# Electrostatic screening in 2D semiconductors: an efficient atomistic implementation

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POLIMA weekly seminar

# Where have I been?

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# Outline

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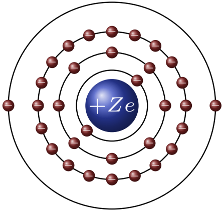
# Screening...

**...in an atom.**

(Bare) Coulomb potential $v_c = \frac{Ze^2}{r}$



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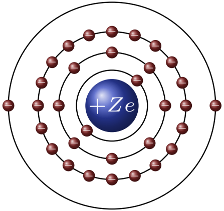


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$$W < v_c$$

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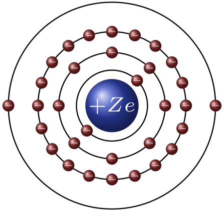


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Phys. Rev. 36, 57, J.C. Slater

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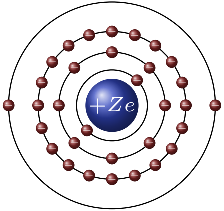


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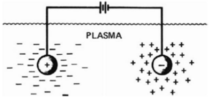
**...in a plasma.**

$\phi(r) \propto e^{-\lambda_D r}/r\,, \lambda_D^2 = \varepsilon_r \varepsilon_0 k_B T / nq^2$




"Intro. to Plasma Physics and Controlled Fusion", F.F. Chen

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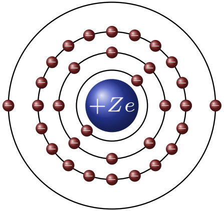


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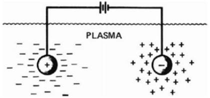


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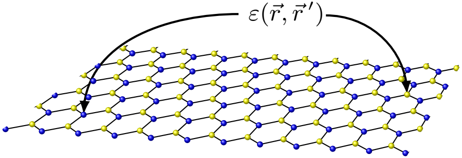
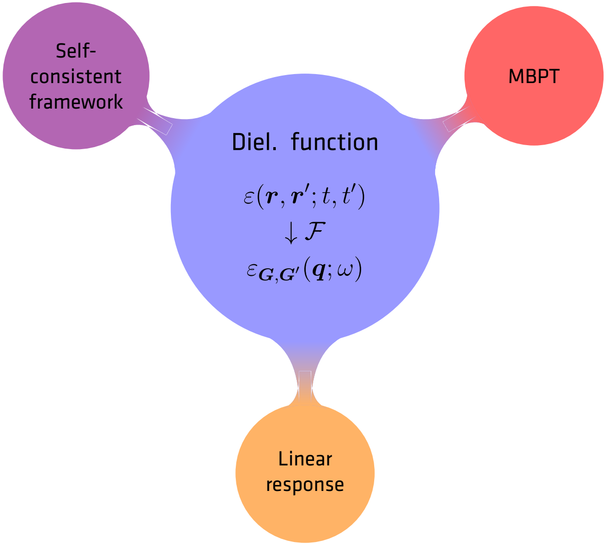
## ...in a crystal.



# Outline

# The dielectric function: technical contexts



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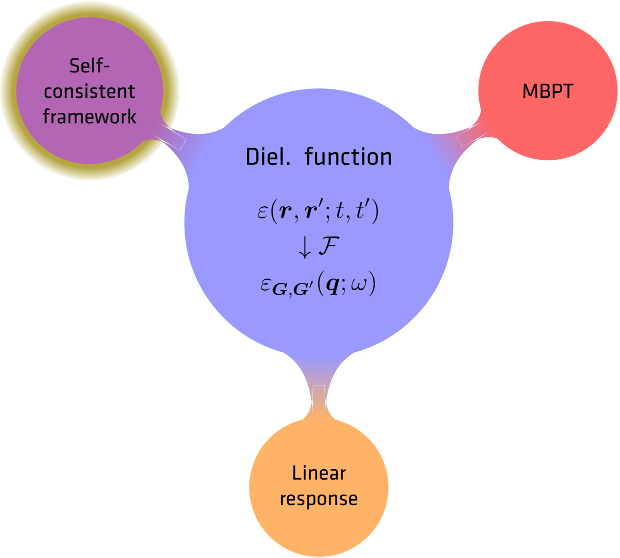

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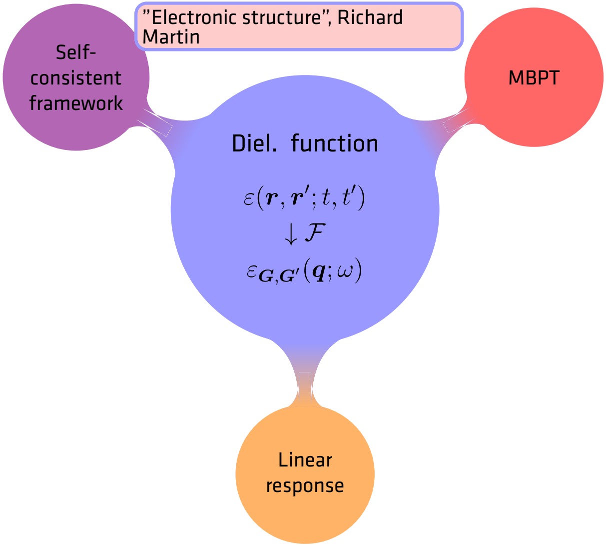

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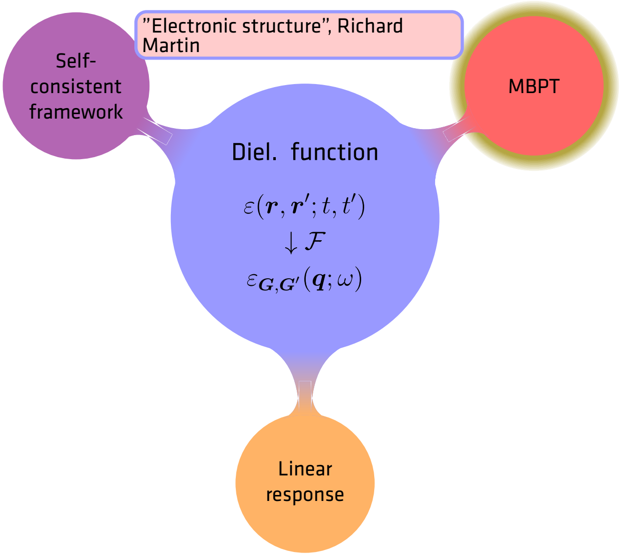

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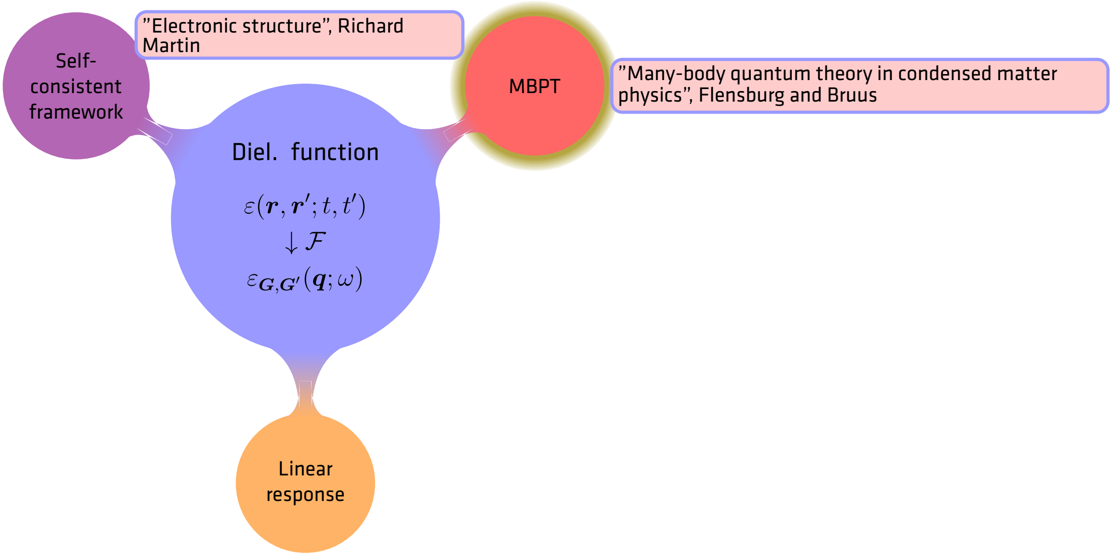

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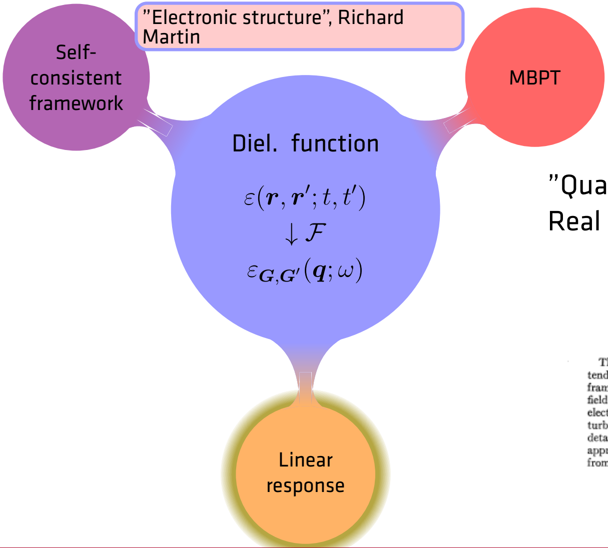
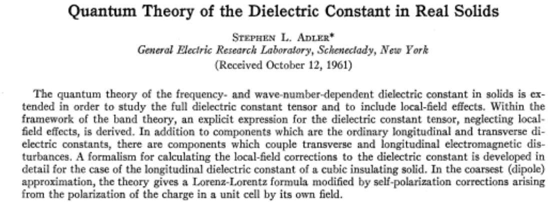



"Many-body quantum theory in condensed matter physics", Flensburg and Bruus

"Quantum Theory of the Dielectric Constant in Real Solids", S.L. Adler, Phys. Rev. 126, 1962



**Quantum Theory of the Dielectric Constant in Real Solids**

STEPHEN L. ADLER*
*General Electric Research Laboratory, Schenectady, New York*
(Received October 12, 1961)

The quantum theory of the frequency- and wave-number-dependent dielectric constant in solids is extended in order to study the full dielectric constant tensor and to include local-field effects. Within the framework of the band theory, an explicit expression for the dielectric constant tensor, neglecting local-field effects, is derived. In addition to components which are the ordinary longitudinal and transverse dielectric constants, there are components which couple transverse and longitudinal electromagnetic disturbances. A formalism for calculating the local-field corrections to the dielectric constant is developed in detail for the case of the longitudinal dielectric constant of a cubic insulating solid. In the coarsest (dipole) approximation, the theory gives a Lorentz-Lorentz formula modified by self-polarization corrections arising from the polarization of the charge in a unit cell by its own field.

# The dielectric function: technical contexts

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Self-consistent framework

"Electronic structure", Richard Martin

MBPT

"Many-body quantum theory in condensed matter physics", Flensburg and Bruus

Diel. function

$$\varepsilon(\boldsymbol{r},\boldsymbol{r}';t,t')$$
$$\downarrow \mathcal{F}$$
$$\varepsilon_{\boldsymbol{G},\boldsymbol{G}'}(\boldsymbol{q};\omega)$$

Linear response

"Many-Particle Physics", Gerald Mahan

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# The dielectric function: full and non-interacting

"Interacting Electrons: Theory and Computational Approaches", Richard Martin et. al, 2016

$$\varepsilon^{-1}(\boldsymbol{r},\boldsymbol{r}';t,t') = \delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t') + \int \mathrm{d}\boldsymbol{r}'' \int_{-\infty}^{t} \mathrm{d}t'' \chi(\boldsymbol{r},\boldsymbol{r}';t-t'') v_c(\boldsymbol{r}-\boldsymbol{r}')$$

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Hedin's equations: ($(1,2) \equiv (\boldsymbol{r}_1, t_1; \boldsymbol{r}_2, t_2)$, f.egs.)

$$W(1,2) = v_c(1,2) + \int \mathrm{d}3\mathrm{d}4 v_c(1,3)P(3,4)W(4,2) \text{ (Dyson's eq.)}$$

$$P(1,2) = -i\int \mathrm{d}3\mathrm{d}4\, G(1,3)G(4,1^+)\Gamma(3,4;2)$$

$$\Sigma(1,2) = \int \mathrm{d}3\mathrm{d}4\, G(1,3)\Gamma(3,2;4)W(4,1^+)$$

$$\Gamma(1,2;3) = \delta(1,2)\delta(1,3) + \int \mathrm{d}4\mathrm{d}5\mathrm{d}6\mathrm{d}7\, \frac{\delta\Sigma(1,2)}{\delta G(4,5)}G(4,6)G(7,5)\Gamma(6,7;3)\,,$$

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# The dielectric function: $GW$ and RPA

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$$P^0(1,2) = -i \int \mathrm{d}3\, G(1,3)G(3,2)$$, Random Phase Approximation

$$\Sigma(1,2) = \int \mathrm{d}3\, G(1,3)W(3,2)$$, $GW$ approximation

$$\Gamma(1,2;3) = \delta(1,2)\delta(1,3) + \cancel{\int \mathrm{d}4\mathrm{d}5\mathrm{d}6\mathrm{d}7 \frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6)G(7,5)\Gamma(6,7;3)},$$

# Outline

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# RPA polarizability: general expression

$$\chi_0(\boldsymbol{r},\boldsymbol{r}';\omega) = \sum_{i,j}(f_i - f_j)\frac{\phi_i^*(\boldsymbol{r})\phi_j(\boldsymbol{r})\phi_j^*(\boldsymbol{r}')\phi_i(\boldsymbol{r}')}{\epsilon_i - \epsilon_j + \hbar\omega + \mathrm{i}\hbar\alpha}$$

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$$\chi_0(\boldsymbol{r},\boldsymbol{r}';\omega) = \sum_{v\boldsymbol{k},c\boldsymbol{k}'}\left[\frac{\psi_{c\boldsymbol{k}'}(\boldsymbol{r})\psi_{v\boldsymbol{k}}^*(\boldsymbol{r})\psi_{v\boldsymbol{k}}(\boldsymbol{r}')\psi_{c\boldsymbol{k}'}^*(\boldsymbol{r}')}{\hbar\omega - (\epsilon_{c\boldsymbol{k}'} - \epsilon_{v\boldsymbol{k}}) + \mathrm{i}\hbar\alpha} - \frac{\psi_{v\boldsymbol{k}}(\boldsymbol{r})\psi_{c\boldsymbol{k}'}^*(\boldsymbol{r})\psi_{c\boldsymbol{k}'}(\boldsymbol{r}')\psi_{v\boldsymbol{k}}^*(\boldsymbol{r}')}{\hbar\omega + (\epsilon_{c\boldsymbol{k}'} - \epsilon_{v\boldsymbol{k}}) + \mathrm{i}\hbar\alpha}\right].$$

$$\langle\boldsymbol{r}|n,\boldsymbol{k}\rangle = \psi_{n\boldsymbol{k}}(\boldsymbol{r})\,,\alpha \to 0^+$$

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{R}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\sum_{i\alpha}C_{i\alpha}^{n\boldsymbol{k}}\phi_\alpha(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{t}_i)\,,$$ in the TB approx.

# RPA polarizability: momentum space

$$\chi^0(\boldsymbol{r},\boldsymbol{r}';\omega) = \frac{1}{N}\sum_{\boldsymbol{q},\boldsymbol{q}'} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\chi^0(\boldsymbol{q},\boldsymbol{q}';\omega)\mathrm{e}^{-\mathrm{i}\boldsymbol{q}'\cdot\boldsymbol{r}'}$$

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$$= \frac{1}{N}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{G}'} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\mathrm{e}^{-\mathrm{i}\boldsymbol{G}'\cdot\boldsymbol{r}'}\chi^0(\boldsymbol{q},\boldsymbol{q}+\boldsymbol{G}';\omega)$$

# RPA polarizability: momentum space

$$\chi^0(\boldsymbol{r},\boldsymbol{r}';\omega) = \frac{1}{N}\sum_{\boldsymbol{q},\boldsymbol{q}'} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\chi^0(\boldsymbol{q},\boldsymbol{q}';\omega)\mathrm{e}^{-\mathrm{i}\boldsymbol{q}'\cdot\boldsymbol{r}'} =$$

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$$= \frac{1}{N}\sum_{\boldsymbol{q}\in\mathrm{BZ}}\sum_{\boldsymbol{G},\boldsymbol{G}'} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\mathrm{e}^{\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{r}}\mathrm{e}^{-\mathrm{i}(\boldsymbol{G}'+\boldsymbol{G})\cdot\boldsymbol{r}'}\chi^0(\boldsymbol{q}+\boldsymbol{G},\boldsymbol{q}+\boldsymbol{G}+\boldsymbol{G}';\omega) =$$

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# RPA polarizability: momentum space

$$
\begin{aligned}
\chi^0(\boldsymbol{r},\boldsymbol{r}';\omega) &= \frac{1}{N}\sum_{\boldsymbol{q},\boldsymbol{q}'} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\chi^0(\boldsymbol{q},\boldsymbol{q}';\omega)\mathrm{e}^{-\mathrm{i}\boldsymbol{q}'\cdot\boldsymbol{r}'} = \\
&= \frac{1}{N}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{G}'} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\mathrm{e}^{-\mathrm{i}\boldsymbol{G}'\cdot\boldsymbol{r}'}\chi^0(\boldsymbol{q},\boldsymbol{q}+\boldsymbol{G}';\omega) = \\
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\end{aligned}
$$

$$
\chi^0_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q};\omega) = \int \mathrm{d}\boldsymbol{r}\int \mathrm{d}\boldsymbol{r}'\mathrm{e}^{-\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}}\chi_0(\boldsymbol{r},\boldsymbol{r}';\omega)\mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G}')\cdot\boldsymbol{r}}
$$

# Static RPA polarizability: $r$ and $q$ spaces

$$\chi_0(\boldsymbol{r},\boldsymbol{r}';\omega)=\sum_{v\boldsymbol{k},c\boldsymbol{k}'}\left[\frac{\psi_{c\boldsymbol{k}'}(\boldsymbol{r})\psi^*_{v\boldsymbol{k}}(\boldsymbol{r})\psi_{v\boldsymbol{k}}(\boldsymbol{r}')\psi^*_{c\boldsymbol{k}'}(\boldsymbol{r}')}{\hbar\omega-(\epsilon_{c\boldsymbol{k}'}-\epsilon_{v\boldsymbol{k}})+\mathrm{i}\hbar\alpha}-\frac{\psi_{v\boldsymbol{k}}(\boldsymbol{r})\psi^*_{c\boldsymbol{k}'}(\boldsymbol{r})\psi_{c\boldsymbol{k}'}(\boldsymbol{r}')\psi^*_{v\boldsymbol{k}}(\boldsymbol{r}')}{\hbar\omega+(\epsilon_{c\boldsymbol{k}'}-\epsilon_{v\boldsymbol{k}})+\mathrm{i}\hbar\alpha}\right].$$

$$\chi_0(\boldsymbol{r},\boldsymbol{r}')=-\sum_{v\boldsymbol{k},c\boldsymbol{k}'}\frac{2\,\mathrm{Re}\left\{\psi_{c\boldsymbol{k}'}(\boldsymbol{r})\psi^*_{v\boldsymbol{k}}(\boldsymbol{r})\psi_{v\boldsymbol{k}}(\boldsymbol{r}')\psi^*_{c\boldsymbol{k}'}(\boldsymbol{r}')\right\}}{\epsilon_{c\boldsymbol{k}'}-\epsilon_{v\boldsymbol{k}}}$$

$$\chi^0_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q};\omega)=\frac{1}{\Omega}\sum_{n,n'}\sum_{\boldsymbol{k}}(f_{n,\boldsymbol{k}+\boldsymbol{q}}-f_{n',\boldsymbol{k}})\frac{\langle n,\boldsymbol{k}+\boldsymbol{q}|\,\mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}}\,|n',\boldsymbol{k}\rangle\,\langle n',\boldsymbol{k}|\,\mathrm{e}^{-\mathrm{i}(\boldsymbol{q}+\boldsymbol{G}')\cdot\boldsymbol{r}}\,|n,\boldsymbol{k}+\boldsymbol{q}\rangle}{\epsilon_{n,\boldsymbol{k}+\boldsymbol{q}}-\epsilon_{n',\boldsymbol{k}}+\hbar\omega+\mathrm{i}\hbar\alpha}$$

$$\chi^0_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})=\frac{1}{\Omega}\sum_{n}^{\text{occ}}\sum_{n'}^{\text{emp}}\sum_{\boldsymbol{k}}\frac{\langle n,\boldsymbol{k}+\boldsymbol{q}|\,\mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}}\,|n',\boldsymbol{k}\rangle\,\langle n',\boldsymbol{k}|\,\mathrm{e}^{-\mathrm{i}(\boldsymbol{q}+\boldsymbol{G}')\cdot\boldsymbol{r}}\,|n,\boldsymbol{k}+\boldsymbol{q}\rangle}{\epsilon_{n,\boldsymbol{k}+\boldsymbol{q}}-\epsilon_{n',\boldsymbol{k}}}$$

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# RPA dielectric function

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$$\varepsilon^{\mathsf{RPA}}(\boldsymbol{r},\boldsymbol{r}';t,t') = \delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t') - \int \mathrm{d}\boldsymbol{r}'' \int_{-\infty}^{t} \mathrm{d}t'' \chi^0(\boldsymbol{r},\boldsymbol{r}';t-t'')v_c(\boldsymbol{r}-\boldsymbol{r}')$$

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$$\chi^0_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}) = \frac{1}{\Omega}\sum_{v,c}\sum_{\boldsymbol{k}} \frac{\langle v,\boldsymbol{k}+\boldsymbol{q}|\,\mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}}\,|c,\boldsymbol{k}\rangle\,\langle c,\boldsymbol{k}|\,\mathrm{e}^{-\mathrm{i}(\boldsymbol{q}+\boldsymbol{G}')\cdot\boldsymbol{r}}\,|v,\boldsymbol{k}+\boldsymbol{q}\rangle}{\epsilon_{v,\boldsymbol{k}+\boldsymbol{q}}-\epsilon_{c,\boldsymbol{k}}}$$ see [1]

[1] Jack Deslippe et al., “BerkeleyGW: A massively parallel computer package for the calculation of the quasiparticle and optical properties of materials and nanostructures”, Computer Physics Communications 183.6 (2012)

# The (RPA) screened electrostatic potential

$$W(\boldsymbol{r}, \boldsymbol{r}') = \int \mathrm{d}\boldsymbol{r}'' \varepsilon^{-1}(\boldsymbol{r}, \boldsymbol{r}'') v_c(\boldsymbol{r}'', \boldsymbol{r}')$$

$$W_{\boldsymbol{G},\boldsymbol{G}'}(\boldsymbol{q}) = \varepsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}) v_c(\boldsymbol{q} + \boldsymbol{G}') \,,$$

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Ignoring local field effects ($\boldsymbol{G} = \boldsymbol{G}' = 0$) and defining $\varepsilon_{\text{mac}}(\boldsymbol{q}) = 1/\varepsilon^{-1}_{\mathbf{00}}(\boldsymbol{q})$

$$W(\boldsymbol{q}) = \frac{v_c(\boldsymbol{q})}{\varepsilon_{\text{mac}}(\boldsymbol{q})} \,,$$

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$$W(\boldsymbol{q}) = \frac{v_c(\boldsymbol{q})}{\varepsilon_{\mathsf{mac}}(\boldsymbol{q})} \,,$$

For a 2D semiconductor/insulator $\varepsilon_{\mathsf{mac}}(\boldsymbol{q}) = \varepsilon_{\mathsf{2D}}(\boldsymbol{q}) \approx 1 + r_0 q \equiv \varepsilon_{\mathsf{RK}}(\boldsymbol{q})$

$$V_{\mathsf{RK}}(q) = \frac{v_c(q)}{\varepsilon_{\mathsf{RK}}(q)} = \frac{e^2}{2\varepsilon_0(1+r_0 q)q} \,,$$

# Outline

# Outline

# Bloch states in the TB approx.

In the linear combination of atomic orbitals (LCAO) method

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \sum_{i\alpha} C_{i\alpha}^{n\boldsymbol{k}} \phi_\alpha(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{t}_i)$$

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Frequently, we work under the tight-binding approximation: retain nearest neighbors and neglect overlap between orbitals.

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$$H\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = E\psi_{n\boldsymbol{k}}(\boldsymbol{r}) \Leftrightarrow \sum_j \psi_j(\boldsymbol{k}) H \Phi_j(\boldsymbol{k}, \boldsymbol{r}) = E \sum_j \psi_j(\boldsymbol{k}) \Phi_j(\boldsymbol{k}, \boldsymbol{r}) \,.$$

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$$\sum_j \psi_j(\boldsymbol{k}) \underbrace{\int \mathrm{d}\boldsymbol{r}\, \Phi_i^*(\boldsymbol{k},\boldsymbol{r}) H \Phi_j(\boldsymbol{k},\boldsymbol{r})}_{H_{ij}(\boldsymbol{k})} = E\sum_j \psi_j(\boldsymbol{k}) \underbrace{\int \mathrm{d}\boldsymbol{r}\, \Phi_i^*(\boldsymbol{k},\boldsymbol{r})\Phi_j(\boldsymbol{k},\boldsymbol{r})}_{S_{ij}(\boldsymbol{k})}$$

# Bloch Hamiltonian in the TB approx.

Defining $H_{ij}(\boldsymbol{k}) = \langle \Phi_i(\boldsymbol{k}, \boldsymbol{r}) | H | \Phi_j(\boldsymbol{k}, \boldsymbol{r}) \rangle$ and $S_{ij}(\boldsymbol{k}) = \langle \Phi_i(\boldsymbol{k}, \boldsymbol{r}) | \Phi_j(\boldsymbol{k}, \boldsymbol{r}) \rangle$

$$\sum_j \psi_j(\boldsymbol{k}) H_{ij}(\boldsymbol{k}) = E \sum_j \psi_j(\boldsymbol{k}) S_{ij}(\boldsymbol{k})$$

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POLIMA

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$$\sum_j \psi_j(\boldsymbol{k}) H_{ij}(\boldsymbol{k}) = E \sum_j \psi_j(\boldsymbol{k}) S_{ij}(\boldsymbol{k})$$

The transfer integral matrix elements read

$$H_{ij}(\boldsymbol{k}) = \langle \Phi_i(\boldsymbol{k},\boldsymbol{r})|H|\Phi_j(\boldsymbol{k},\boldsymbol{r})\rangle = \sum_{ij} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_j-\boldsymbol{R}_i)} \langle \phi(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{t}_i)|H|\phi(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{t}_j)\rangle =$$

$$= \sum_{\boldsymbol{R}_j} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j} \langle \phi_i(\boldsymbol{r})|H|\phi_j(\boldsymbol{r}-\boldsymbol{R}_j)\rangle = \underbrace{\sum_{\boldsymbol{R}_j} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j} H_{ij}(\boldsymbol{R}_j)}_{\text{Bloch Ham.}}\,, H(\boldsymbol{R}_j) \rightarrow \text{Fock matrix at } \boldsymbol{R}_j$$

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TB approx. $\Rightarrow S_{ij}(\boldsymbol{k}) \approx \delta_{ij}$ and eigenvalue/eigenvector problem:

$$H(\boldsymbol{k})\psi(\boldsymbol{k}) = E\psi(\boldsymbol{k})$$

# Tight-Binding coefficients

POLIMA

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \sum_{i\alpha} C_{i\alpha}^{n\boldsymbol{k}} \phi_\alpha(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{t}_i)$$

$$H(\boldsymbol{k})\underline{C}^{n\boldsymbol{k}} = \epsilon_{n\boldsymbol{k}}\underline{C}^{n\boldsymbol{k}}$$

$$H(\boldsymbol{k}) \begin{bmatrix} C_{1,1}^{n\boldsymbol{k}} \\ C_{1,2}^{n\boldsymbol{k}} \\ \vdots \\ C_{1,N_o^1}^{n\boldsymbol{k}} \\ C_{2,1}^{n\boldsymbol{k}} \\ \vdots \\ C_{2,N_o^2}^{n\boldsymbol{k}} \\ \vdots \\ C_{N_a,N_o^{N_a}-1}^{n\boldsymbol{k}} \\ C_{N_a,N_o^{N_a}}^{n\boldsymbol{k}} \end{bmatrix} = \epsilon_{n\boldsymbol{k}} \begin{bmatrix} C_{1,1}^{n\boldsymbol{k}} \\ C_{1,2}^{n\boldsymbol{k}} \\ \vdots \\ C_{1,N_o^1}^{n\boldsymbol{k}} \\ C_{2,1}^{n\boldsymbol{k}} \\ \vdots \\ C_{2,N_o^2}^{n\boldsymbol{k}} \\ \vdots \\ C_{N_a,N_o^{N_a}-1}^{n\boldsymbol{k}} \\ C_{N_a,N_o^{N_a}}^{n\boldsymbol{k}} \end{bmatrix}$$

# Outline

# Polarizability in the TB approximation

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \sum_{i\alpha} C_{i\alpha}^{n\boldsymbol{k}} \phi_\alpha(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{t}_i)$$

$$\chi^0_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}) = \frac{1}{\Omega} \sum_{v,c} \sum_{\boldsymbol{k}} \frac{\langle v, \boldsymbol{k}+\boldsymbol{q}| \, \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}} \, |c, \boldsymbol{k}\rangle \langle c, \boldsymbol{k}+\boldsymbol{q}| \, \mathrm{e}^{-\mathrm{i}(\boldsymbol{q}+\boldsymbol{G}')\cdot\boldsymbol{r}} \, |v, \boldsymbol{k}\rangle}{\epsilon_{v,\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{c,\boldsymbol{k}}} =$$

$$= \frac{1}{\Omega} \sum_{v,c} \sum_{\boldsymbol{k}} \frac{M_{vc}(\boldsymbol{k},\boldsymbol{q},\boldsymbol{G}) M^*_{vc}(\boldsymbol{k},\boldsymbol{q},\boldsymbol{G}')}{\epsilon_{v,\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{c,\boldsymbol{k}}}$$

# Polarizability in the TB approximation

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \sum_{i\alpha} C_{i\alpha}^{n\boldsymbol{k}} \phi_\alpha(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{t}_i)$$

$$\chi^0_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}) = \frac{1}{\Omega} \sum_{v,c} \sum_{\boldsymbol{k}} \frac{\langle v, \boldsymbol{k}+\boldsymbol{q}|\, \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}}\, |c, \boldsymbol{k}\rangle \langle c, \boldsymbol{k}+\boldsymbol{q}|\, \mathrm{e}^{-\mathrm{i}(\boldsymbol{q}+\boldsymbol{G}')\cdot\boldsymbol{r}}\, |v, \boldsymbol{k}\rangle}{\epsilon_{v,\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{c,\boldsymbol{k}}} =$$

$$= \frac{1}{\Omega} \sum_{v,c} \sum_{\boldsymbol{k}} \frac{M_{vc}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G}) M^*_{vc}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G}')}{\epsilon_{v,\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{c,\boldsymbol{k}}}$$

Point-like orbitals approximation $\phi^*_\alpha(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{t}_i)\phi_\beta(\boldsymbol{r} - \boldsymbol{R}' - \boldsymbol{t}_j) \approx \delta_{ij}\delta_{\alpha\beta}\delta_{\boldsymbol{R}\boldsymbol{R}'}\delta(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{t}_i)$:

$$M_{nn'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G}) \equiv \langle n, \boldsymbol{k}+\boldsymbol{q}|\, \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}}\, |n', \boldsymbol{k}\rangle = \int \mathrm{d}\boldsymbol{r}\, \psi^*_{n,\boldsymbol{k}+\boldsymbol{q}}(\boldsymbol{r}) \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}} \psi_{n'\boldsymbol{k}}(\boldsymbol{r}) =$$

$$= \sum_{i\alpha} (C_{i\alpha}^{n\boldsymbol{k}+\boldsymbol{q}})^* C_{i\alpha}^{n'\boldsymbol{k}} \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{t}_i} \equiv I^{\boldsymbol{G}}_{n\boldsymbol{k}+\boldsymbol{q},n'\boldsymbol{k}}$$

# Polarizability in the TB approximation

POLIMA

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \sum_{i\alpha} C^{n\boldsymbol{k}}_{i\alpha} \phi_\alpha(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{t}_i)$$

$$\chi^0_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}) = \frac{1}{\Omega} \sum_{v,c} \sum_{\boldsymbol{k}} \frac{\langle v, \boldsymbol{k}+\boldsymbol{q}| \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}} |c, \boldsymbol{k}\rangle \langle c, \boldsymbol{k}+\boldsymbol{q}| \mathrm{e}^{-\mathrm{i}(\boldsymbol{q}+\boldsymbol{G}')\cdot\boldsymbol{r}} |v, \boldsymbol{k}\rangle}{\epsilon_{v,\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{c,\boldsymbol{k}}} =$$

$$= \frac{1}{\Omega} \sum_{v,c} \sum_{\boldsymbol{k}} \frac{M_{vc}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G}) M^*_{vc}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G}')}{\epsilon_{v,\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{c,\boldsymbol{k}}} = \frac{1}{A_{\mathsf{UC}} N_k} \sum_{vc} \sum_{\boldsymbol{k}} \frac{I^{\boldsymbol{G}}_{v\boldsymbol{k}+\boldsymbol{q},c\boldsymbol{k}} (I^{\boldsymbol{G}'}_{v\boldsymbol{k}+\boldsymbol{q},c\boldsymbol{k}})^*}{\epsilon_{v,\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{c,\boldsymbol{k}}}$$

Point-like orbitals approximation $\phi^*_\alpha(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{t}_i)\phi_\beta(\boldsymbol{r} - \boldsymbol{R}' - \boldsymbol{t}_j) \approx \delta_{ij}\delta_{\alpha\beta}\delta_{\boldsymbol{R}\boldsymbol{R}'}\delta(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{t}_i)$:

$$M_{nn'}(\boldsymbol{k}, \boldsymbol{q}, \boldsymbol{G}) \equiv \langle n, \boldsymbol{k}+\boldsymbol{q}| \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}} |n', \boldsymbol{k}\rangle = \int \mathrm{d}\boldsymbol{r}\, \psi^*_{n,\boldsymbol{k}+\boldsymbol{q}}(\boldsymbol{r}) \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{r}} \psi_{n'\boldsymbol{k}}(\boldsymbol{r}) =$$

$$= \sum_{i\alpha} (C^{n\boldsymbol{k}+\boldsymbol{q}}_{i\alpha})^* C^{n'\boldsymbol{k}}_{i\alpha} \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{G})\cdot\boldsymbol{t}_i} \equiv I^{\boldsymbol{G}}_{n\boldsymbol{k}+\boldsymbol{q},n'\boldsymbol{k}}$$

# Dielectric function computation scheme

POLIMA

1. Diagonalize $H(\boldsymbol{k})$ and store all $\{\epsilon_{n\boldsymbol{k}}\}$,$\{\underline{C}^{n\boldsymbol{k}}\}$ in a BZ mesh
2. Compute dielectric matrix $\varepsilon_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}) = \delta_{\boldsymbol{G}\boldsymbol{G}'} - v_c(\boldsymbol{q}+\boldsymbol{G})\chi^0_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q}),\ \forall \boldsymbol{q} \in \mathrm{BZ}$
3. Invert $\varepsilon_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})\,\forall \boldsymbol{q} \in \mathrm{BZ}$
4. Compute $W_{\boldsymbol{G},\boldsymbol{G}'}(\boldsymbol{q}) = \varepsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\boldsymbol{q})v_c(\boldsymbol{q}+\boldsymbol{G}')\,\forall \boldsymbol{q} \in \mathrm{BZ}$
5. Compute the exciton (details for another time)

# Outline

# Polarizability convergence

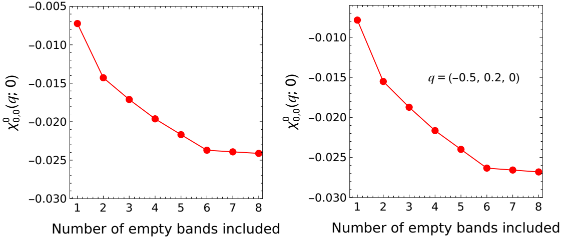


**Figure:** *$MoS_2$ tight-binding model by Ridolfi [1].*

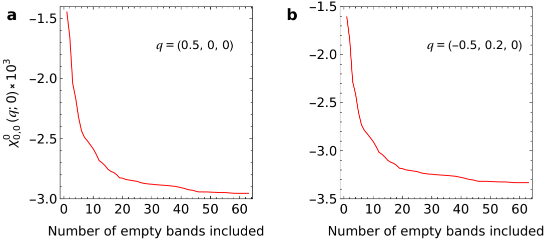


**Figure:** *hBN, DFT (HSE06 functional) using CRYSTAL [2].*


- [1] E. Ridolfi et al., Journal of Physics: Condensed Matter 27.36 (2015)
- [2] A. Erba et al., Journal of Chemical Theory and Computation 19.20 (2023)

# Polarizability convergence: comparing models

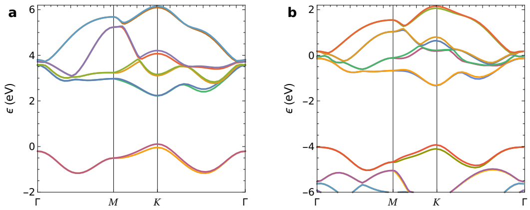

**Figure:** *$MoS_2$ bands,* ***a****-Ridolfi's TB model,* ***b****-Wannier90 [1].*

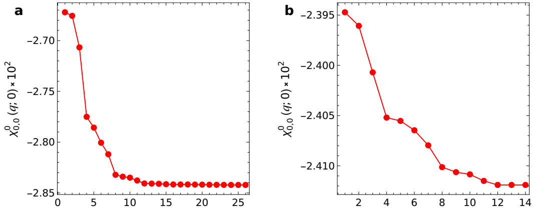

**Figure:** $\chi_{00}(\boldsymbol{q})$, $\boldsymbol{q} = (0.5, 0)$. *(a->b, b->a)*

Convergence of the polarizability with the number of included valence bands, including all the conduction bands. Different values justified by a different band structure.

- [1] G. Pizzi et al., Journal of Physics: Condensed Matter 32.16 (2020)

# Polarizability in the Brillouin Zone

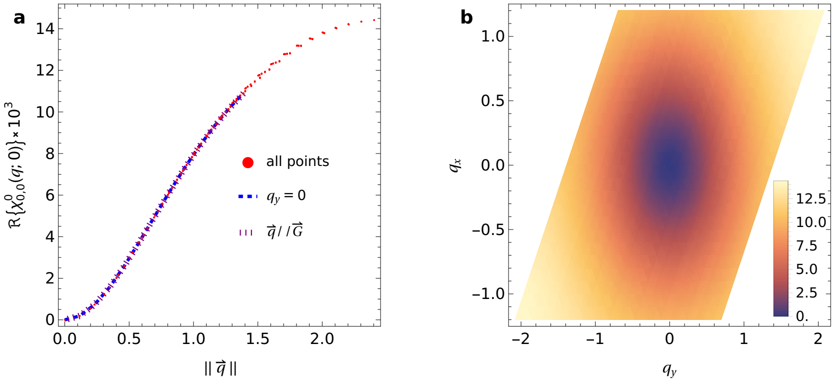


**Figure:** *Panel **a**: $\chi^0_{\mathbf{00}}(\boldsymbol{q})$ vs. $|\boldsymbol{q}|$; Panel **b**: $\chi^0_{\mathbf{00}}(\boldsymbol{q})$ vs. $\boldsymbol{q} \in$ BZ. Calculation for hBN, whose bands were obtained within DFT with the HSE06 functional.*

# Convergence of the inverse dielectric function

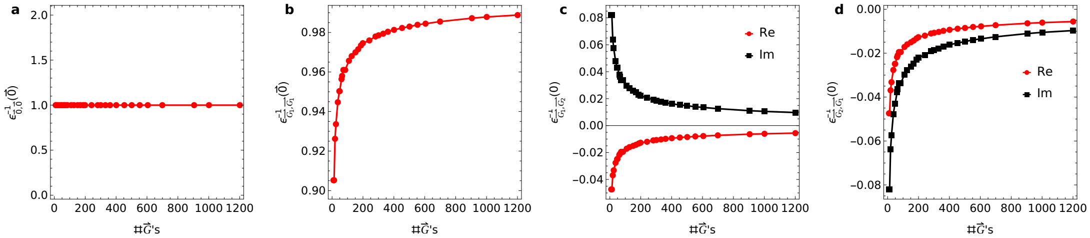


**Figure:** *Selection of matrix elements* $\varepsilon^{-1}_{\boldsymbol{G}\boldsymbol{G}'}(\mathbf{0})$ *for* $MoS_2$ *using Ridolfi's tight-binding model. All bands included, and with a BZ mesh with 20 momentum points in each direction.* ***a*** $(\boldsymbol{G},\boldsymbol{G}')=(\mathbf{0},\mathbf{0})$, ***b*** $(\boldsymbol{G},\boldsymbol{G}')=(\boldsymbol{G}_1,\boldsymbol{G}_1)$, ***c*** $(\boldsymbol{G},\boldsymbol{G}')=(\boldsymbol{G}_1,\boldsymbol{G}_2)$, **d** $(\boldsymbol{G},\boldsymbol{G}')=(\boldsymbol{G}_2,\boldsymbol{G}_1)$. $\boldsymbol{G}_1=(-1.98835, 1.14797)$*(Å$^{-1}$) and* $\boldsymbol{G}_2=-\boldsymbol{G}_1$.

# Macroscopic dielectric function

$$\varepsilon_{\mathsf{2D}}(\boldsymbol{q}) \equiv \frac{1}{\varepsilon^{-1}_{\mathbf{00}}(\boldsymbol{q})}$$

$$\varepsilon_{\mathsf{RK}}(\boldsymbol{q}) = 1 + r_0 q$$

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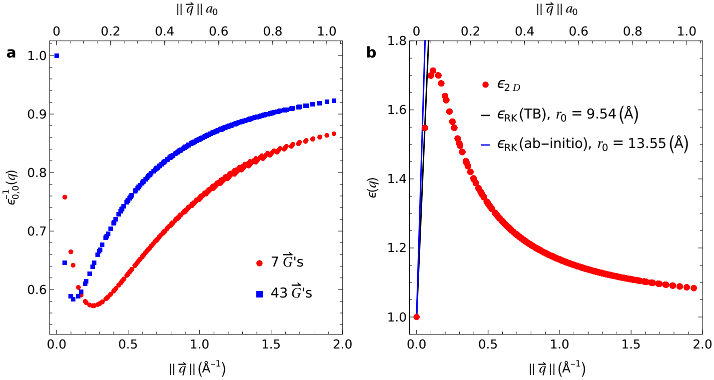


**Figure:** ***a*** $\varepsilon_{\mathbf{00}}^{-1}(|\boldsymbol{q}|)$ *and* ***b*** $\varepsilon_{2D}(|\boldsymbol{q}|)$*. For* $MoS_2$ *using Ridolfi's tight-binding model. In* ***b*** *we display the numerical* $\varepsilon_{2D}$*, the Rytova-Keldysh dielectric function with an estimated* $r_0 \approx 9.54$ *Å and with the ab-initio one* $r_0 = 13.55$ *Å.*

# Screened potential

$$v_c(\boldsymbol{q}) = \frac{e^2}{2\varepsilon_0 q}$$

$$V_{\mathsf{RK}}(\boldsymbol{q}) = \frac{e^2}{2\varepsilon_0(1 + r_0 q)q}$$

$$W_{\mathbf{00}}(\boldsymbol{q}) = \varepsilon^{-1}_{\mathbf{00}}(\boldsymbol{q}) v_c(\boldsymbol{q})$$

# Screened potential

$$v_c(\boldsymbol{q}) = \frac{e^2}{2\varepsilon_0 q} \text{ (black dots)}$$

$$V_{\mathrm{RK}}(\boldsymbol{q}) = \frac{e^2}{2\varepsilon_0(1 + r_0 q)q} \text{ (blue dots)}$$

$$W_{\mathbf{00}}(\boldsymbol{q}) = \varepsilon^{-1}_{\mathbf{00}}(\boldsymbol{q}) v_c(\boldsymbol{q}) \text{ (red dots)}$$

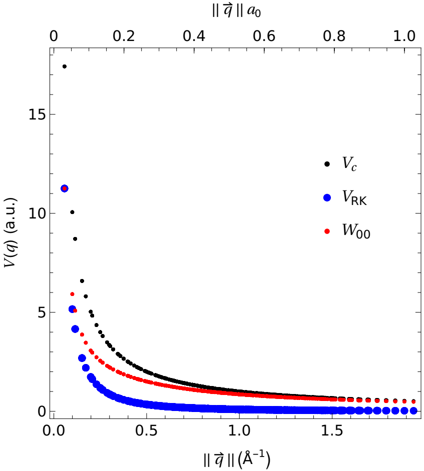


**Figure:** *Bare and screened potentials for* $MoS_2$ *using Ridolfi's TB model. 43* $\boldsymbol{G}$*s included.*

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$$v_c(\boldsymbol{q}) = \frac{e^2}{2\varepsilon_0 q}$$ (black dots)

$$V_{\mathrm{RK}}(\boldsymbol{q}) = \frac{e^2}{2\varepsilon_0(1+r_0 q)q}$$ (blue dots)

$$W_{\mathbf{00}}(\boldsymbol{q}) = \varepsilon^{-1}_{\mathbf{00}}(\boldsymbol{q})v_c(\boldsymbol{q})$$ (red dots)

- $W_{\mathbf{00}}(\boldsymbol{q}) \xrightarrow{q\nearrow} v_c(\boldsymbol{q})$
- RK approx. overestimates screening

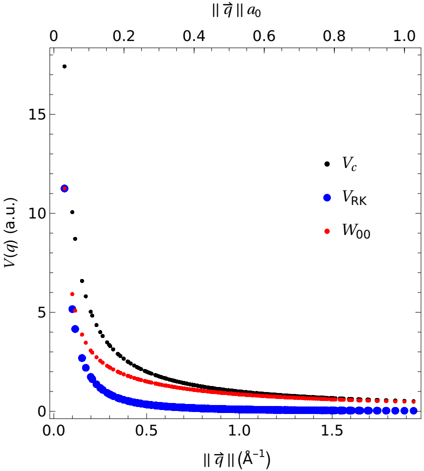



**Figure:** *Bare and screened potentials for $MoS_2$ using Ridolfi's TB model. 43 $\mathbf{G}$s included.*

# A use case: excitons in $MoS_2$

Please consult: Alejandro José Uría-Álvarez et al. “Efficient computation of optical excitations in 2D materials with the Xatu code”, Computer Physics Communications 295 (2024)

| State | Energy (RK) (eV) | B. energy (RK) (eV) | Energy ($\varepsilon_{\boldsymbol{G},\boldsymbol{G}'}$) (eV) | B. energy ($\varepsilon_{\boldsymbol{G},\boldsymbol{G}'}$) (eV) |
|---|---|---|---|---|
| 1a | 1.15051 | -0.96949 | 0.858549 | -1.261451 |
| 1b | | | 0.858551 | -1.261449 |
| 2a | 1.187938 | -0.932062 | 0.900934 | -1.219066 |
| 2b | | | 0.900936 | -1.219064 |
| 3a | 1.266467 | -0.853533 | 0.971518 | -1.148482 |
| 3b | | | 0.971520 | -1.14848 |
| 4a | 1.305554 | -0.814446 | 1.015683 | -1.104317 |
| 4b | | | 1.015685 | -1.104315 |

**Table:** *Exciton spectrum of $MoS_2$ described by Ridolfi's tight-binding model, using the Rytova-Keldysh potential and the computed inverse dielectric matrix to compute the interaction matrix elements, at the left and right, respectively.* $N_k = 40^2$, $N_c = N_v = 2$ *for the exciton,* $N_G = 43$. *Excludes the exchange interaction term in both approaches to screening.*

# Outline

# Revisiting Dyson's equation

$$\chi_0(\boldsymbol{r},\boldsymbol{r}';\omega) = \sum_{v\boldsymbol{k},c\boldsymbol{k}'} \left[ \frac{\psi_{c\boldsymbol{k}'}(\boldsymbol{r})\psi^*_{v\boldsymbol{k}}(\boldsymbol{r})\psi_{v\boldsymbol{k}}(\boldsymbol{r}')\psi^*_{c\boldsymbol{k}'}(\boldsymbol{r}')}{\hbar\omega - (\epsilon_{c\boldsymbol{k}'} - \epsilon_{v\boldsymbol{k}}) + \mathrm{i}\hbar\alpha} - \frac{\psi_{v\boldsymbol{k}}(\boldsymbol{r})\psi^*_{c\boldsymbol{k}'}(\boldsymbol{r})\psi_{c\boldsymbol{k}'}(\boldsymbol{r}')\psi^*_{v\boldsymbol{k}}(\boldsymbol{r}')}{\hbar\omega + (\epsilon_{c\boldsymbol{k}'} - \epsilon_{v\boldsymbol{k}}) + \mathrm{i}\hbar\alpha} \right].$$

$$W(\boldsymbol{r},\boldsymbol{r}') = \int \mathrm{d}\boldsymbol{r}''\varepsilon^{-1}(\boldsymbol{r},\boldsymbol{r}'')v_c(\boldsymbol{r}'',\boldsymbol{r}') = v_c(\boldsymbol{r},\boldsymbol{r}') + \int \mathrm{d}\boldsymbol{x} \int \mathrm{d}\boldsymbol{y}\, v_c(\boldsymbol{r},\boldsymbol{x})\chi_0(\boldsymbol{x},\boldsymbol{y})W(\boldsymbol{y},\boldsymbol{r}')$$

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \sum_{i\alpha} C^{n\boldsymbol{k}}_{i\alpha}\phi_\alpha(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{t}_i),$$

# Revisiting Dyson's equation

In the continuum

$$W(\boldsymbol{r},\boldsymbol{r}') = \int \mathrm{d}\boldsymbol{r}''\varepsilon^{-1}(\boldsymbol{r},\boldsymbol{r}'')v_c(\boldsymbol{r}'',\boldsymbol{r}') = v_c(\boldsymbol{r},\boldsymbol{r}') + \int \mathrm{d}\boldsymbol{x} \int \mathrm{d}\boldsymbol{y}\, v_c(\boldsymbol{r},\boldsymbol{x})\chi_0(\boldsymbol{x},\boldsymbol{y})W(\boldsymbol{y},\boldsymbol{r}')$$

Discretized version, in the point-like orbital approximation

$$W(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{t}_j) = v_c(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{t}_j) + \sum_{i',\boldsymbol{R}_1}^{\boldsymbol{R}_1+\boldsymbol{t}_{i'}\neq\boldsymbol{R}+\boldsymbol{t}_i} v_c(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{R}_1+\boldsymbol{t}_{i'}) \sum_{j',\boldsymbol{R}''}^{\boldsymbol{R}''+\boldsymbol{t}_{j'}\neq\boldsymbol{t}_j} \mathcal{T}^{i',j'}_{\boldsymbol{R}_1,\boldsymbol{R}''} W(\boldsymbol{R}''+\boldsymbol{t}_{j'},\boldsymbol{t}_j)$$

$$\mathcal{T}^{i,j}_{\boldsymbol{R},\boldsymbol{R}'} \equiv \frac{1}{N^2}\sum_{v\boldsymbol{k},c\boldsymbol{k}'}\sum_{\alpha\beta} \frac{-2\,\mathrm{Re}\left\{(C^{c\boldsymbol{k}'}_{i\alpha})^* C^{v\boldsymbol{k}}_{i\alpha}(C^{v\boldsymbol{k}}_{j\beta})^* C^{c\boldsymbol{k}'}_{j\beta}\,\mathrm{e}^{-\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot(\boldsymbol{R}-\boldsymbol{R}')}\right\}}{\epsilon_{c\boldsymbol{k}'}-\epsilon_{v\boldsymbol{k}}}$$

# Screened potential in real space

$$W(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{t}_j) = v_c(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{t}_j) + \sum_{i',\boldsymbol{R}_1}^{\boldsymbol{R}_1+\boldsymbol{t}_{i'}\neq\boldsymbol{R}+\boldsymbol{t}_i} v_c(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{R}_1+\boldsymbol{t}_{i'}) \sum_{j',\boldsymbol{R}''}^{\boldsymbol{R}''+\boldsymbol{t}_{j'}\neq\boldsymbol{t}_j} \mathcal{T}^{i',j'}_{\boldsymbol{R}_1,\boldsymbol{R}''} W(\boldsymbol{R}''+\boldsymbol{t}_{j'},\boldsymbol{t}_j)$$

is equivalent to

$$W(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{t}_j) - \sum_{j',\boldsymbol{R}''}^{\boldsymbol{R}''+\boldsymbol{t}_{j'}\neq\boldsymbol{t}_j} \left[ \sum_{i',\boldsymbol{R}_1}^{\boldsymbol{R}_1+\boldsymbol{t}_{i'}\neq\boldsymbol{R}+\boldsymbol{t}_i} v_c(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{R}_1+\boldsymbol{t}_{i'}) \mathcal{T}^{i',j'}_{\boldsymbol{R}_1,\boldsymbol{R}''} \right] W(\boldsymbol{R}''+\boldsymbol{t}_{j'},\boldsymbol{t}_j) = v_c(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{t}_j)$$

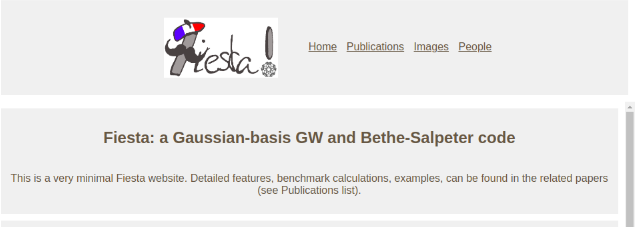
System of linear equations, however....

- $W(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{t}_j) > 0$ sometimes, $W(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{t}_j) < 0$ other times;
- Situation improves including the term $\boldsymbol{R}_1+\boldsymbol{t}_{i'} = \boldsymbol{R}+\boldsymbol{t}_i$, but result is regularization dependent.

# Screened potential in real space: what to do?

- Look at what chemists do.
- Self-consistent approach?

$$W(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{t}_j) =$$
$$v_c(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{t}_j)+\sum_{i',\boldsymbol{R}_1}^{\boldsymbol{R}_1+\boldsymbol{t}_{i'}\neq\boldsymbol{R}+\boldsymbol{t}_i} v_c(\boldsymbol{R}+\boldsymbol{t}_i,\boldsymbol{R}_1+\boldsymbol{t}_{i'})\sum_{j',\boldsymbol{R}''}^{\boldsymbol{R}''+\boldsymbol{t}_{j'}\neq\boldsymbol{t}_j}\mathcal{T}^{i',j'}_{\boldsymbol{R}_1,\boldsymbol{R}''}v_c(\boldsymbol{R}''+\boldsymbol{t}_{j'},\boldsymbol{t}_j)+\ldots.$$



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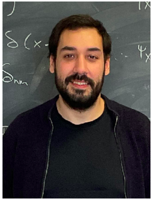

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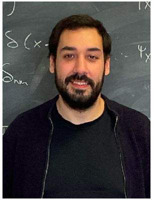

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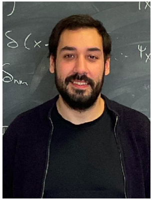

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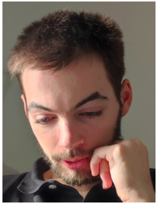

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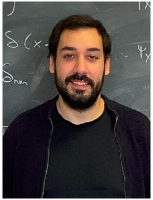

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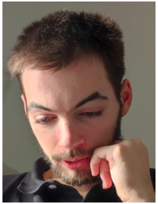

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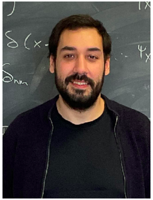

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