

Electrostatic screening in 2D semiconductors: an efficient atomistic implementation

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POLIMA weekly seminar

Where have I been?



Where have I been?



Outline

1 Screening

- Screening (what is it?)
- The dielectric function

2 The screened potential

- RPA polarizability: useful expressions
- RPA dielectric function and screened potential

3 Dielectric function in the Tight-Binding approximation

- Tight-Binding approximation
- Dielectric function within TB

4 Numerical results

5 What is in order? Real space approach

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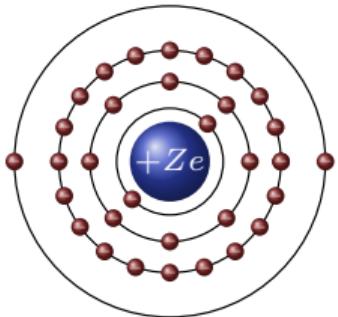
4 Numerical results

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Screening...

...in an atom.

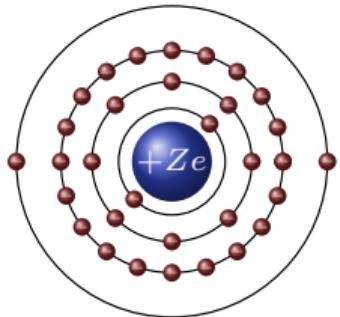
(Bare) Coulomb potential $v_c = \frac{Ze^2}{r}$



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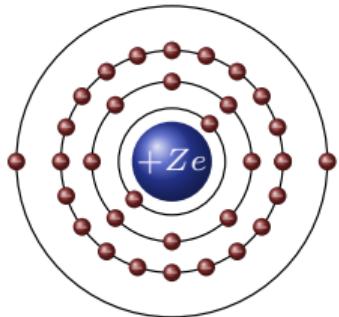
$$Z_{\text{eff}} = Z - \sigma$$

$$W < v_c$$

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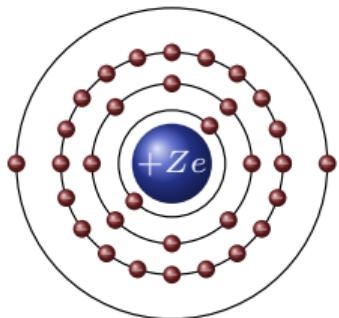
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Phys. Rev. 36, 57, J.C. Slater

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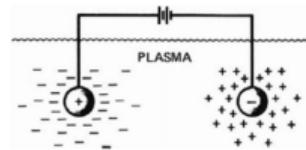


$$Z_{\text{eff}} = Z - \sigma$$

$$W < v_c$$

...in a plasma.

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



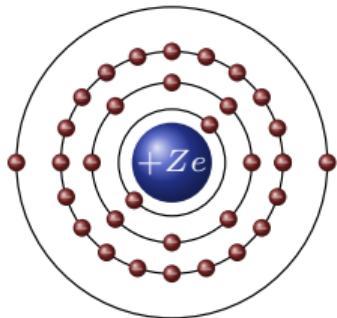
"Intro. to Plasma Physics and Controlled Fusion",
F.F. Chen

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...in an atom.

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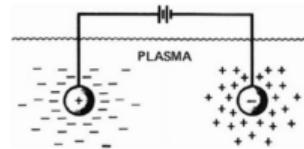
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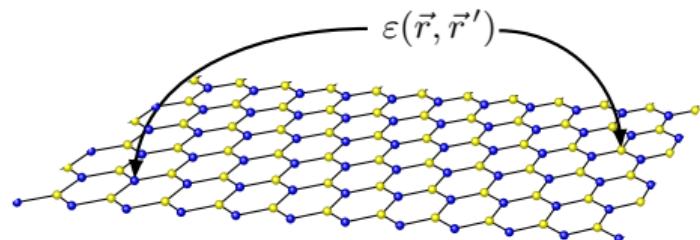
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"Intro. to Plasma Physics and Controlled Fusion",
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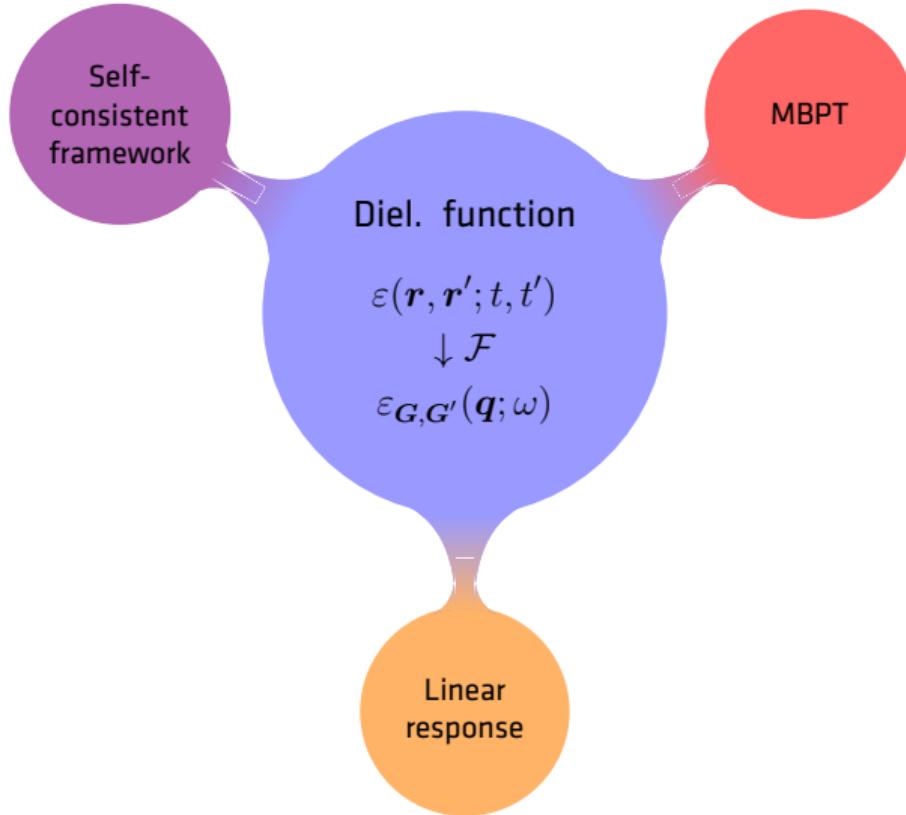
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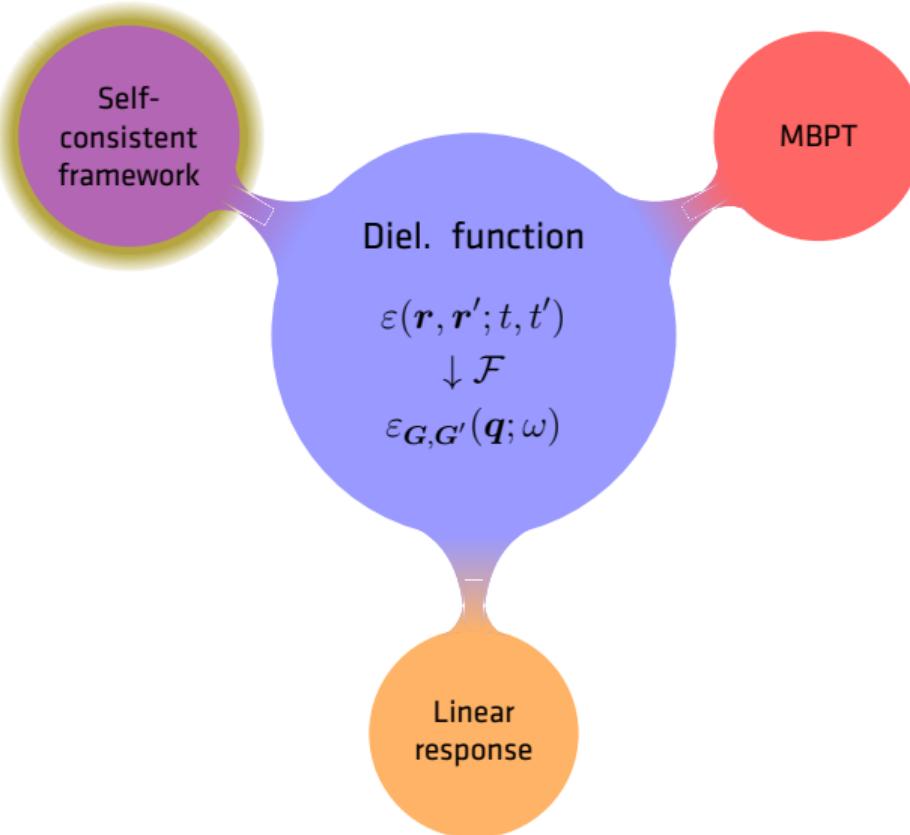
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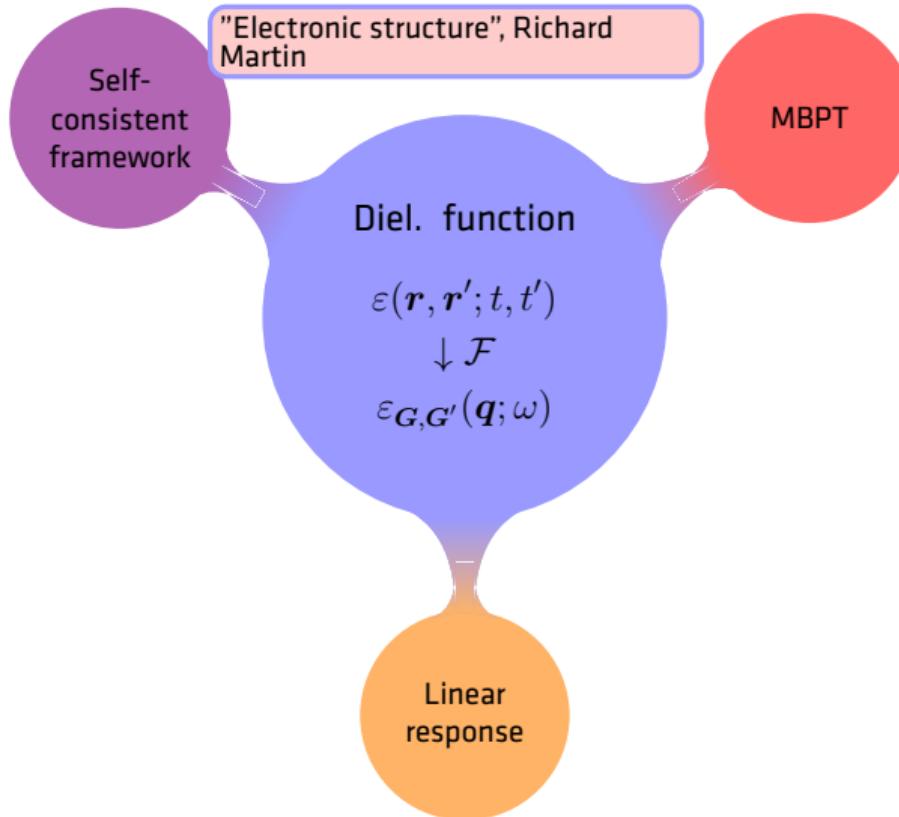
The dielectric function: technical contexts



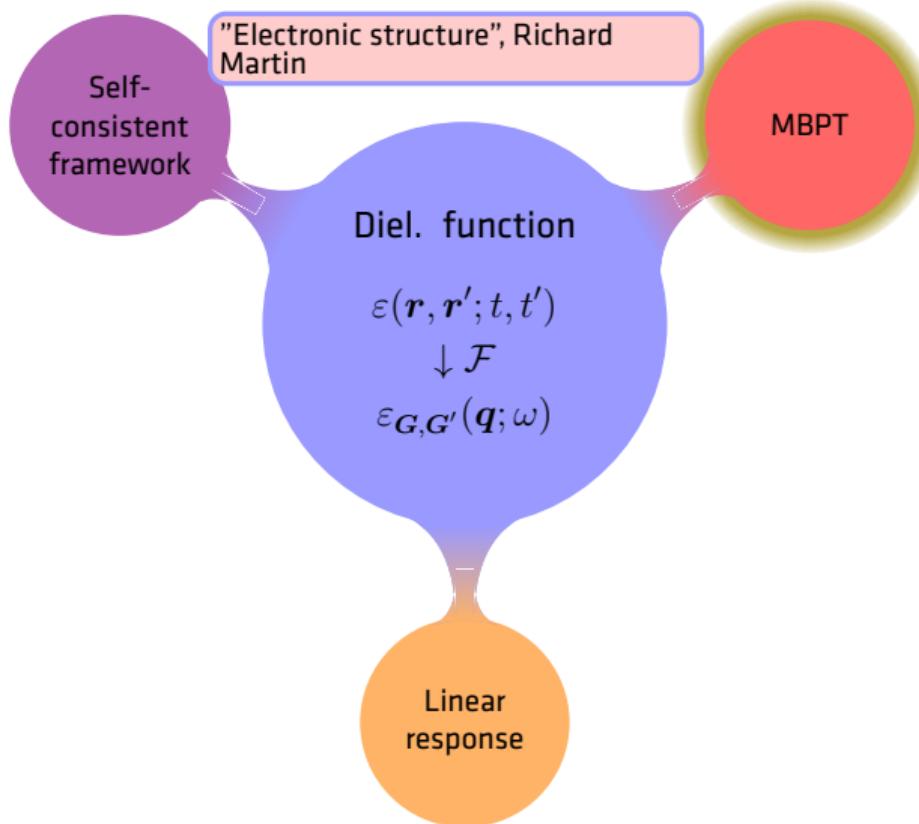
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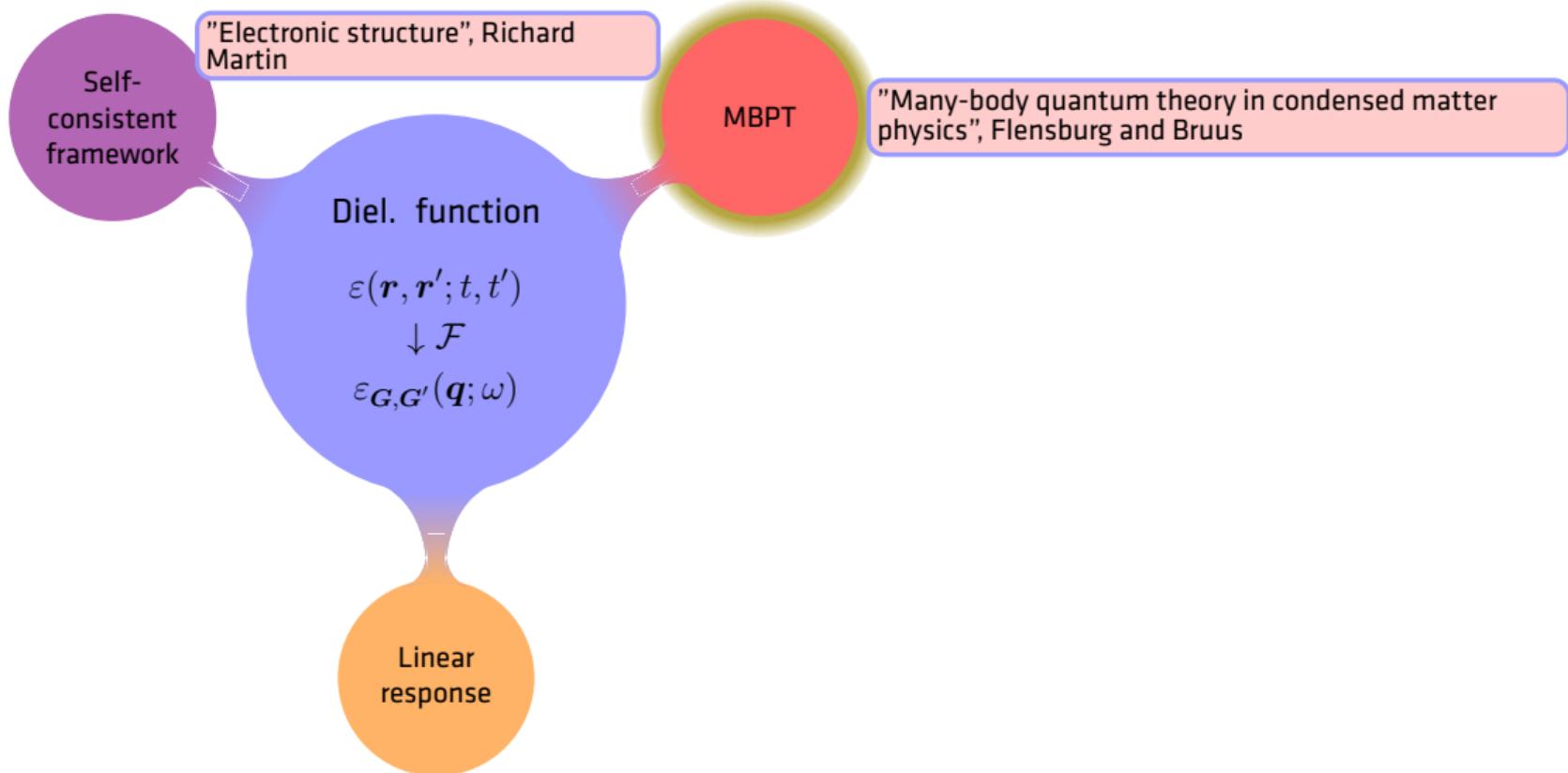
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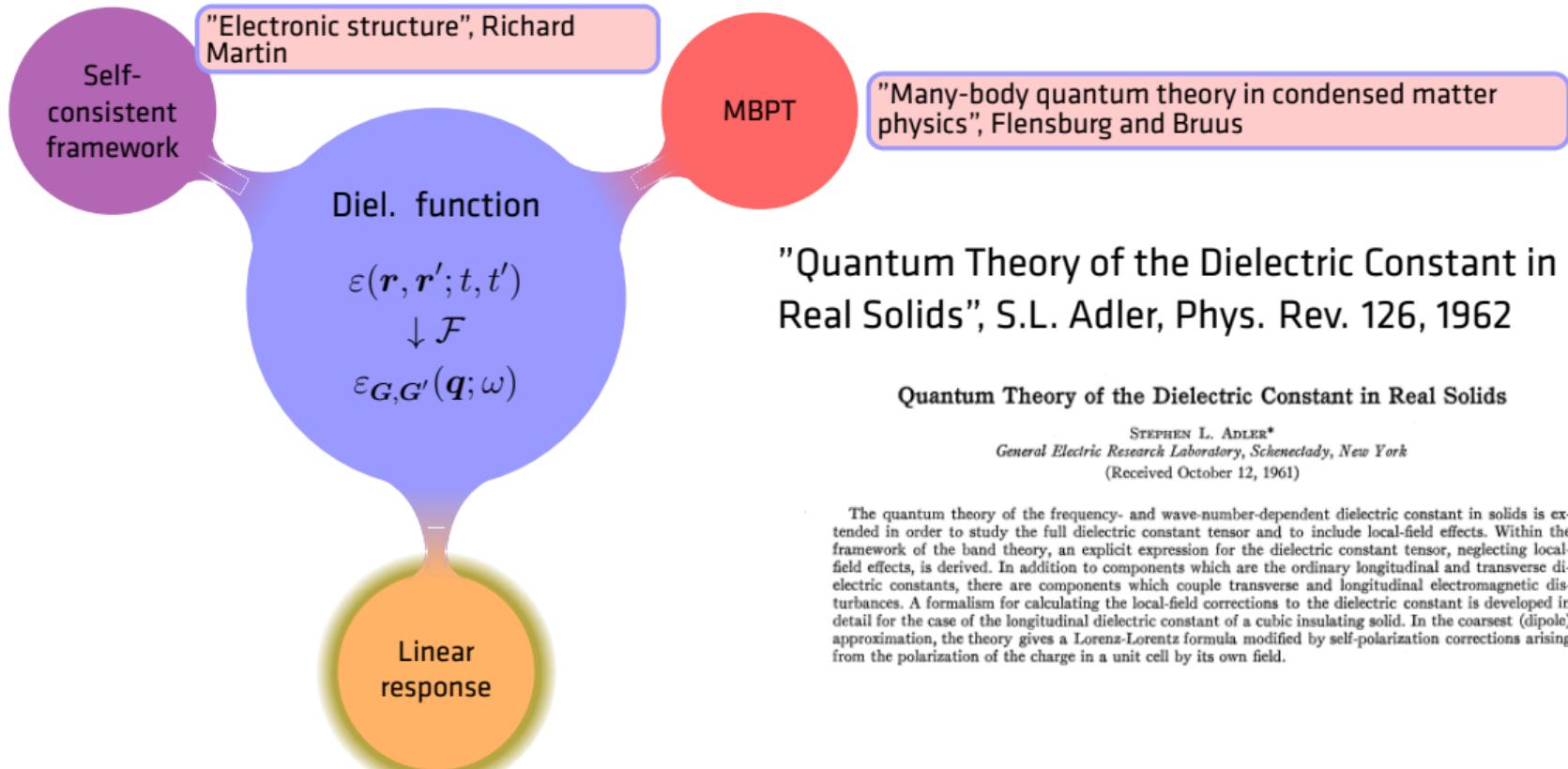
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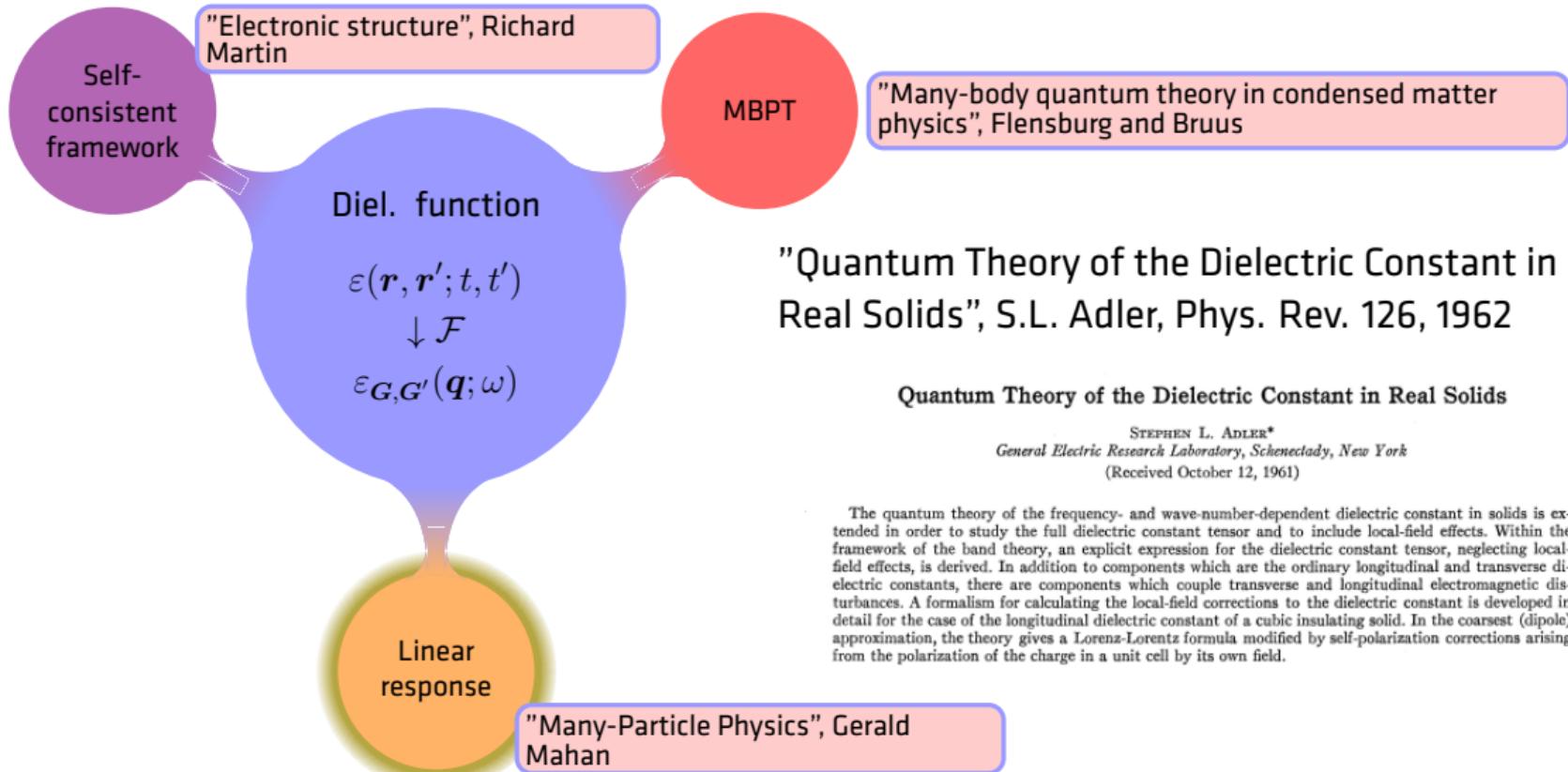
The dielectric function: technical contexts



The dielectric function: technical contexts



The dielectric function: technical contexts



The dielectric function: full and non-interacting

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

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

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

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

$$W(1, 2) = v_c(1, 2) + \int d3d4 v_c(1, 3) P(3, 4) W(4, 2) \text{ (Dyson's eq.)}$$

$$P(1, 2) = -i \int d3d4 G(1, 3) G(4, 1^+) \Gamma(3, 4; 2)$$

$$\Sigma(1, 2) = \int d3d4 G(1, 3) \Gamma(3, 2; 4) W(4, 1^+)$$

$$\Gamma(1, 2; 3) = \delta(1, 2)\delta(1, 3) + \int d4d5d6d7 \frac{\delta\Sigma(1, 2)}{\delta G(4, 5)} G(4, 6) G(7, 5) \Gamma(6, 7; 3) ,$$

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The dielectric function: GW and RPA

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

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

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

$$W(1, 2) = v_c(1, 2) + \int d3 d4 v_c(1, 3) P^0(3, 4) W(4, 2)$$

$$P^0(1, 2) = -i \int d3 G(1, 3) G(3, 2), \text{Random Phase Approximation}$$

$$\Sigma(1, 2) = \int d3 G(1, 3) W(3, 2), \text{GW approximation}$$

$$\Gamma(1, 2; 3) = \delta(1, 2)\delta(1, 3) + \cancel{\int d4 d5 d6 d7} \frac{\delta\Sigma(1, 2)}{\delta G(4, 5)} G(4, 6) G(7, 5) \Gamma(6, 7; 3),$$

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RPA polarizability: general expression

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

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

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

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

RPA polarizability: momentum space

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

RPA polarizability: momentum space

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

RPA polarizability: momentum space

$$\begin{aligned}\chi^0(\mathbf{r}, \mathbf{r}'; \omega) &= \frac{1}{N} \sum_{\mathbf{q}, \mathbf{q}'} e^{i\mathbf{q} \cdot \mathbf{r}} \chi^0(\mathbf{q}, \mathbf{q}'; \omega) e^{-i\mathbf{q}' \cdot \mathbf{r}'} = \\ &= \frac{1}{N} \sum_{\mathbf{q}} \sum_{\mathbf{G}'} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} e^{-i\mathbf{G}' \cdot \mathbf{r}'} \chi^0(\mathbf{q}, \mathbf{q} + \mathbf{G}'; \omega) = \\ &= \frac{1}{N} \sum_{\mathbf{q} \in \text{BZ}} \sum_{\mathbf{G}, \mathbf{G}'} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} e^{i\mathbf{G} \cdot \mathbf{r}} e^{-i(\mathbf{G}' + \mathbf{G}) \cdot \mathbf{r}'} \chi^0(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G} + \mathbf{G}'; \omega) = \\ &= \frac{1}{N} \sum_{\mathbf{q} \in \text{BZ}} \sum_{\mathbf{G}, \mathbf{G}'} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} e^{i\mathbf{G} \cdot \mathbf{r}} e^{-i\mathbf{G}' \cdot \mathbf{r}'} \underbrace{\chi^0(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}'; \omega)}_{\chi^0_{\mathbf{G}, \mathbf{G}'}(\mathbf{q}; \omega)},\end{aligned}$$

RPA polarizability: momentum space

$$\begin{aligned}\chi^0(\mathbf{r}, \mathbf{r}'; \omega) &= \frac{1}{N} \sum_{\mathbf{q}, \mathbf{q}'} e^{i\mathbf{q} \cdot \mathbf{r}} \chi^0(\mathbf{q}, \mathbf{q}'; \omega) e^{-i\mathbf{q}' \cdot \mathbf{r}'} = \\ &= \frac{1}{N} \sum_{\mathbf{q}} \sum_{\mathbf{G}'} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} e^{-i\mathbf{G}' \cdot \mathbf{r}'} \chi^0(\mathbf{q}, \mathbf{q} + \mathbf{G}'; \omega) = \\ &= \frac{1}{N} \sum_{\mathbf{q} \in \text{BZ}} \sum_{\mathbf{G}, \mathbf{G}'} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} e^{i\mathbf{G} \cdot \mathbf{r}} e^{-i(\mathbf{G}' + \mathbf{G}) \cdot \mathbf{r}'} \chi^0(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G} + \mathbf{G}'; \omega) = \\ &= \frac{1}{N} \sum_{\mathbf{q} \in \text{BZ}} \sum_{\mathbf{G}, \mathbf{G}'} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} e^{i\mathbf{G} \cdot \mathbf{r}} e^{-i\mathbf{G}' \cdot \mathbf{r}'} \underbrace{\chi^0(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}'; \omega)}_{\chi^0_{\mathbf{G}, \mathbf{G}'}(\mathbf{q}; \omega)},\end{aligned}$$

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

Static RPA polarizability: r and q spaces

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

$$\chi_0(\mathbf{r}, \mathbf{r}') = - \sum_{v\mathbf{k}, c\mathbf{k}'} \frac{2 \operatorname{Re}\{\psi_{c\mathbf{k}'}(\mathbf{r})\psi_{v\mathbf{k}}^*(\mathbf{r})\psi_{v\mathbf{k}}(\mathbf{r}')\psi_{c\mathbf{k}'}^*(\mathbf{r}')\}}{\epsilon_{c\mathbf{k}'} - \epsilon_{v\mathbf{k}}}$$

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

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

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RPA dielectric function

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

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$$\varepsilon_{GG'}(\mathbf{q}) = \delta_{GG'} - v_c(\mathbf{q} + \mathbf{G}) \chi^0_{GG'}(\mathbf{q}), v_c(\mathbf{q}) = \frac{e^2}{2\varepsilon_0 |\mathbf{q}|}$$

RPA dielectric function

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$$\varepsilon_{GG'}(\mathbf{q}) = \delta_{GG'} - v_c(\mathbf{q} + \mathbf{G}) \chi_{GG'}^0(\mathbf{q}), v_c(\mathbf{q}) = \frac{e^2}{2\varepsilon_0 |\mathbf{q}|}$$

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

[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

$$W(\mathbf{r}, \mathbf{r}') = \int d\mathbf{r}'' \varepsilon^{-1}(\mathbf{r}, \mathbf{r}'') v_c(\mathbf{r}'', \mathbf{r}')$$
$$W_{\mathbf{G}, \mathbf{G}'}(\mathbf{q}) = \varepsilon_{\mathbf{G}\mathbf{G}'}^{-1}(\mathbf{q}) v_c(\mathbf{q} + \mathbf{G}'),$$

The (RPA) screened electrostatic potential

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

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

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

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

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

Outline

1 Screening

- Screening (what is it?)
- The dielectric function

2 The screened potential

- RPA polarizability: useful expressions
- RPA dielectric function and screened potential

3 Dielectric function in the Tight-Binding approximation

- Tight-Binding approximation
- Dielectric function within TB

4 Numerical results

5 What is in order? Real space approach

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5 What is in order? Real space approach

Bloch states in the TB approx.

In the linear combination of atomic orbitals (LCAO) method

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

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

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_j} \psi_j(\mathbf{k}) \Phi_j(\mathbf{k}, \mathbf{r}), \quad \Phi_j(\mathbf{k}, \mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{R}} \phi(\mathbf{r} - \mathbf{R} - \mathbf{t}_j)$$

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

Bloch states in the TB approx.

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

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

Bloch Hamiltonian in the TB approx.

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

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

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

The transfer integral matrix elements read

$$\begin{aligned} H_{ij}(\mathbf{k}) &= \langle \Phi_i(\mathbf{k}, \mathbf{r}) | H | \Phi_j(\mathbf{k}, \mathbf{r}) \rangle = \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_i)} \langle \phi(\mathbf{r} - \mathbf{R} - \mathbf{t}_i) | H | \phi(\mathbf{r} - \mathbf{R} - \mathbf{t}_j) \rangle = \\ &= \sum_{\mathbf{R}_j} e^{i\mathbf{k}\cdot\mathbf{R}_j} \langle \phi_i(\mathbf{r}) | H | \phi_j(\mathbf{r} - \mathbf{R}_j) \rangle = \underbrace{\sum_{\mathbf{R}_j} e^{i\mathbf{k}\cdot\mathbf{R}_j} H_{ij}(\mathbf{R}_j)}_{\text{Bloch Ham.}}, H(\mathbf{R}_j) \rightarrow \text{Fock matrix at } \mathbf{R}_j \end{aligned}$$

Bloch Hamiltonian in the TB approx.

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

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

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

Tight-Binding coefficients

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

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

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

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Polarizability in the TB approximation

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

$$\begin{aligned} \chi_{GG'}^0(\mathbf{q}) &= \frac{1}{\Omega} \sum_{v,c} \sum_{\mathbf{k}} \frac{\langle v, \mathbf{k} + \mathbf{q} | e^{i(\mathbf{q} + \mathbf{G}) \cdot \mathbf{r}} | c, \mathbf{k} \rangle \langle c, \mathbf{k} + \mathbf{q} | e^{-i(\mathbf{q} + \mathbf{G}') \cdot \mathbf{r}} | v, \mathbf{k} \rangle}{\epsilon_{v,\mathbf{k}+\mathbf{q}} - \epsilon_{c,\mathbf{k}}} = \\ &= \frac{1}{\Omega} \sum_{v,c} \sum_{\mathbf{k}} \frac{M_{vc}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{vc}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')}{\epsilon_{v,\mathbf{k}+\mathbf{q}} - \epsilon_{c,\mathbf{k}}} \end{aligned}$$

Polarizability in the TB approximation

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

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

$$\begin{aligned} M_{nn'}(\mathbf{k}, \mathbf{q}, \mathbf{G}) &\equiv \langle n, \mathbf{k} + \mathbf{q} | e^{i(\mathbf{q} + \mathbf{G}) \cdot \mathbf{r}} | n', \mathbf{k} \rangle = \int d\mathbf{r} \psi_{n,\mathbf{k}+\mathbf{q}}^*(\mathbf{r}) e^{i(\mathbf{q} + \mathbf{G}) \cdot \mathbf{r}} \psi_{n'\mathbf{k}}(\mathbf{r}) = \\ &= \sum_{i\alpha} (C_{i\alpha}^{n\mathbf{k}+\mathbf{q}})^* C_{i\alpha}^{n'\mathbf{k}} e^{i(\mathbf{q} + \mathbf{G}) \cdot \mathbf{t}_i} \equiv I_{n\mathbf{k}+\mathbf{q}, n'\mathbf{k}}^{\mathbf{G}} \end{aligned}$$

Polarizability in the TB approximation

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

$$\begin{aligned} \chi_{GG'}^0(\mathbf{q}) &= \frac{1}{\Omega} \sum_{v,c} \sum_{\mathbf{k}} \frac{\langle v, \mathbf{k} + \mathbf{q} | e^{i(\mathbf{q} + \mathbf{G}) \cdot \mathbf{r}} | c, \mathbf{k} \rangle \langle c, \mathbf{k} + \mathbf{q} | e^{-i(\mathbf{q} + \mathbf{G}') \cdot \mathbf{r}} | v, \mathbf{k} \rangle}{\epsilon_{v,\mathbf{k}+\mathbf{q}} - \epsilon_{c,\mathbf{k}}} = \\ &= \frac{1}{\Omega} \sum_{v,c} \sum_{\mathbf{k}} \frac{M_{vc}(\mathbf{k}, \mathbf{q}, \mathbf{G}) M_{vc}^*(\mathbf{k}, \mathbf{q}, \mathbf{G}')}{\epsilon_{v,\mathbf{k}+\mathbf{q}} - \epsilon_{c,\mathbf{k}}} = \frac{1}{A_{\text{UC}} N_k} \sum_{vc} \sum_{\mathbf{k}} \frac{I_{v\mathbf{k}+\mathbf{q}, c\mathbf{k}}^{\mathbf{G}} (I_{v\mathbf{k}+\mathbf{q}, c\mathbf{k}}^{\mathbf{G}'})^*}{\epsilon_{v,\mathbf{k}+\mathbf{q}} - \epsilon_{c,\mathbf{k}}} \end{aligned}$$

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

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Dielectric function computation scheme

- ➊ Diagonalize $H(\mathbf{k})$ and store all $\{\epsilon_{n\mathbf{k}}\}, \{\underline{C}^{n\mathbf{k}}\}$ in a BZ mesh
- ➋ Compute dielectric matrix $\varepsilon_{GG'}(\mathbf{q}) = \delta_{GG'} - v_c(\mathbf{q} + \mathbf{G})\chi_{GG'}^0(\mathbf{q}), \forall \mathbf{q} \in \text{BZ}$
- ➌ Invert $\varepsilon_{GG'}(\mathbf{q}) \forall \mathbf{q} \in \text{BZ}$
- ➍ Compute $W_{G,G'}(\mathbf{q}) = \varepsilon_{GG'}^{-1}(\mathbf{q})v_c(\mathbf{q} + \mathbf{G}') \forall \mathbf{q} \in \text{BZ}$
- ➎ Compute the exciton (details for another time)

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4 Numerical results

5 What is in order? Real space approach

Polarizability convergence

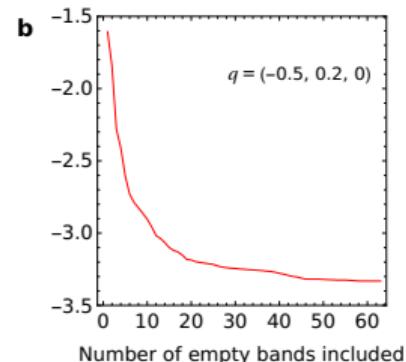
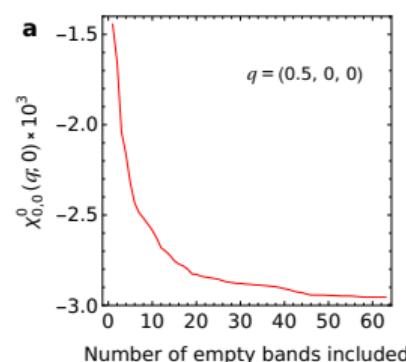
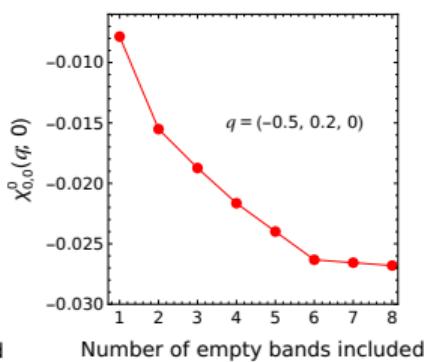
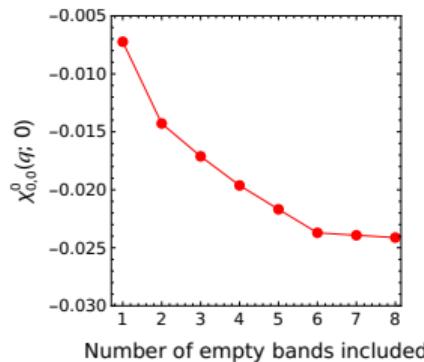


Figure: MoS_2 tight-binding model by Ridolfi [1].

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

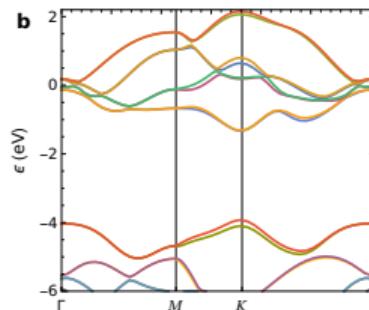
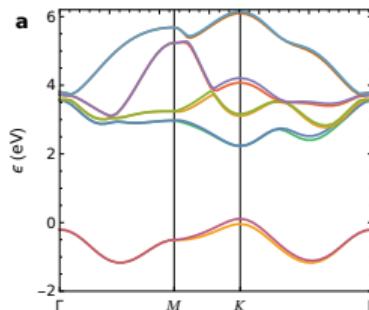


Figure: MoS₂ bands, **a**-Ridolfi's TB model, **b**-Wannier90 [1].

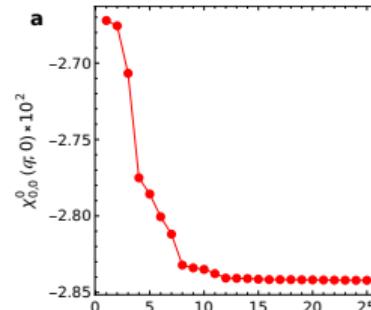
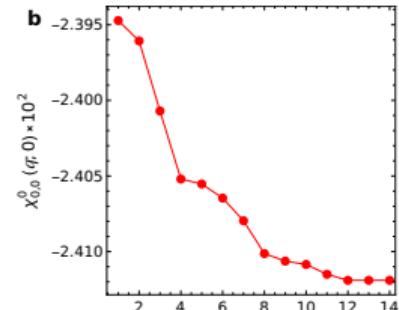


Figure: $\chi_{00}(\mathbf{q})$, $\mathbf{q} = (0.5, 0)$. (**a**->**b**, **b**->**a**)



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

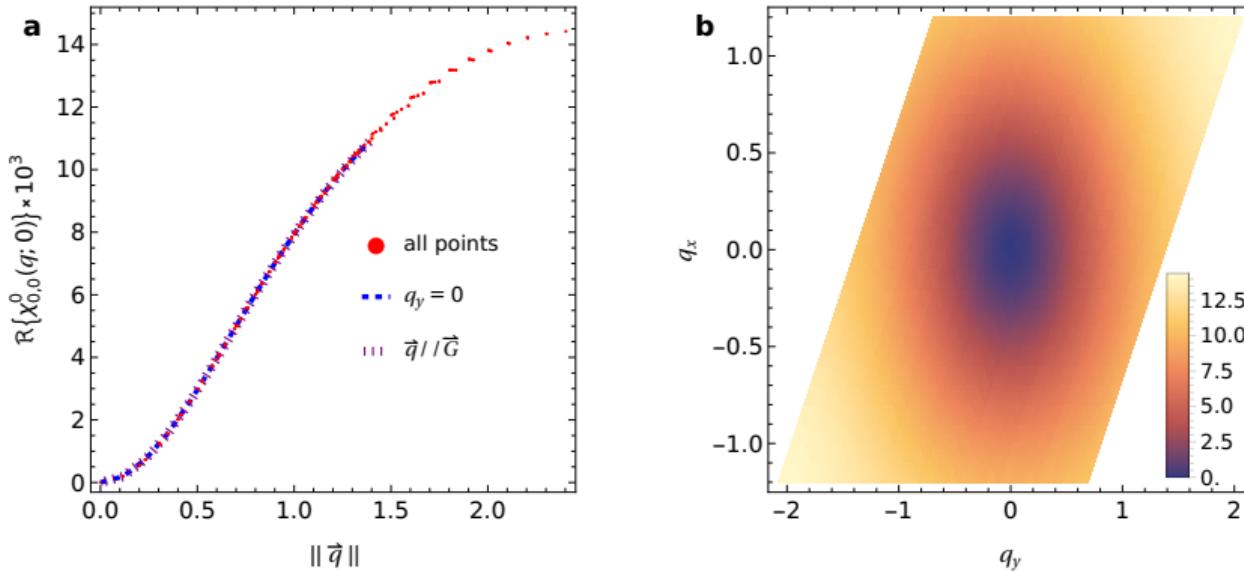


Figure: Panel **a**: $\chi_{00}^0(\vec{q})$ vs. $|\vec{q}|$; Panel **b**: $\chi_{00}^0(\vec{q})$ vs. $\vec{q} \in BZ$. Calculation for hBN, whose bands were obtained within DFT with the HSE06 functional.

Convergence of the inverse dielectric function

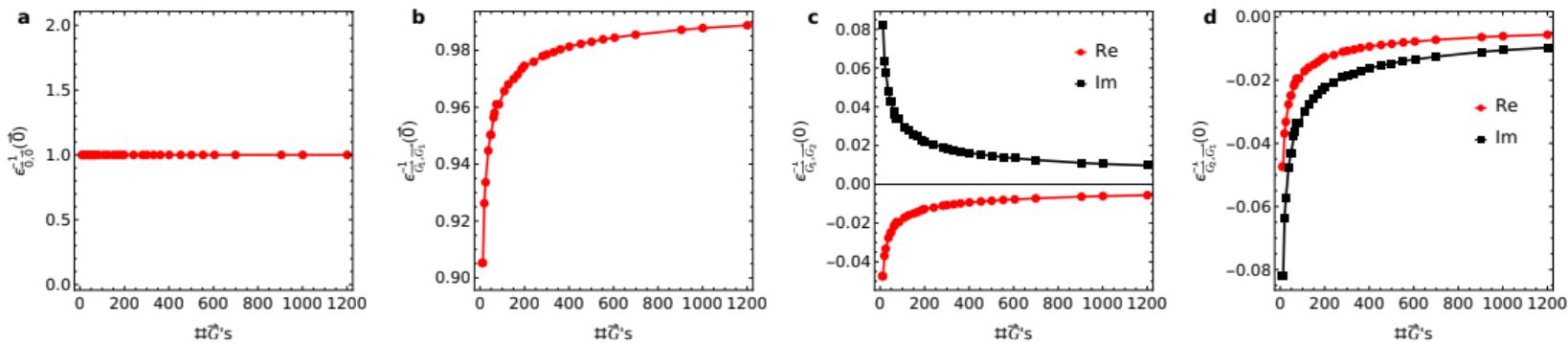


Figure: Selection of matrix elements $\epsilon_{GG'}^{-1}(0)$ for MoS₂ using Ridolfi's tight-binding model. All bands included, and with a BZ mesh with 20 momentum points in each direction. **a** ($G, G' = (0, 0)$), **b** ($G, G' = (G_1, G_1)$), **c** ($G, G' = (G_1, G_2)$), **d** ($G, G' = (G_2, G_1)$). $G_1 = (-1.98835, 1.14797)(\text{\AA}^{-1})$ and $G_2 = -G_1$.

Macroscopic dielectric function

$$\varepsilon_{\text{2D}}(\mathbf{q}) \equiv \frac{1}{\varepsilon_{\mathbf{00}}^{-1}(\mathbf{q})}$$

$$\varepsilon_{\text{RK}}(\mathbf{q}) = 1 + r_0 q$$

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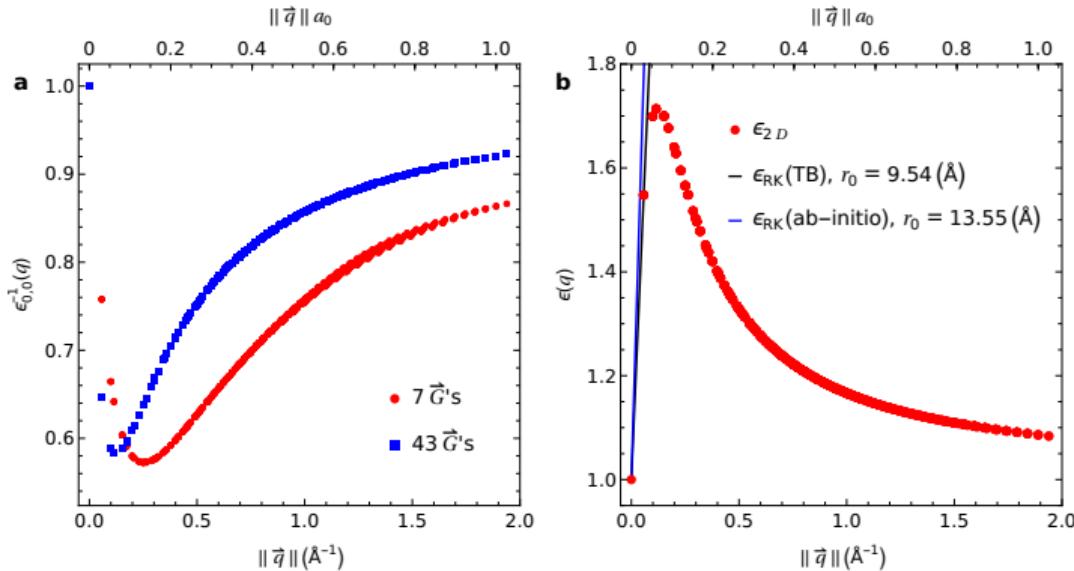


Figure: **a** $\varepsilon_{00}^{-1}(|\mathbf{q}|)$ and **b** $\varepsilon_{2D}(|\mathbf{q}|)$. For MoS₂ using Ridolfi's tight-binding model. In **b** we display the numerical ε_{2D} , the Rytova-Keldysh dielectric function with an estimated $r_0 \approx 9.54 \text{\AA}$ and with the ab-initio one $r_0 = 13.55 \text{\AA}$.

Screened potential

$$v_c(\mathbf{q}) = \frac{e^2}{2\epsilon_0 q}$$

$$V_{RK}(\mathbf{q}) = \frac{e^2}{2\epsilon_0(1 + r_0 q)q}$$

$$W_{00}(\mathbf{q}) = \epsilon_{00}^{-1}(\mathbf{q}) v_c(\mathbf{q})$$

Screened potential

$$v_c(\mathbf{q}) = \frac{e^2}{2\epsilon_0 q} \text{ (black dots)}$$

$$V_{RK}(\mathbf{q}) = \frac{e^2}{2\epsilon_0(1 + r_0 q)q} \text{ (blue dots)}$$

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

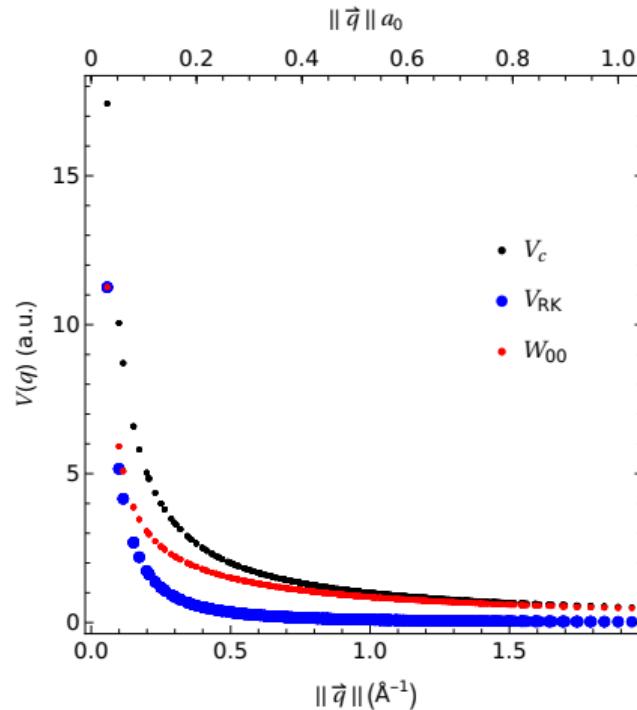


Figure: Bare and screened potentials for MoS₂ using Ridolfi's TB model. 43 Gs included.

Screened potential

$$v_c(\mathbf{q}) = \frac{e^2}{2\epsilon_0 q} \text{ (black dots)}$$

$$V_{RK}(\mathbf{q}) = \frac{e^2}{2\epsilon_0(1 + r_0q)q} \text{ (blue dots)}$$

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

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

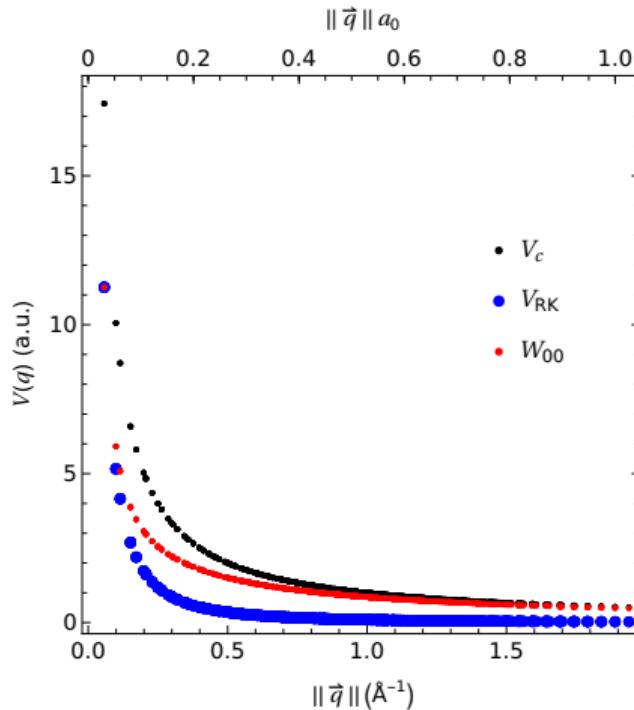


Figure: Bare and screened potentials for MoS₂ using Ridolfi's TB model. 43 Gs included.

A use case: excitons in MoS₂

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 ($\varepsilon_{G,G'}$) (eV)	B. energy ($\varepsilon_{G,G'}$) (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 MoS₂ 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.

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Revisiting Dyson's equation

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

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

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

Revisiting Dyson's equation

In the continuum

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

Discretized version, in the point-like orbital approximation

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

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

Screened potential in real space

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

is equivalent to

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

System of linear equations, however....

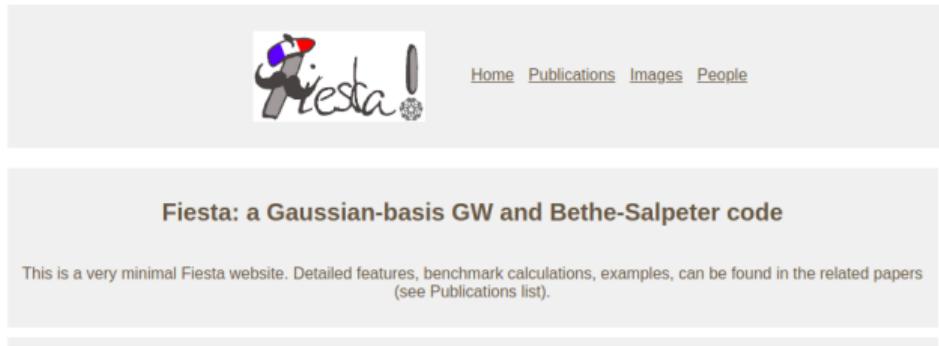
- $W(\mathbf{R} + \mathbf{t}_i, t_j) > 0$ sometimes, $W(\mathbf{R} + \mathbf{t}_i, t_j) < 0$ other times;
- Situation improves including the term $\mathbf{R}_1 + \mathbf{t}_{i'} = \mathbf{R} + \mathbf{t}_i$, but result is regularization dependent.

Screened potential in real space: what to do?

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

$$W(\mathbf{R} + \mathbf{t}_i, \mathbf{t}_j) =$$

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



The screenshot shows the homepage of the Fiesta code. At the top, there is a navigation bar with links to Home, Publications, Images, and People. The main content area features a large logo with the word "Fiesta!" in a stylized font, accompanied by a small atomic model icon. Below the logo, the text "Fiesta: a Gaussian-basis GW and Bethe-Salpeter code" is displayed. A descriptive paragraph follows, stating: "This is a very minimal Fiesta website. Detailed features, benchmark calculations, examples, can be found in the related papers (see Publications list)." A horizontal scrollbar is visible on the right side of the content area.

Acknowledgments

Juan José Palacios



Alex



Acknowledgments

Juan José Palácios



Alex



Juanjo



Manuel António



Simran

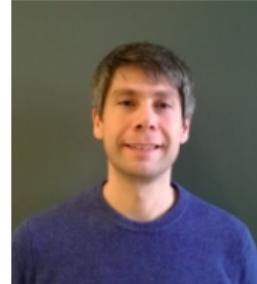
David

Acknowledgments

Juan José Palácios



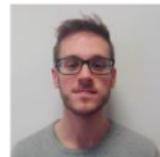
António Picón



Alex



Juanjo



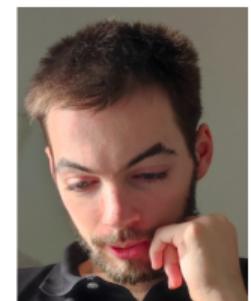
Manuel António



Miguel



Maurício



Simran

David

Acknowledgments

Vinicius



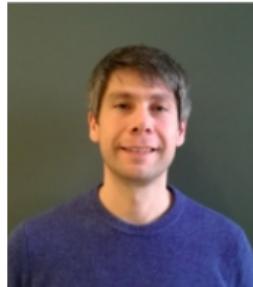
Juan José Palacios



Guilherme



António Picón



Alex



Juanjo



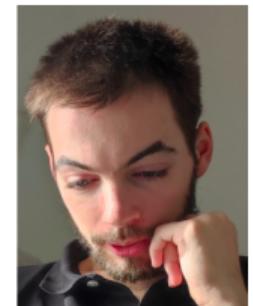
Manuel António



Miguel



Maurício



Simran

David

Acknowledgments

Vinicius



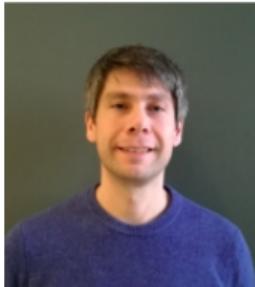
Juan José Palacios



Guilherme



António Picón



Johan



Alex



Juanjo



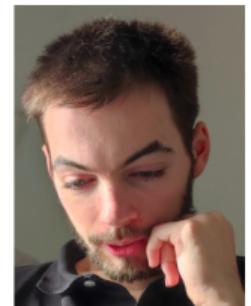
Manuel António



Miguel



Maurício



Simran

David