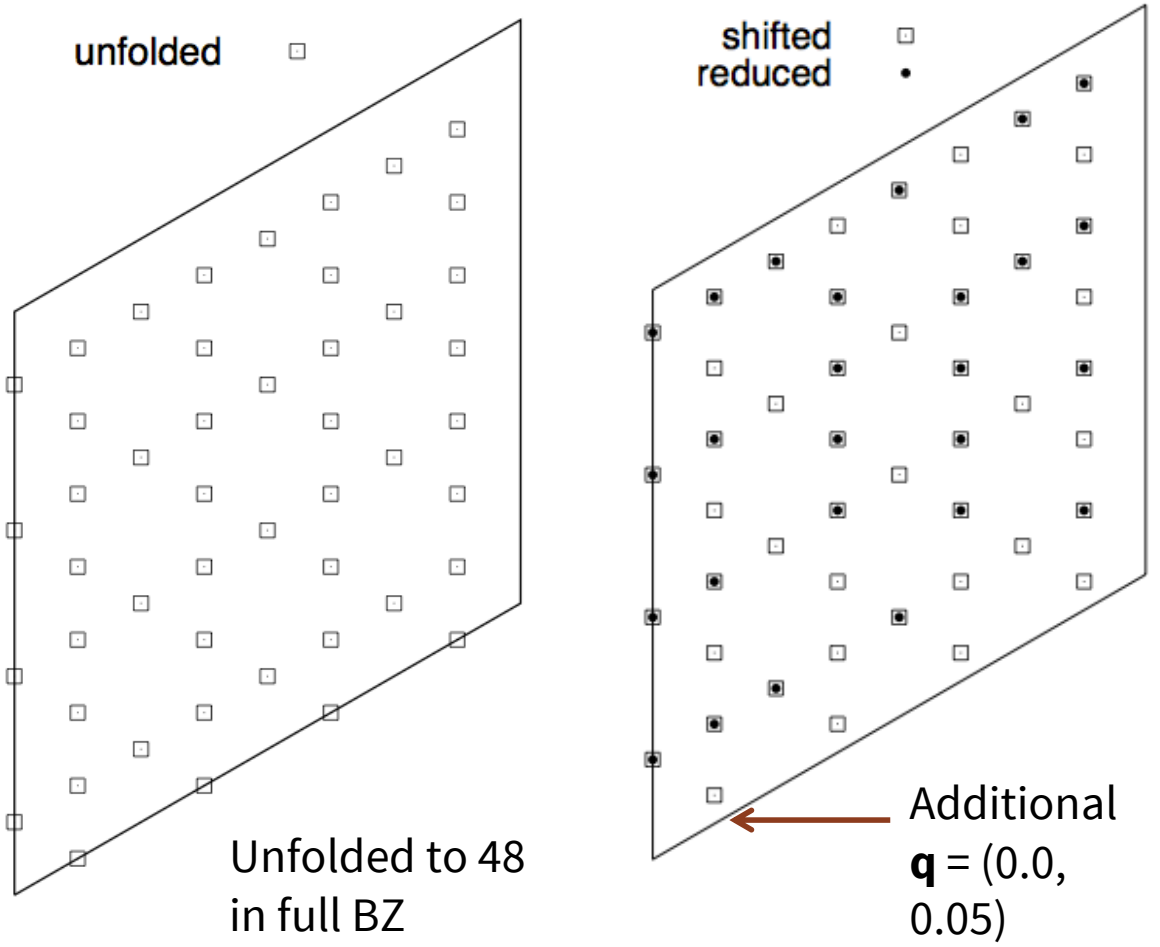
Unfolded to 48
in full BZ

Unfolding gives more points!

k-grid construction: 4 × 4 shifted grid for graphene

`kgrid.x`

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



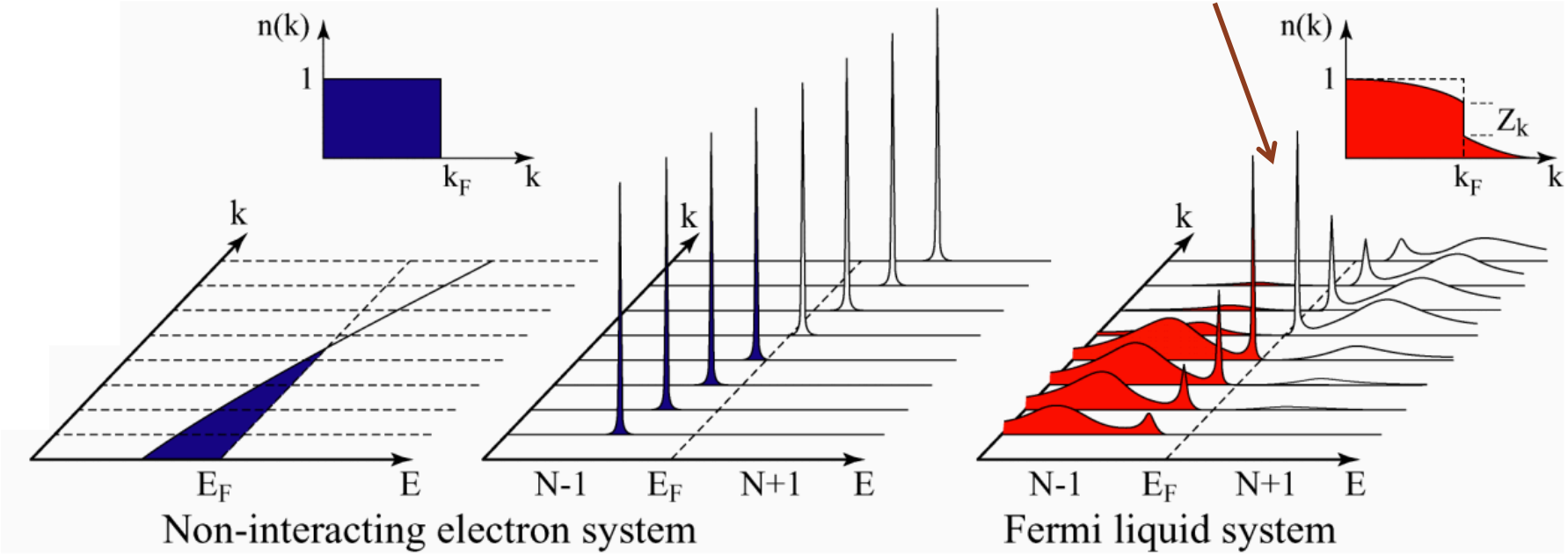
Unfolding and breaking symmetry gives more points!

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)

Special treatment for metals

Coefficients depend critically on sampling DOS at Fermi surface for intraband transitions.

Two separate runs of Epsilon

eps0mat: $\epsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q}_0)$

WFN = WFNq
only a small number of bands for intra-band transitions around Fermi surface
very fine: grid spacing is $\mathbf{q}_0$ *e.g.* grid = 32 × 32 × 32 unshifted, $\mathbf{q}_0$ = (0, 0, 1/32)

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

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

WFN = WFNq. unshifted, many bands, ordinary fineness. *e.g.* grid = 12 × 12 × 12.

epsilon.inp for metals

```
begin qpoints
  0.000000000  0.000000000  0.031250000 1.0 2
end
```

eps0mat:

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

```
begin qpoints
  0.000000000  0.000000000  0.083333333 1.0 0
  0.000000000  0.000000000  0.166666667 1.0 0
  0.000000000  0.000000000  0.250000000 1.0 0
…
end
```

epsmat:

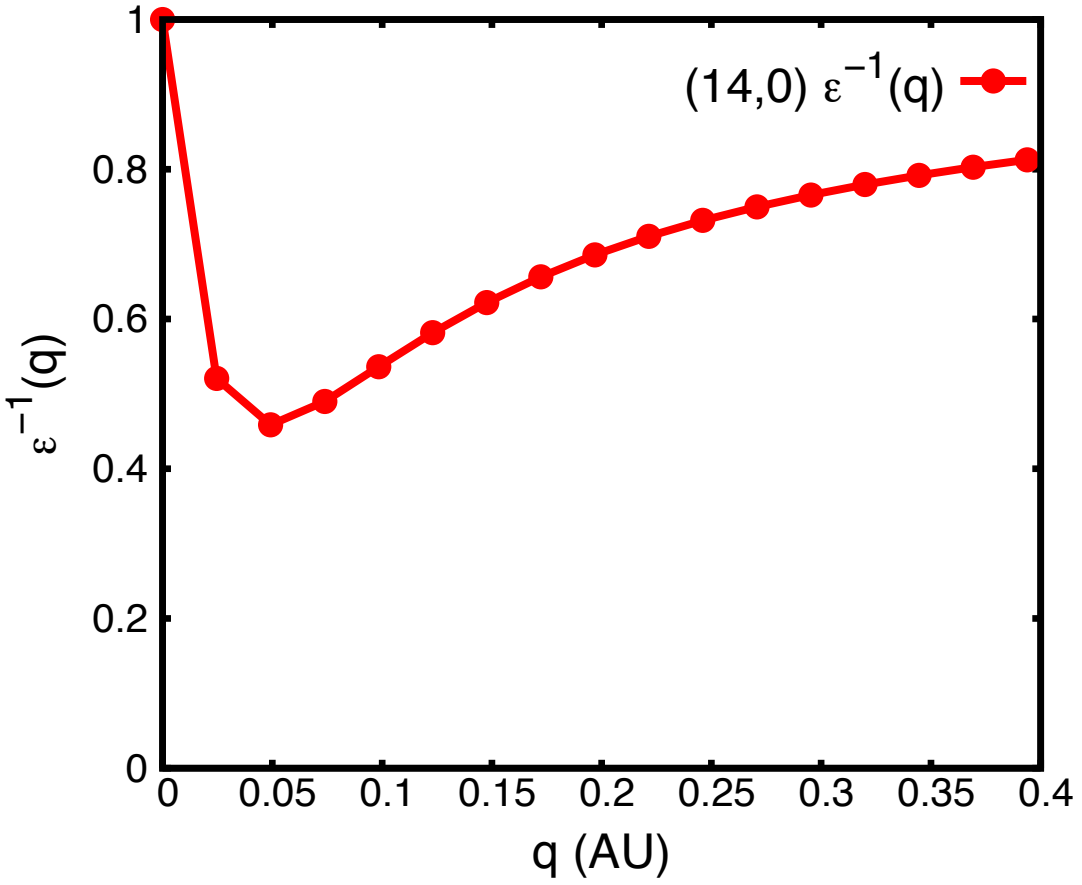
$\epsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q} \neq \mathbf{q}_0)$

Problem 1: Non-smooth behavior around q = 0

(14, 0) carbon nanotube wire truncation

Systems with reduced dimensionality are harder to converge!

Not covered in this tutorial
See example 4 from 2019 BerkeleyGW Workshop



See BerkeleyGW paper: arXiv:1111.4429