Graphene Nanophotonics
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Spatial Dispersion and the Tensor Intraband Conductivity of Graphene: Importance for Modeling Graphene Nanoribbons

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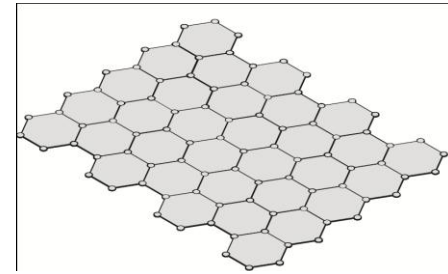
Giampiero Lovat, Rodolfo Araneo, Paolo Burghignoli, University of Rome "Sapienza", Italy



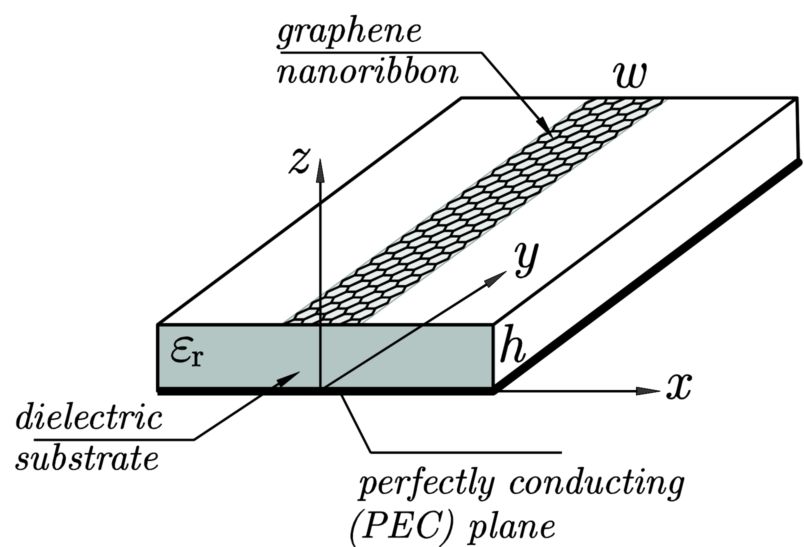
Introduction

The main focus is propagation properties of **graphene nanoribbons** (GNR).

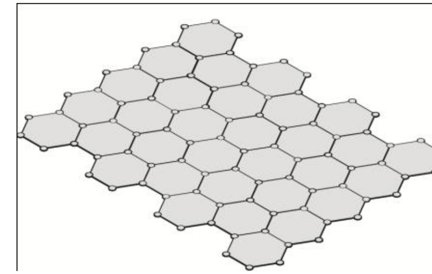
We concentrate on the frequency range 1-1000 GHz:

Less explored (since a lot of the interesting stuff happens from 1-50 THz)

However, the low GHz range is important for possible graphene interconnects and/or all-graphene circuits.

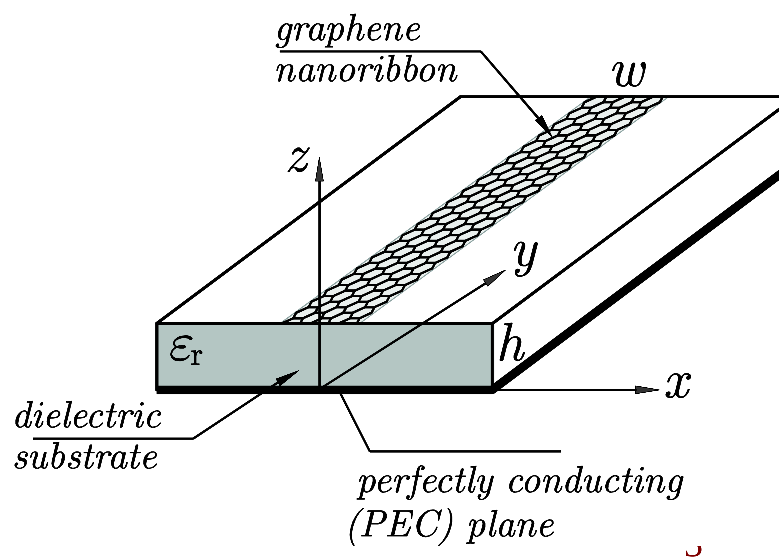


Introduction

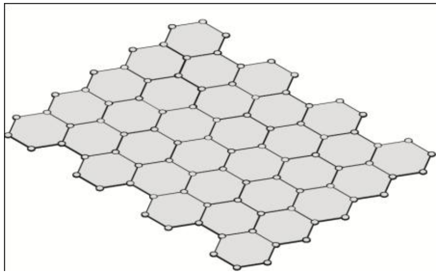


Based on the need to consider very slow modes on GNR, we derived analytical expressions for the spatially-dispersive intraband conductivity tensor of graphene, valid for any wavevector.

Derived from the semi-classical Boltzmann transport equation under the Bhatnagar-Gross-Krook model (allowing for number conservation – the Mermin correction).



Previous work – surface plasmons on local graphene



There has been a lot of previous work on **surface waves on infinite graphene sheets.**

An early and important paper is
S. A. Mikhailov and K. Ziegler, PRL **99**, 016803 2007.

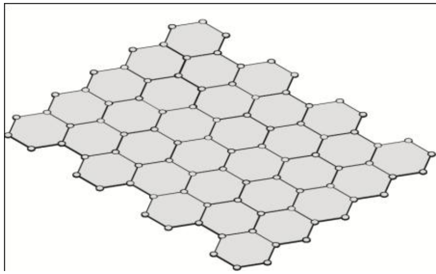
Interplay of intra- and interband conductivity governs the sign of Im(σ):

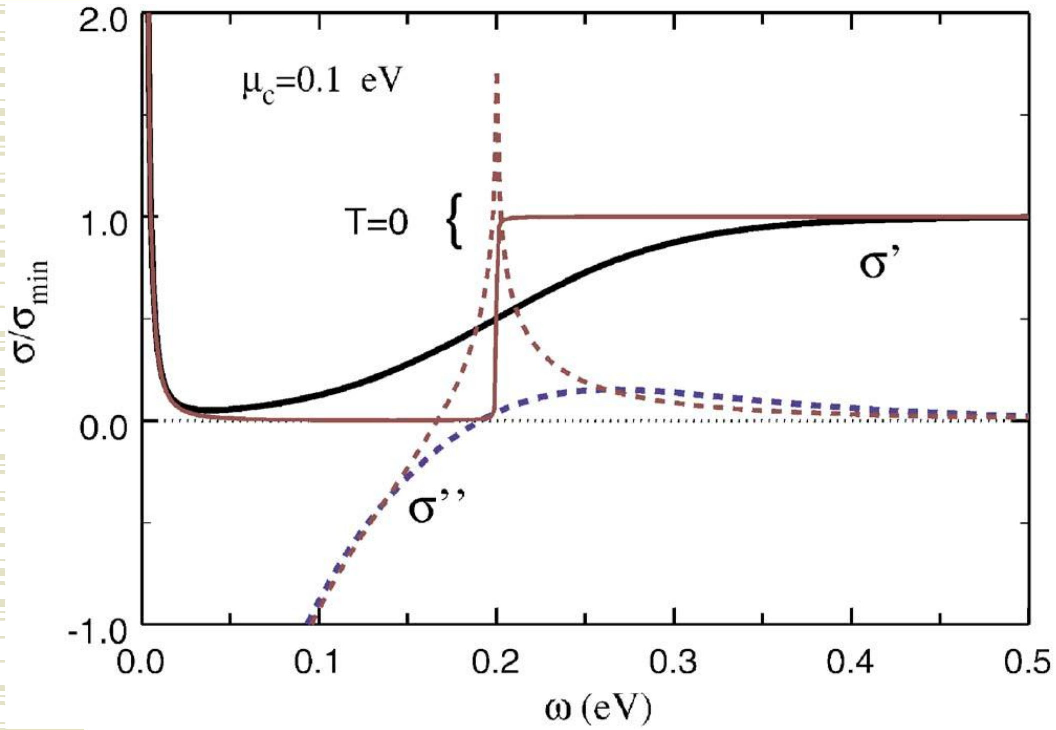
Im(σ)>0: intraband contribution dominates, only TM modes allowed

Im(σ)<0: interband contribution dominates, only TE modes allowed

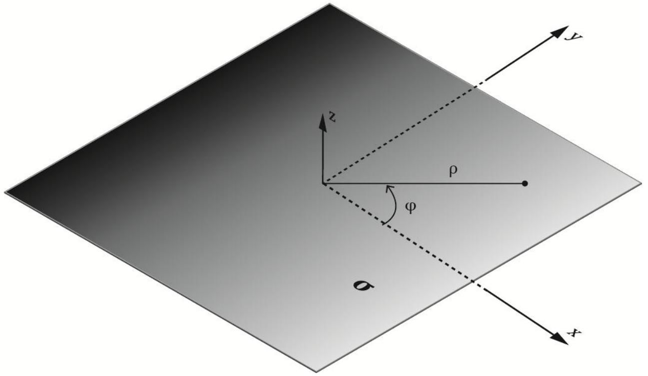
($e^{-i\omega t}$ assumed)

Previous work – surface plasmons on local graphene

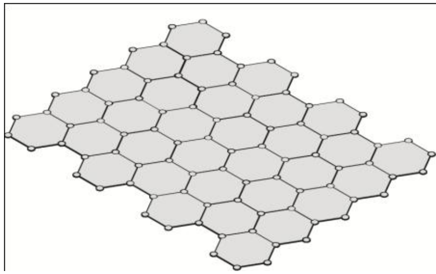


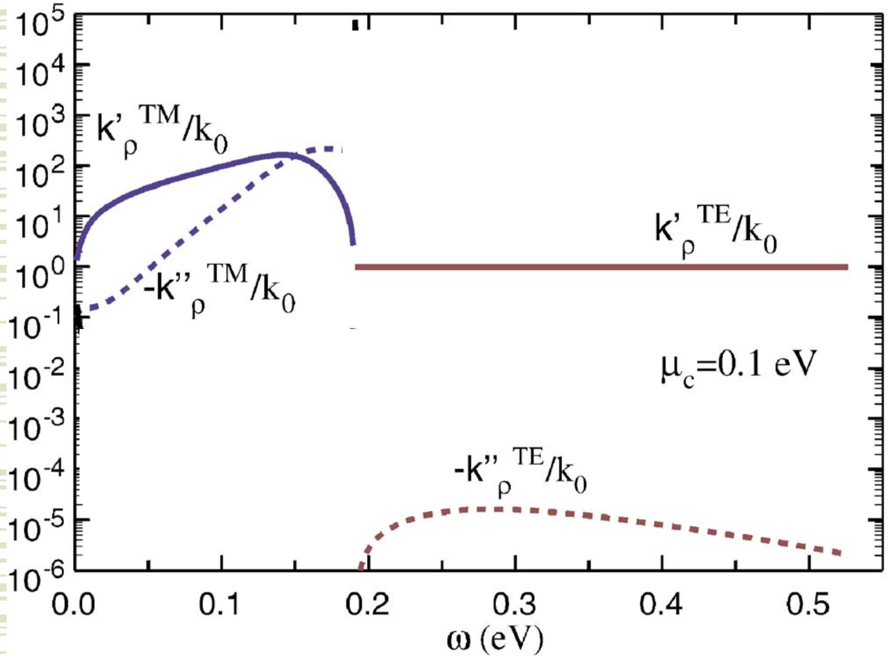


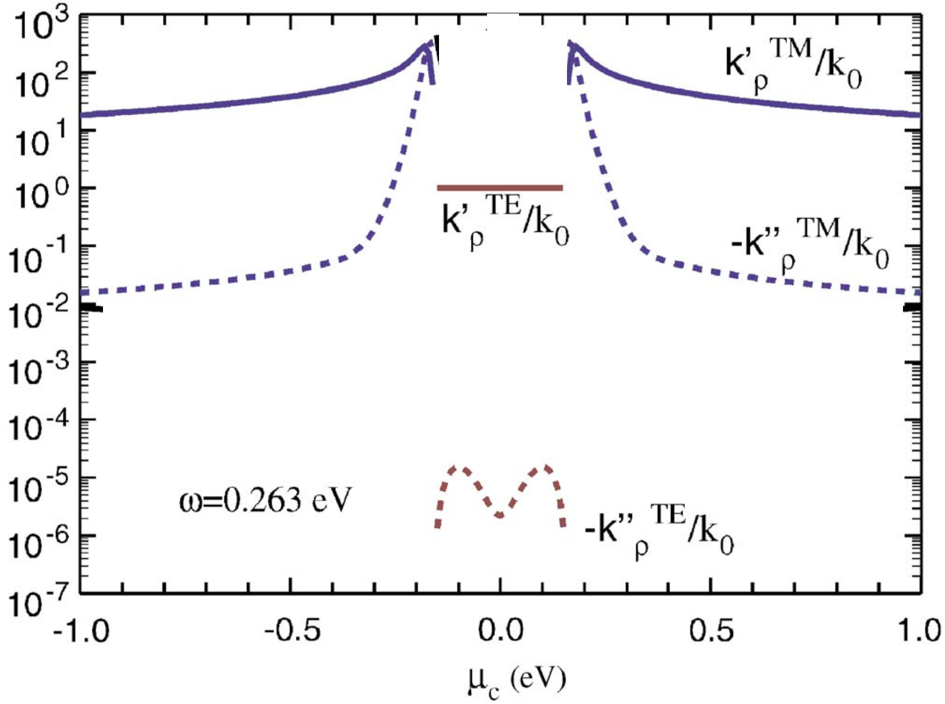
Local conductivity model



Previous work – surface plasmon propagation on local graphene

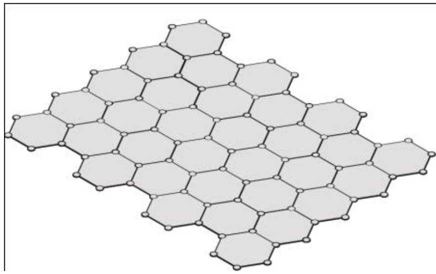


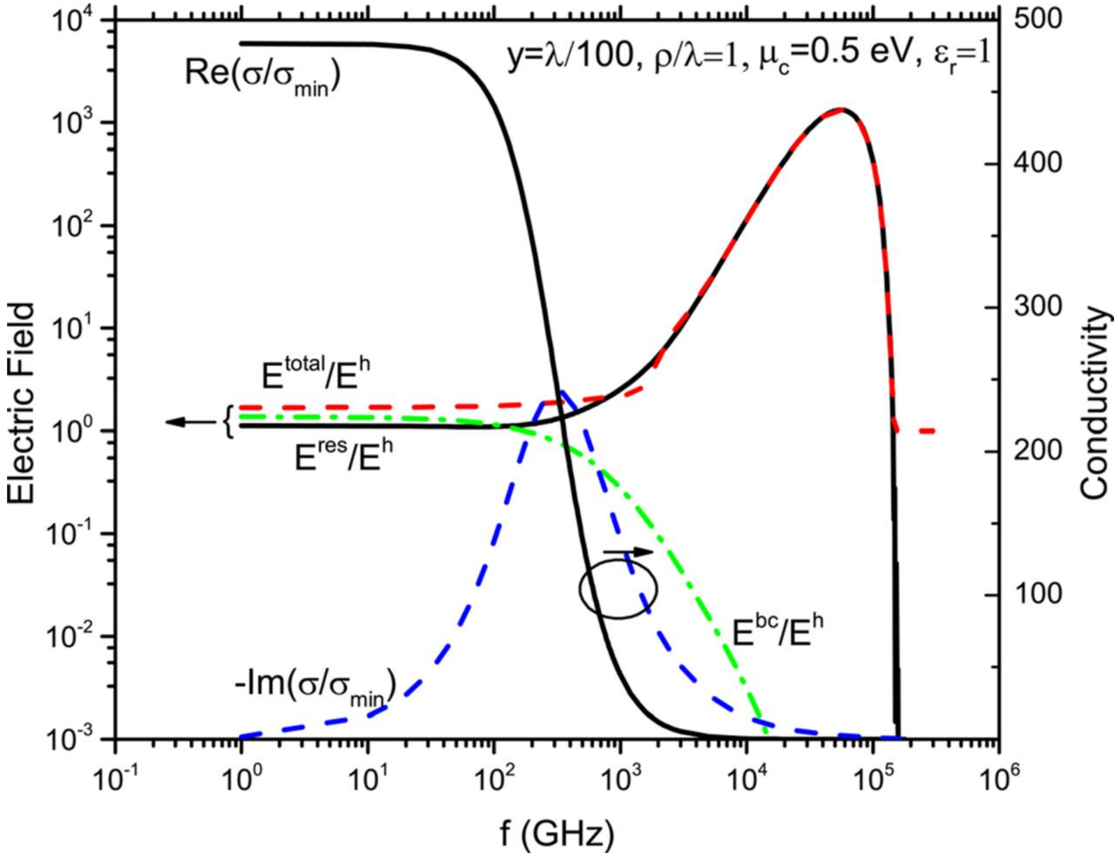




Hanson, J. Appl. Phys., v. 103, pp. 064302 (1-7), 2008.

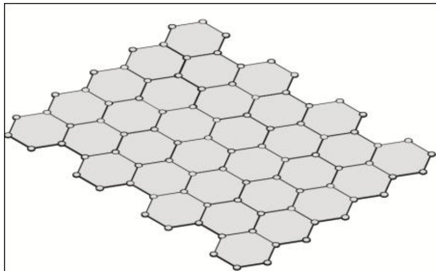
Previous work – **excitation amplitude** of surface plasmons on local graphene





G.W. Hanson, E. Forati, W. Linz, and A.B. Yakovlev, PRB **86**, 235440 (1-9), 2012.
G.W. Hanson, A.B. Yakovlev, and A. Mafi, JAP 110, 114305 (1-8), 2011.

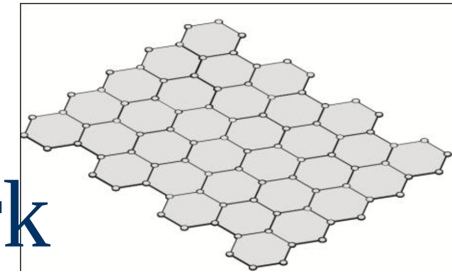
Introduction – previous work – spatial dispersion



Previous work on spatial dispersion in graphene:

L.A. Falkovsky and S.S. Pershoguba, Phys. Rev. B, 76, 153410 (2007).
S.A. Mikhailov and K. Ziegler, Phys. Rev. Lett. 99, 016803 (2007).
V.P. Gusynin and S.G. Sharapov, Phy. Rev. B., 73, 245411 (2006).
V.P. Gusynin, S.G. Sharapov, and J.P. Carbotte, Phys. Rev. Lett., 96, 256802 (2006).
N.M.R. Peres, F. Guinea, and A.H. Castro Neto, Phys. Rev. B, 73, 125411 (2006).
N.M.R. Peres, A.H. Castro Neto, and F. Guinea, Phys. Rev. B, 73, 195411 (2006).
K. Ziegler, Phys. Rev. B, 75, 233407 (2007).
L. A. Falkovsky and A.A. Varlamov, Eur. Phys. J. B, 56, 281 (2007).
V.P. Gusynin, S.G. Sharapov, and J.P. Carbotte, J. Phy.: Condens Matter, 19, 026222 (2007).
V.P. Gusynin, S.G. Sharapov, and J.P. Carbotte, Phys. Rev. B 75, 165407 (2007).

Introduction – Previous Work



PHYSICAL REVIEW B **75**, 205418 (2007)

Dielectric function, screening, and plasmons in two-dimensional graphene

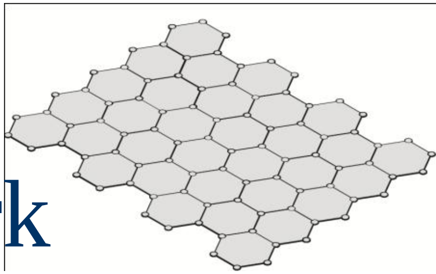
E. H. Hwang and S. Das Sarma
Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA
(Received 4 October 2006; published 11 May 2007)

In the RPA, the dynamical screening function (dielectric function) becomes

$$\varepsilon(q,\omega) = 1 + v_c(q)\Pi(q,\omega), \qquad (2)$$

where $v_c(q) = 2\pi e^2/\kappa q$ is the 2D Coulomb interaction, and $\Pi(q,\omega)$, the 2D polarizability.

Analytical formulas are presented for the scalar permittivity for T=0, τ^{-1}=0, and q real.



Introduction – Previous Work

Our previous work on tensor intraband spatial dispersion in graphene

G.W. Hanson, IEEE Trans. Antennas Propagat., v. 56, pp. 747-757, Mar., 2008.

$$\sigma_{xx} = \sigma + \alpha \frac{\partial^2}{\partial x^2} + \beta \frac{\partial^2}{\partial y^2},$$

$$\sigma_{xy} = 2\beta \frac{\partial^2}{\partial x \partial y},$$

$$\sigma_{yx} = \sigma_{xy},$$

$$\sigma_{yy} = \sigma + \beta \frac{\partial^2}{\partial x^2} + \alpha \frac{\partial^2}{\partial y^2},$$

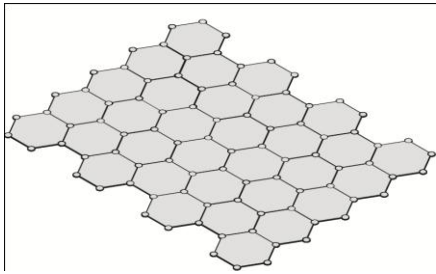
$$\sigma = \frac{-j2\ln(2)e^2 k_B T}{\pi(\omega - i\tau^{-1})\hbar^2},$$

$$\alpha = -\frac{3}{4}\frac{v_F^2}{(\omega - i\tau^{-1})^2}\sigma, \quad \beta = \frac{1}{3}\alpha$$

valid for small-q

only implemented the RTA approximation

Need for spatial dispersion – very slow modes

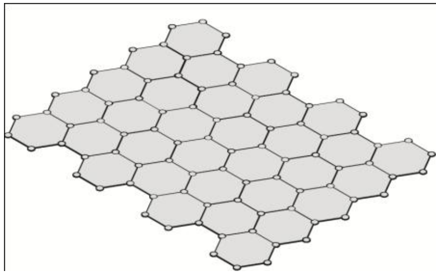


$$\boldsymbol{\sigma}^{\mathrm{RTA}}(\mathbf{q},\omega) = \frac{j2e^2}{(2\pi)^2}\iint \frac{\mathbf{v}\mathbf{v}}{\omega - \mathbf{v}\cdot\mathbf{q} - j\tau^{-1}}\frac{\partial f_0(\mathbf{k})}{\partial \varepsilon}\, d^2\mathbf{k},$$

If $|\mathbf{q}| << \omega/v_F$, then $\sigma^{RTA}(\mathbf{q},\omega) \approx \sigma^{RTA}(\omega)$ and we can assume the local response.

If $|\mathbf{q}| \geq \omega/v_F$, then $\sigma^{RTA}(\mathbf{q},\omega)$ and we need to include spatial dispersion.

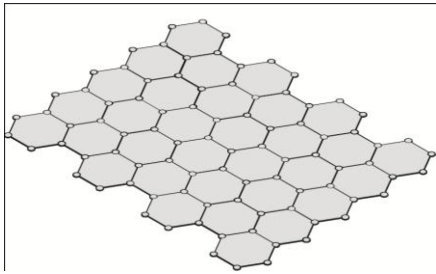
$|\mathbf{q}|/k_0 \geq c/v_F \approx 300$



We found that for surface waves on infinite graphene sheets, spatial dispersion seems to be **unimportant**.

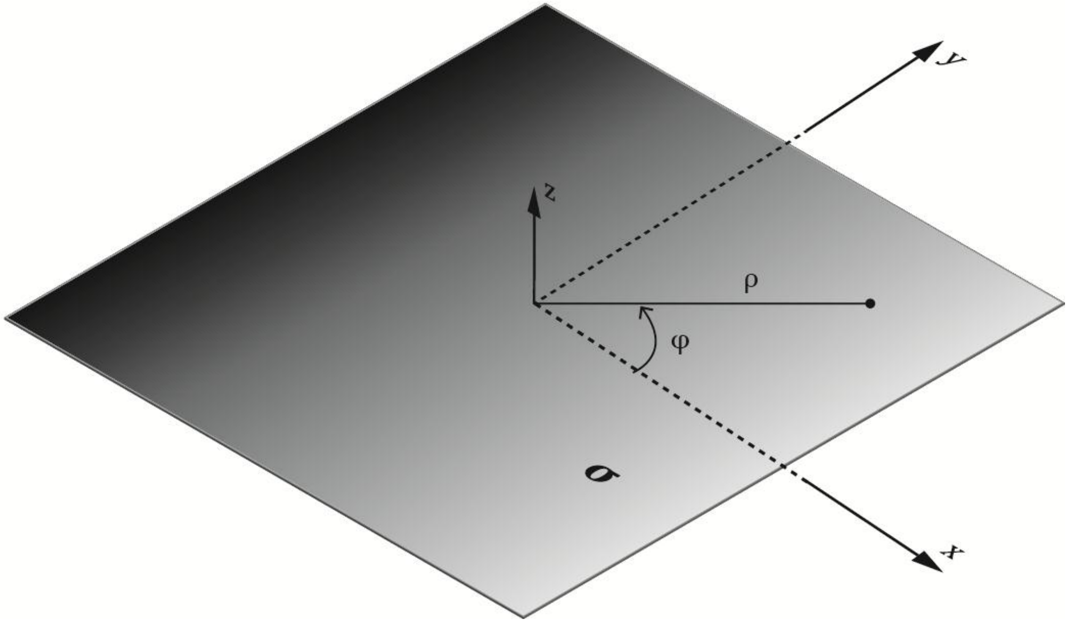
For graphene nanoribbons, above a few THz spatial dispersion may be **unimportant** (at least for phase constant).

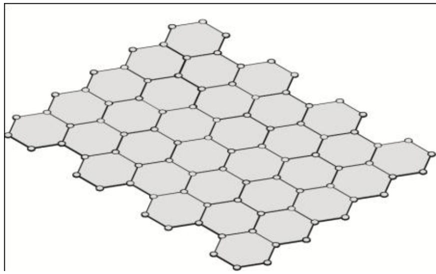
For graphene nanoribbons, below a THz spatial dispersion seems to be **very important**.



Formulation

Infinite contiguous graphene sheet modeled by surface conductivity σ (S)





Formulation

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0 e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}$$

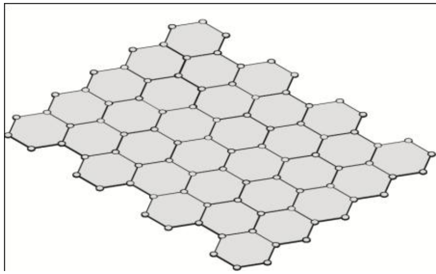
Space-time dependence of field

Energy relationship (tight-binding)

$$\varepsilon^{\pm}(\mathbf{k}) = \varepsilon^{\pm}(k_x,k_y) \simeq \pm\gamma_0 \frac{w(k_x,k_y)}{1 \mp s_0 w(k_x,k_y)}$$

$$w(k_x,k_y) = \sqrt{1 + 4\cos\frac{\sqrt{3}\,a}{2}k_x \cos\frac{a}{2}k_y + 4\cos^2\frac{a}{2}k_y}\ .$$

Formulation



$$\mathbf{v}^{\pm} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon^{\pm}(\mathbf{k})$$

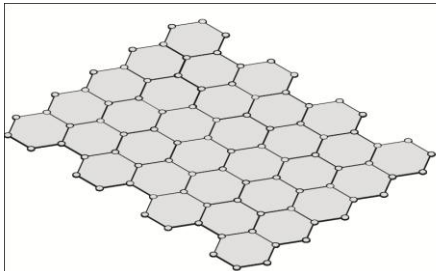
Electron velocity

Current density

$$\mathbf{J}(\mathbf{q}) = \mathbf{J}|_{\pi^*\,\mathrm{band}} + \mathbf{J}|_{\pi\,\mathrm{band}} = \mathbf{J}_{\mathrm{e}} + \mathbf{J}_{\mathrm{h}}$$

$$= 2\frac{e}{(2\pi)^2}\iint_{\mathrm{B.Z.}} \mathbf{v}^{+}(\mathbf{k}) f_{\mathrm{e}}(\mathbf{k},\mathbf{q})\,\mathrm{d}^2\mathbf{k}\Bigg|_{\pi^*\,\mathrm{band}} + 2\frac{(-e)}{(2\pi)^2}\iint_{\mathrm{B.Z.}} \mathbf{v}^{-}(\mathbf{k}) f_{\mathrm{h}}(\mathbf{k},\mathbf{q})\,\mathrm{d}^2\mathbf{k}\Bigg|_{\pi\,\mathrm{band}}$$

Formulation



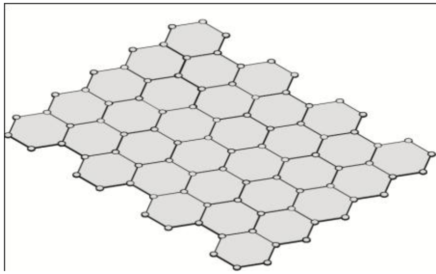
A perturbation approach leads to $f_{\mathrm{e}} = f_{\mathrm{e}}^{(0)} + f_{\mathrm{e}}^{(1)}$ and $f_{\mathrm{h}} = 1 - f_{\mathrm{e}} = f_{\mathrm{h}}^{(0)} + f_{\mathrm{h}}^{(1)}$, where $\left|f_{\mathrm{e/h}}^{(1)}\right| \ll \left|f_{\mathrm{e/h}}^{(0)}\right|$,

Non-equilibrium distribution function from Boltzmann's equation:

$$f_{e/h}^{(1)}(\mathbf{k},\mathbf{q}) = \frac{ih_{e/h}(\mathbf{k})\tau^{-1} - ie\mathbf{E}(\mathbf{q},\omega)\cdot\mathbf{v}^{\pm}(\mathbf{k})\frac{\partial f_e^{(0)}}{\partial\varepsilon}}{\omega - \mathbf{v}^{\pm}(\mathbf{k})\cdot\mathbf{q} + i\tau^{-1}}$$

$$h_{\mathrm{e/h}}(\mathbf{k}) = \left.\frac{\partial f_{e/h}}{\partial n_{e/h}}\right|_0 \left(n_{e/h} - n_{e/h}^{(0)}\right)$$

$$n_{\mathrm{e/h}} = \frac{2}{(2\pi)^2}\iint_{\mathrm{B.Z.}} f_{\mathrm{e/h}}(\mathbf{k})\,\mathrm{d}^2\mathbf{k}, \qquad n_{\mathrm{e/h}}^{(0)} = \frac{2}{(2\pi)^2}\iint_{\mathrm{B.Z.}} f_{\mathrm{e/h}}^{(0)}(\mathbf{k})\,\mathrm{d}^2\mathbf{k}$$



Formulation

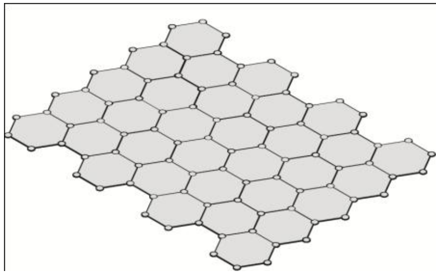
Resulting current density

$$\mathbf{J}(\mathbf{q}) = \underline{\boldsymbol{\sigma}}^{BGK}(\mathbf{q}) \cdot \mathbf{E}_0 e^{i\mathbf{q}\cdot\mathbf{r}}$$

$$\sigma_{rs}^{\mathrm{BGK}}(\mathbf{q}) = \sigma_{rs}^{\mathrm{e}}(\mathbf{q}) + \sigma_{rs}^{\mathrm{h}}(\mathbf{q}), \qquad r,s = x,y$$

$$\sigma_{\alpha\alpha}^{e/h}(\mathbf{q}) = \frac{\sigma_{e/h_{\alpha\alpha}}^{\mathrm{RTA}} + q_\beta\left(\sigma_{e/h_{\alpha\alpha}}^{\mathrm{RTA}} d_{e/h_\beta} - \sigma_{e/h_{\beta\alpha}}^{\mathrm{RTA}} d_{e/h_\alpha}\right)}{1 + (q_\alpha d_{e/h_\alpha} + q_\beta d_{e/h_\beta})}, \quad \alpha,\beta = x,y, \quad \beta \neq \alpha$$

$$\sigma_{\alpha\beta}^{e/h}(\mathbf{q}) = \frac{\sigma_{e/h_{\alpha\beta}}^{\mathrm{RTA}} + q_\beta\left(\sigma_{e/h_{\alpha\beta}}^{\mathrm{RTA}} d_{e/h_\beta} - \sigma_{e/h_{\beta\beta}}^{\mathrm{RTA}} d_{e/h_\alpha}\right)}{1 + (q_\alpha d_{e/h_\alpha} + q_\beta d_{e/h_\beta})}, \quad \alpha,\beta = x,y, \quad \beta \neq \alpha$$



Formulation

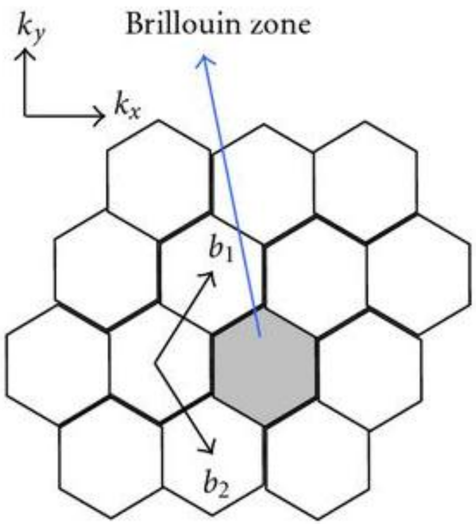
Terms involving numerical integration over first BZ:

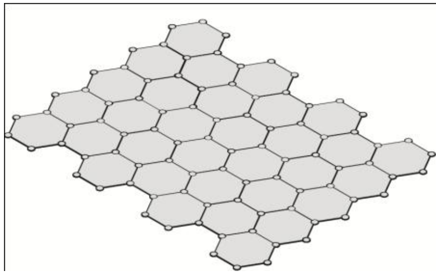
$$\underline{\boldsymbol{\sigma}}^{\mathrm{RTA}}_{\mathrm{e/h}} = \frac{ie^2}{8k_B T\pi^2}\underline{\mathbf{A}}_{\mathrm{ee/hh}}(\mathbf{q})$$

$$\underline{\mathbf{A}}_{\mathrm{ee/hh}}(\mathbf{q}) = \iint\limits_{\mathrm{B.Z.}} \frac{\mathbf{v}^{\pm}\mathbf{v}^{\pm}}{\cosh^2\left(\frac{\varepsilon^{\pm}(\mathbf{k})-\mu}{2k_BT}\right)(\omega - \mathbf{v}^{\pm}\cdot\mathbf{q} + i\tau^{-1})}\,\mathrm{d}^2\mathbf{k}$$

$$\underline{\mathbf{d}}_{\mathrm{e/h}}(\mathbf{q}) = -\frac{i}{\omega\tau F_{e/h}}\iint\limits_{\mathrm{B.Z.}} \frac{\mathbf{v}^{\pm}}{\cosh^2\left(\frac{\varepsilon^{\pm}(\mathbf{k})-\mu}{2k_BT}\right)(\omega - \mathbf{v}^{\pm}\cdot\mathbf{q} + i\tau^{-1})}\,\mathrm{d}^2\mathbf{k}$$

$$F_{\mathrm{e/h}}(\mathbf{q}) = \iint\limits_{\mathrm{B.Z.}} \frac{1}{\cosh^2\left(\frac{\varepsilon^{\pm}(\mathbf{k})-\mu}{2k_BT}\right)}\,\mathrm{d}^2\mathbf{k}$$



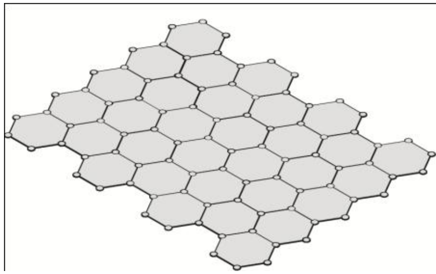


Formulation

We have evaluated the integrals numerically, resulting in what we call the **exact solution** (within a Boltzmann model assuming tight-binding energy dispersion).

Assuming linear dispersion throughout the first BZ , approximate **analytical evaluation** of the integrals can be performed.

This replaces our previous RTA power-series solution valid for small |q| values.



Formulation

The conductivity tensor has a diagonal form in a polar coordinate system.

$$\underline{\mathbf{M}} = \frac{1}{q}\begin{bmatrix} q_x & -q_y \\ q_y & q_x \end{bmatrix}$$

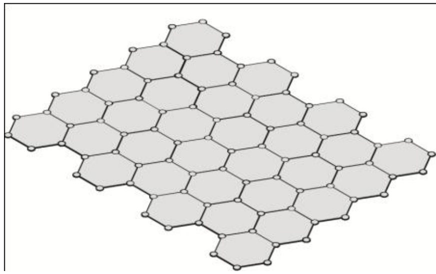
Matrix of eigenvectors

$$\underline{\boldsymbol{\sigma}}^{\mathrm{BGK}}(q) = \begin{bmatrix} \sigma_{\rho}^{\mathrm{BGK}}(q) & 0 \\ 0 & \sigma_{\phi}^{\mathrm{BGK}}(q) \end{bmatrix}$$

Resulting diagonalized conductivity

This implies that the electric field-surface current relationship is invariant under arbitrary rotations of the sheet in that plane.

Formulation



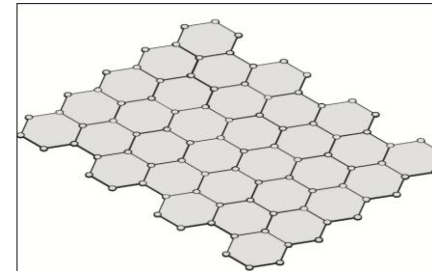
Approximate analytical evaluation of the graphene conductivity: the BGK and RTA forms for low-q values

$$\sigma_{xx} \simeq \gamma \frac{\pi}{\omega + i\tau^{-1}} \left\{ 1 + \left(\left(3 + i\frac{2}{\omega\tau} \right) q_x^2 + q_y^2 \right) \frac{v_F^2}{4(\omega + i\tau^{-1})^2} \right\}$$

$$\sigma_{xy} \simeq \gamma \frac{\pi}{\omega + i\tau^{-1}} \left(1 + \frac{1}{\omega\tau} \right) \frac{v_F^2}{2(\omega - i\tau^{-1})^2} q_x q_y = \sigma_{yx}$$

$$\sigma_{yy} \simeq \gamma \frac{\pi}{\omega + i\tau^{-1}} \left\{ 1 + \left(\left(3 + i\frac{2}{\omega\tau} \right) q_y^2 + q_x^2 \right) \frac{v_F^2}{4(\omega + i\tau^{-1})^2} \right\}$$

Formulation



Quantum Capacitance of a Graphene Sheet

It is natural to define the graphene distributed impedance as

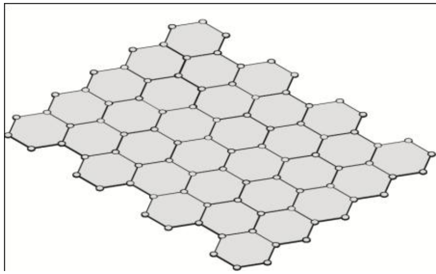
$$z = E_\rho / J_\rho$$

In the low-q approximation, $\sigma_\rho = \gamma \frac{\pi}{\omega + i\tau^{-1}}(1 + a_0 q^2)$

$$a_0^{\mathrm{BGK}} = \left(\frac{3}{4} + i\frac{1}{2\omega\tau}\right)\frac{v_F^2}{(\omega + i\tau^{-1})^2}$$

$$a_0^{\mathrm{RTA}} = \frac{3}{4}\frac{v_F^2}{(\omega + i\tau^{-1})^2}$$

Formulation



$$z = \frac{1}{\sigma_\rho} \simeq R - i\omega L_{\mathrm{k}} - \frac{q^2}{i\omega C_{\mathrm{q}}}\xi$$

Distributed impedance

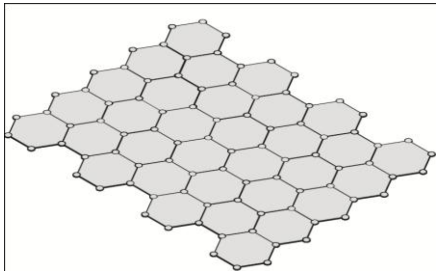
$$R = \frac{\pi\hbar^2}{e^2\tau k_B T \ln\left(2\left[1 + \cosh\left(\frac{\mu}{k_B T}\right)\right]\right)}$$

$$L_{\mathrm{k}} = \tau R$$

$$C_{\mathrm{q}} = \frac{2e^2 k_B T \ln\left(2\left[1 + \cosh\left(\frac{\mu}{k_B T}\right)\right]\right)}{\pi\hbar^2 v_F^2}$$

Agrees with the results of others for the quantum capacitance

Formulation



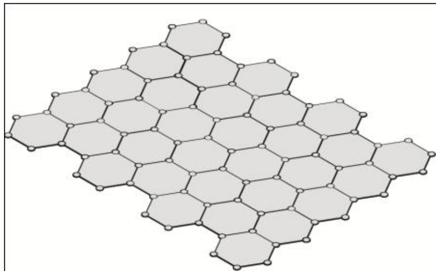
The presence of quantum capacitance is a consequence of including spatial dispersion.

The parameter ξ is dramatically different in the BGK and the RTA models, such that the low-frequency impedance is

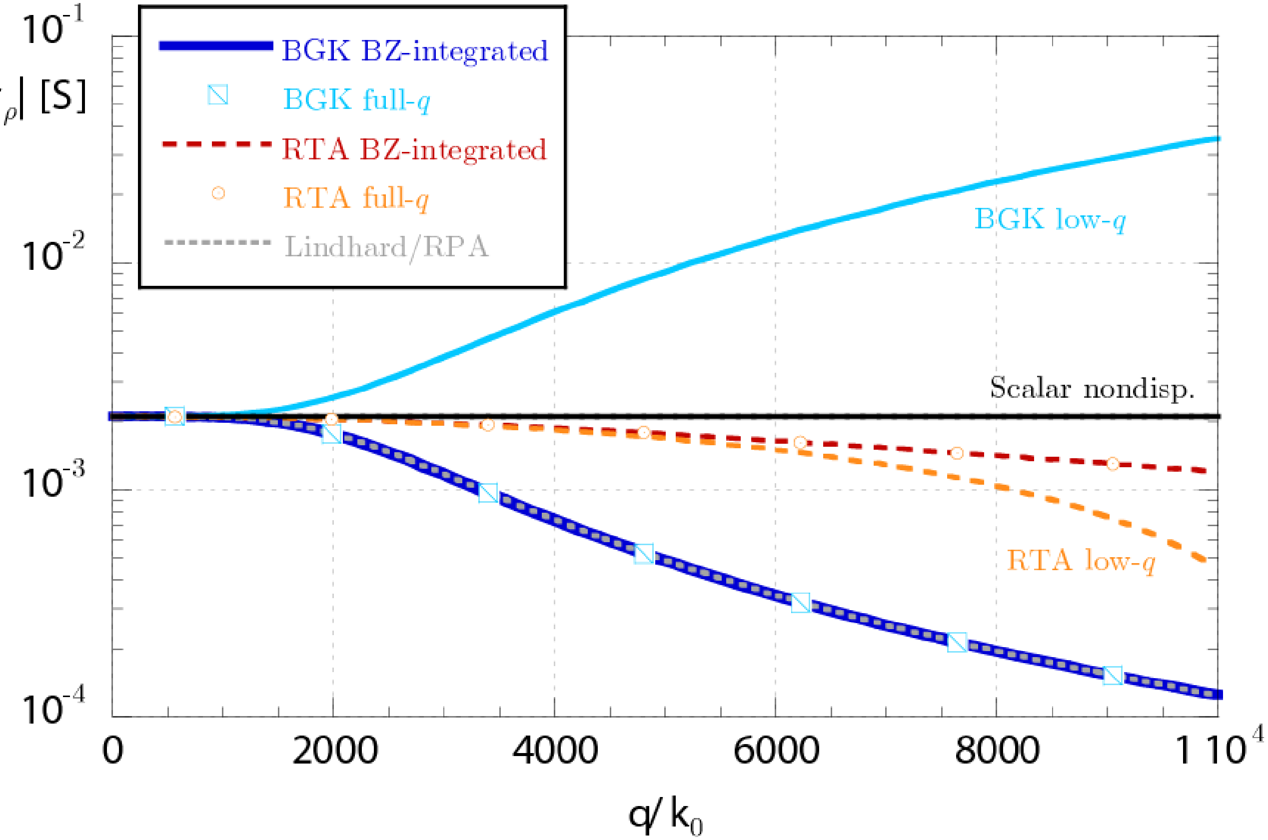
$$z^{\mathrm{BGK}} \to R - i\omega L_{\mathrm{k}} - \frac{q^2}{i\omega C_{\mathrm{q}}}$$

$$z^{\mathrm{RTA}} \to R - i\omega L_{\mathrm{k}}$$

Graphene Conductivity

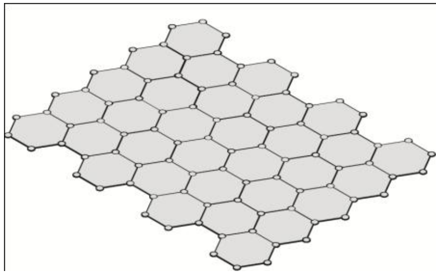


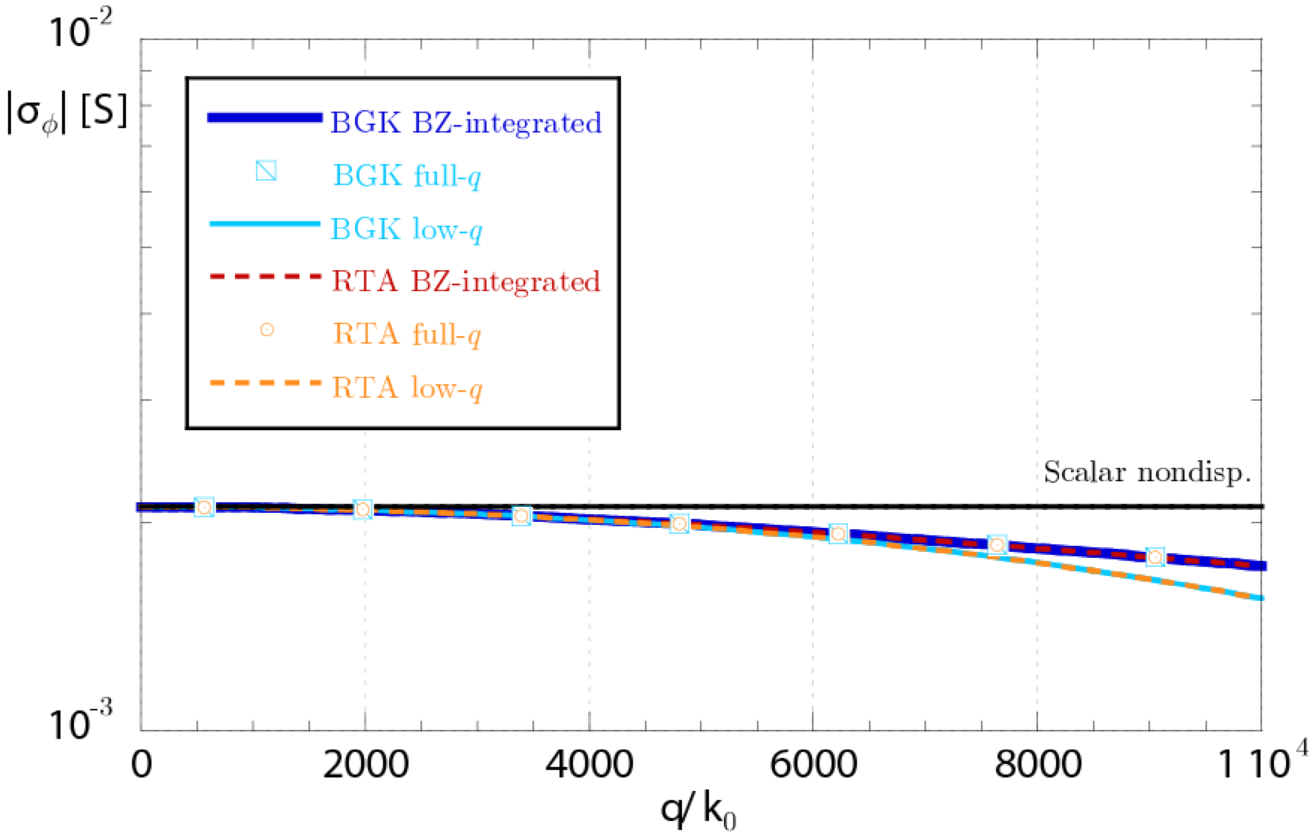
In all cases τ=0.5 ps, μ=0 eV, and T=300 K.



f=10 GHz

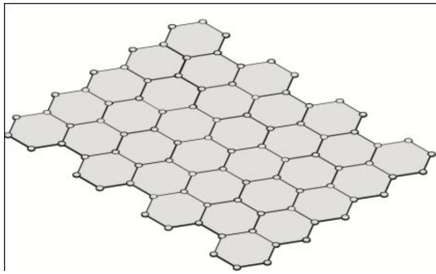
Graphene Conductivity

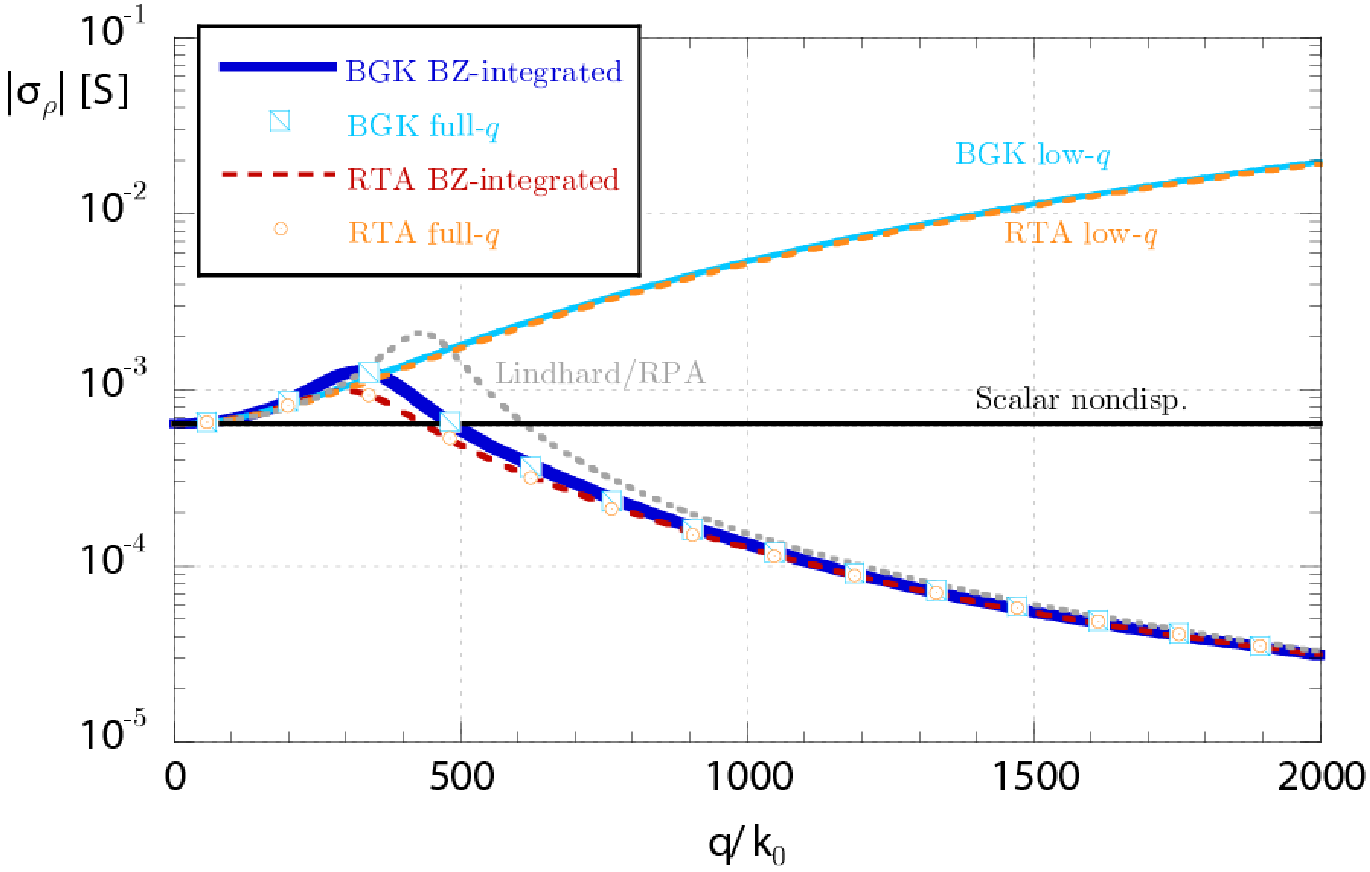




f=10 GHz

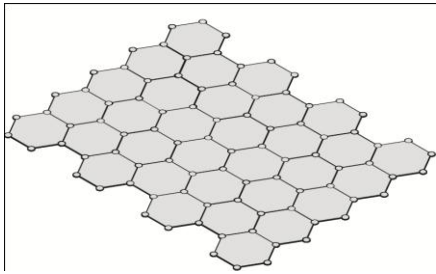
Graphene Conductivity

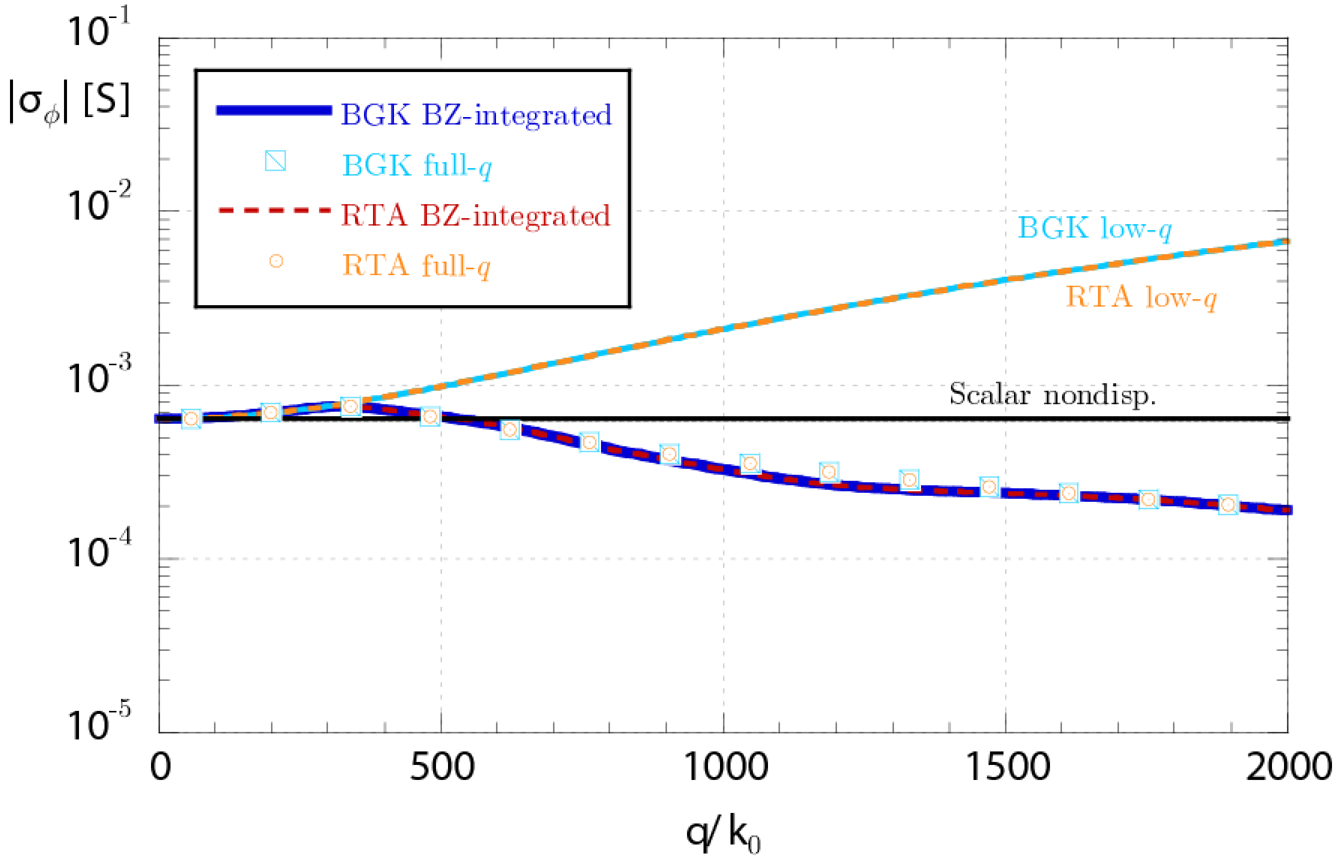




f=1 THz

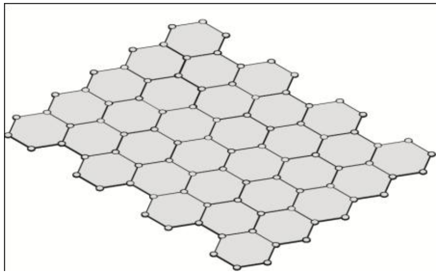
Graphene Conductivity

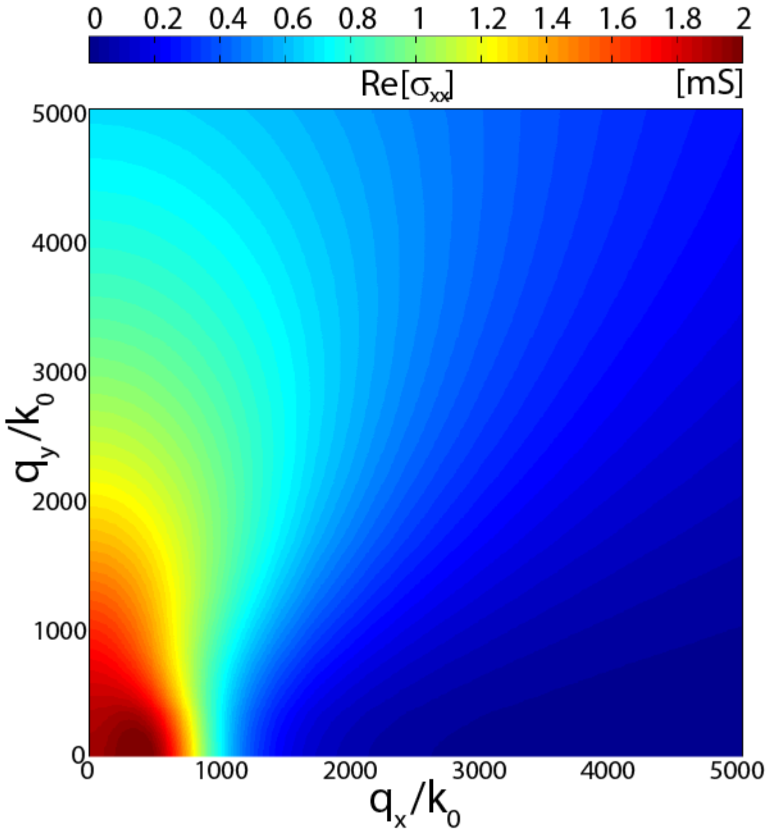


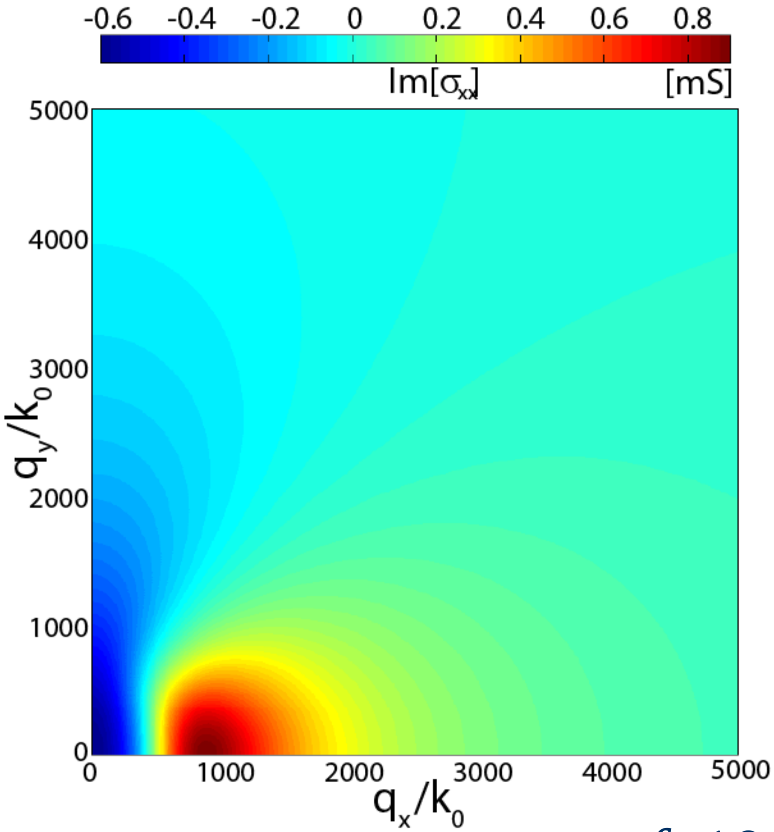


f=1 THz

Graphene Conductivity

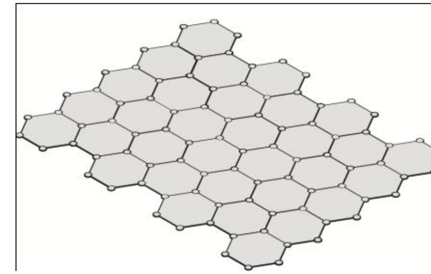


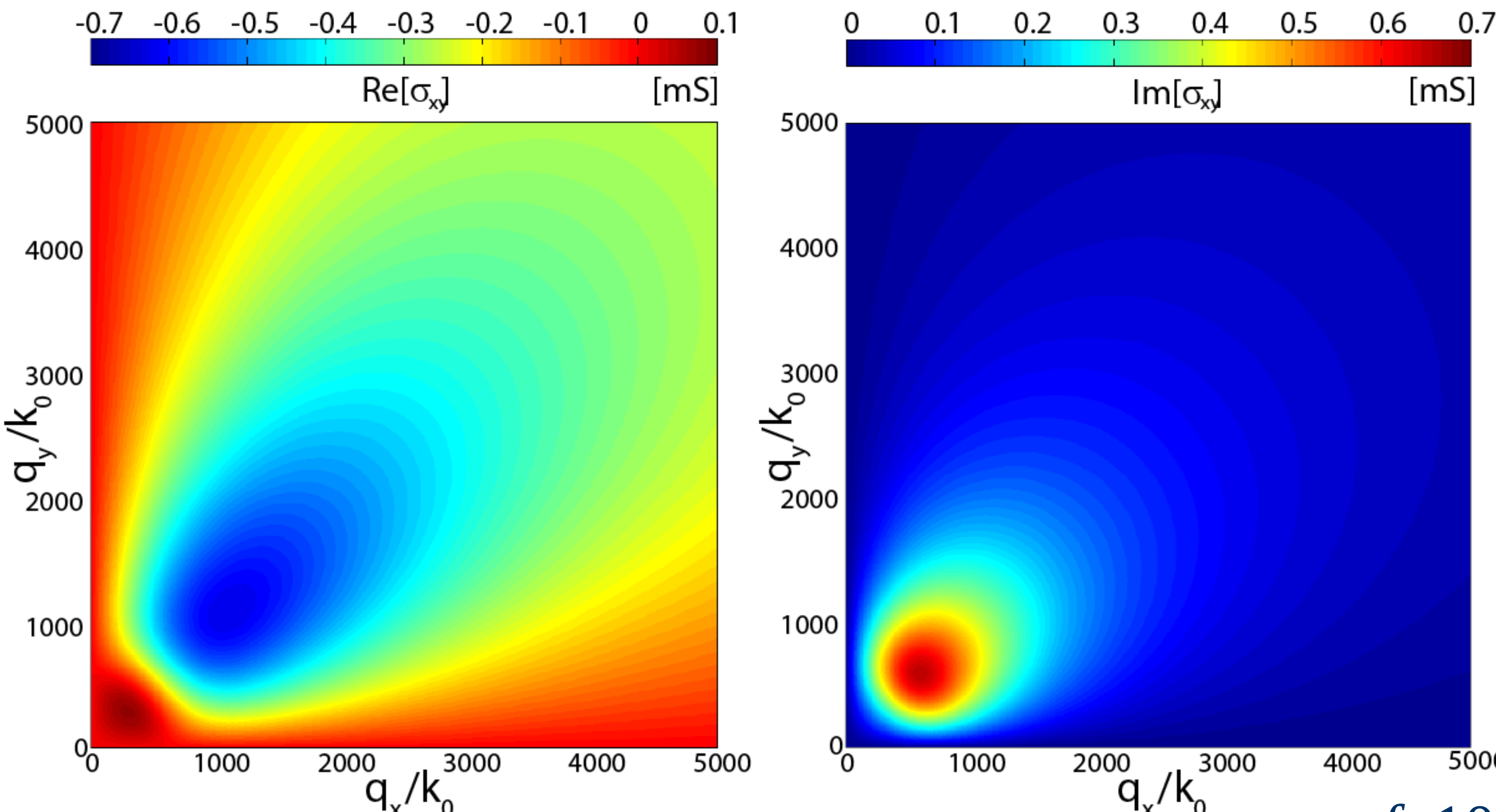




f=100 GHz

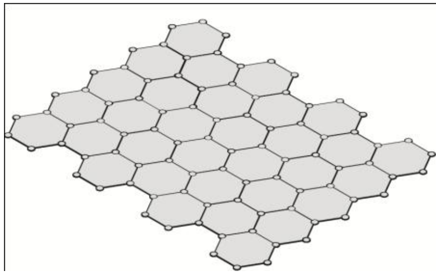
Graphene Conductivity

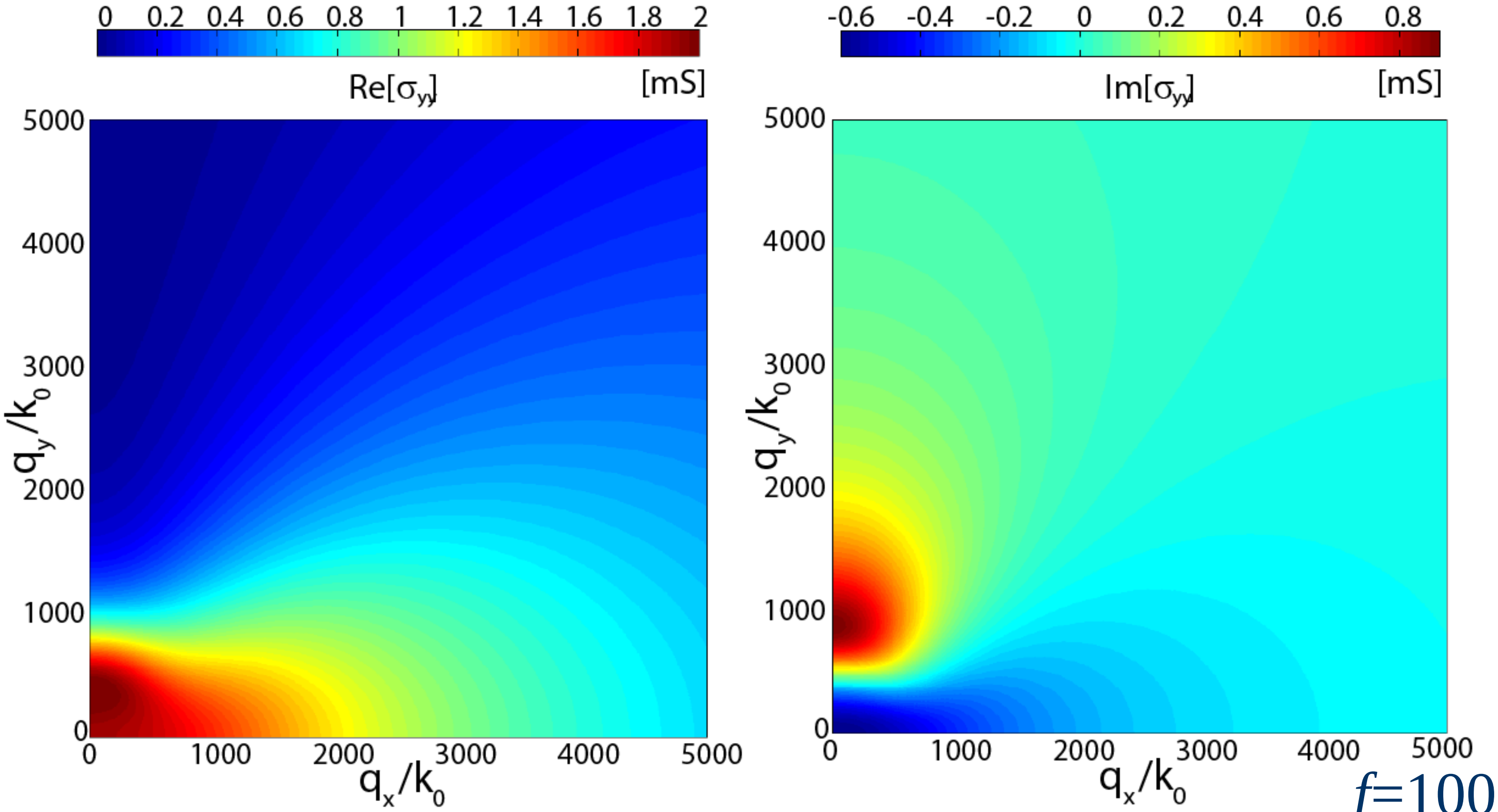




f=100 GHz

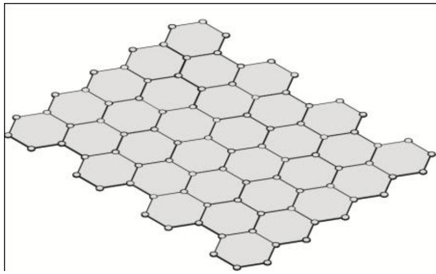
Graphene Conductivity

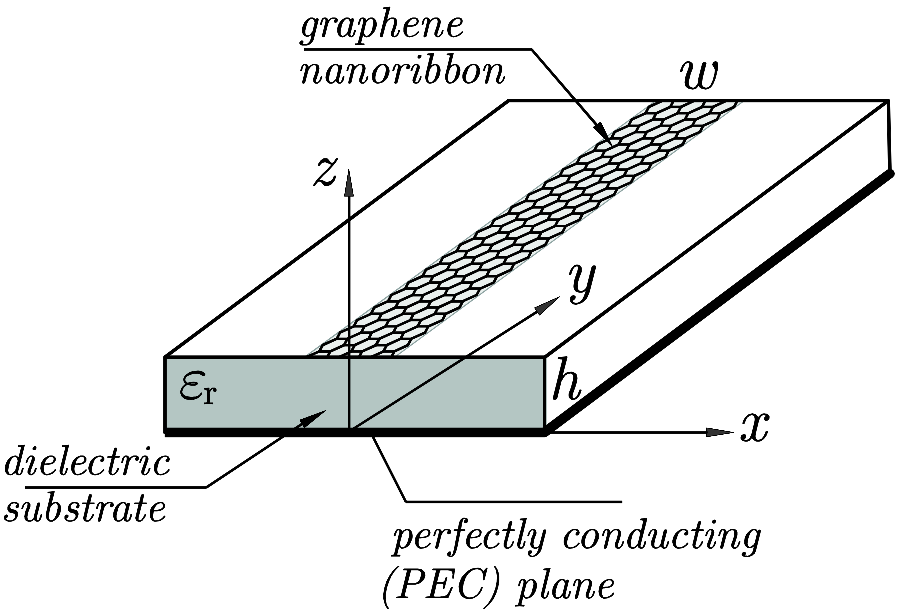




f=100 GHz

Graphene Nanoribbon (GNR)

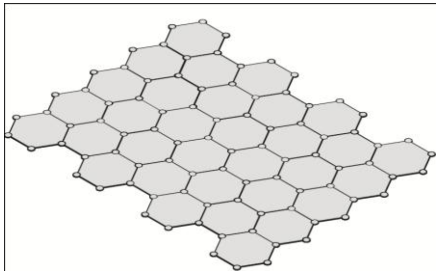




GNR modes are found using dyadic Green's functions and forming a homogeneous integral equation.

Numerical root search leads to the longitudinal eigenvalues.

Graphene Nanoribbon (GNR)



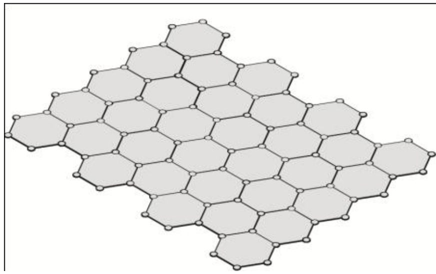
Some previous GNR simulation work:

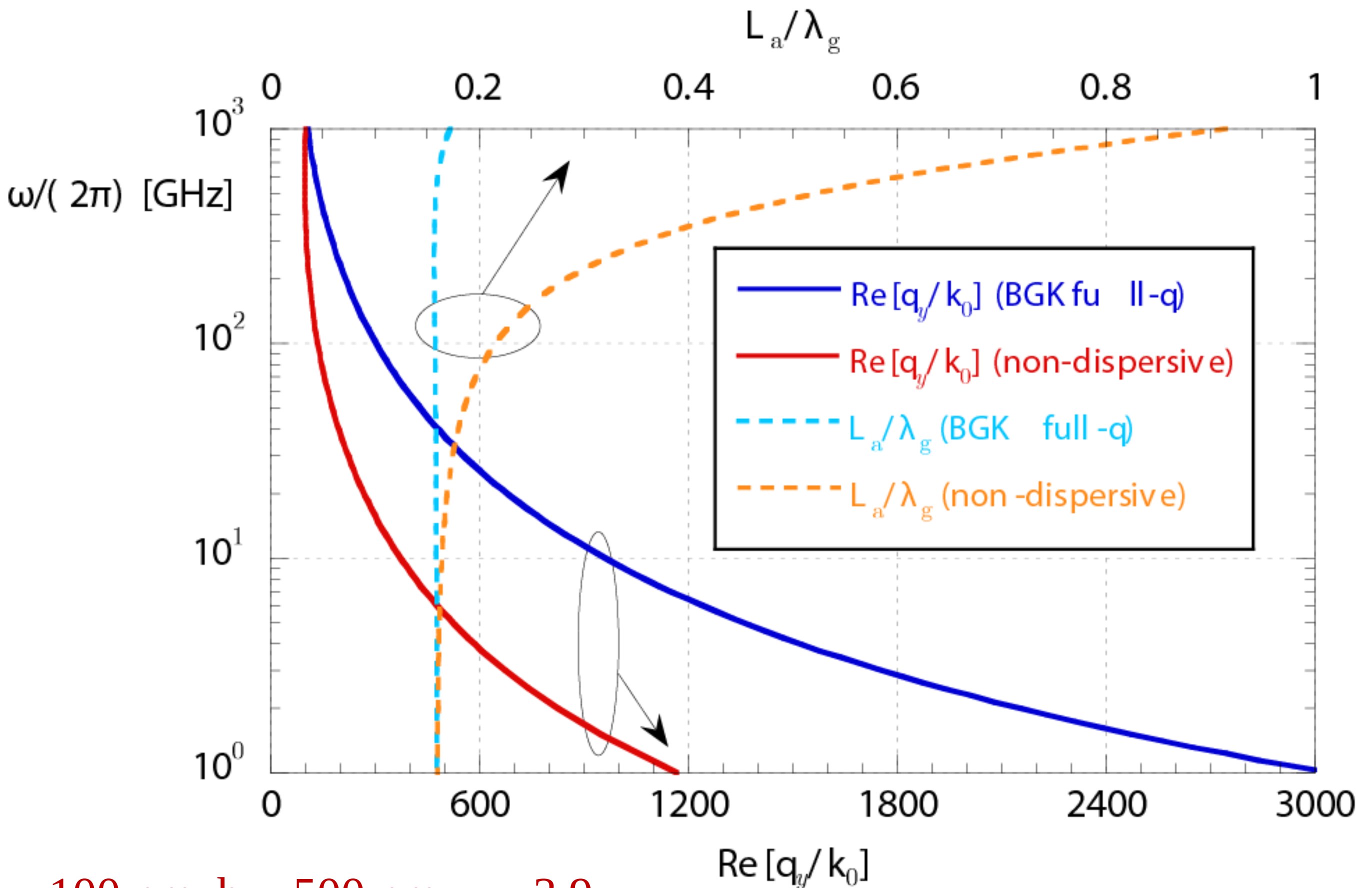
J. Christensen, A. Manjavacas, S. Thongrattanasiri, F.H.L. Koppens, and F. J. García de Abajo, ACS Nano 6, 431-440, 2012.

A. Y. Nikitin, F. Guinea, F. J. García-Vidal, and L. Martín-Moreno, Phys. Rev. B 84, 161407, 2011.

We found good agreement with previous work in the THz range.

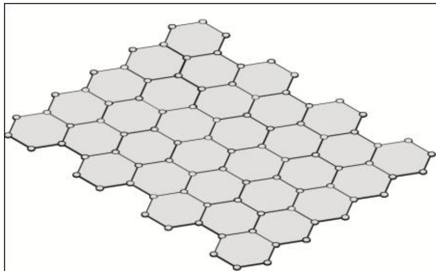
Graphene Nanoribbon (GNR)

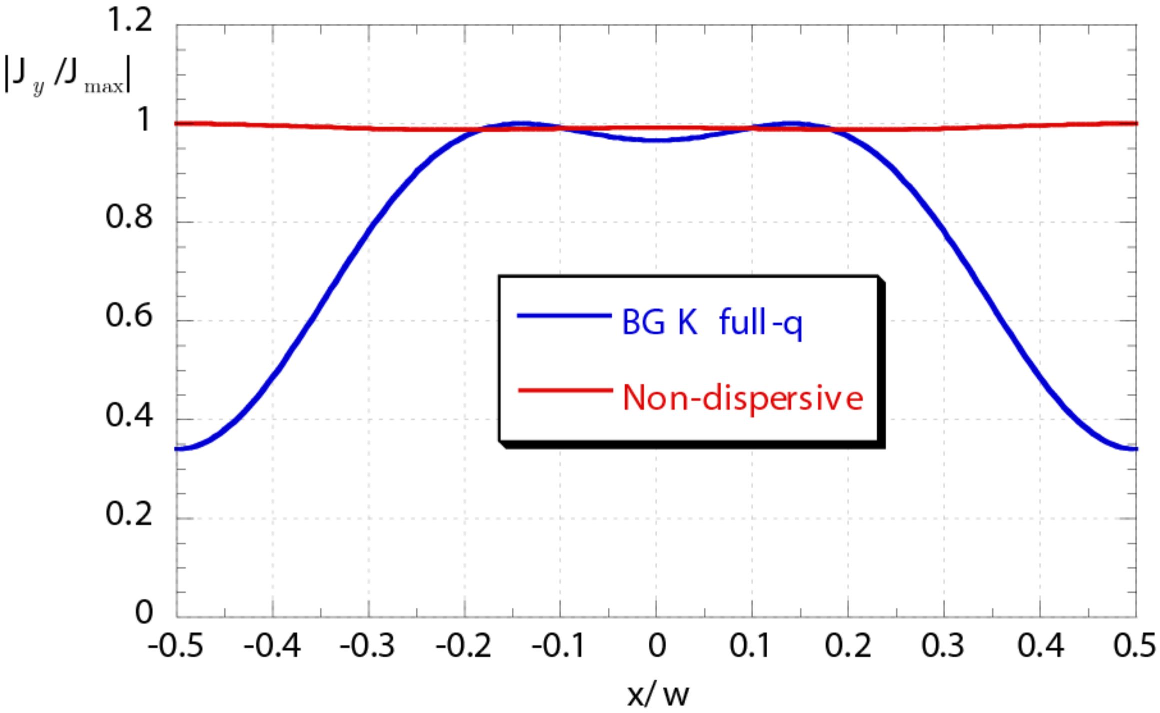




w = 100 nm, h = 500 nm, ε= 3.9

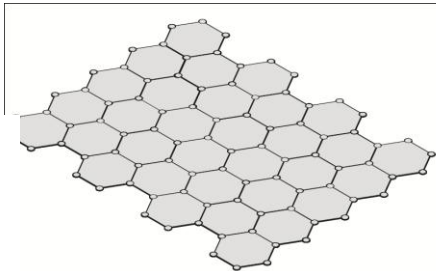
Graphene Nanoribbon (GNR)

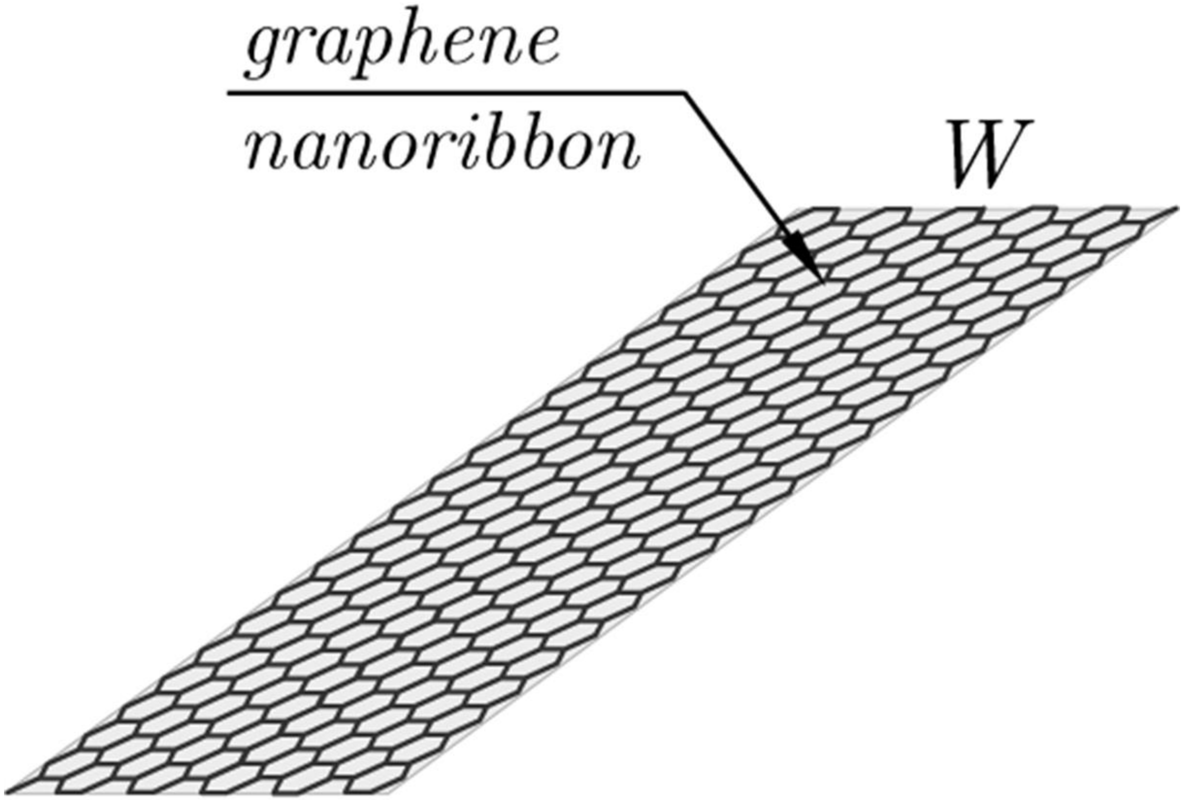




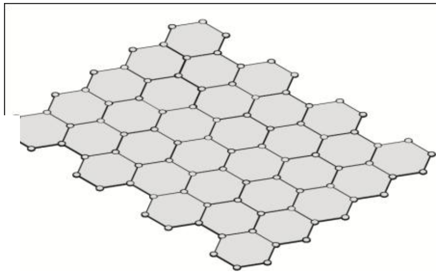
w = 100 nm, h = 500 nm, ε= 3.9

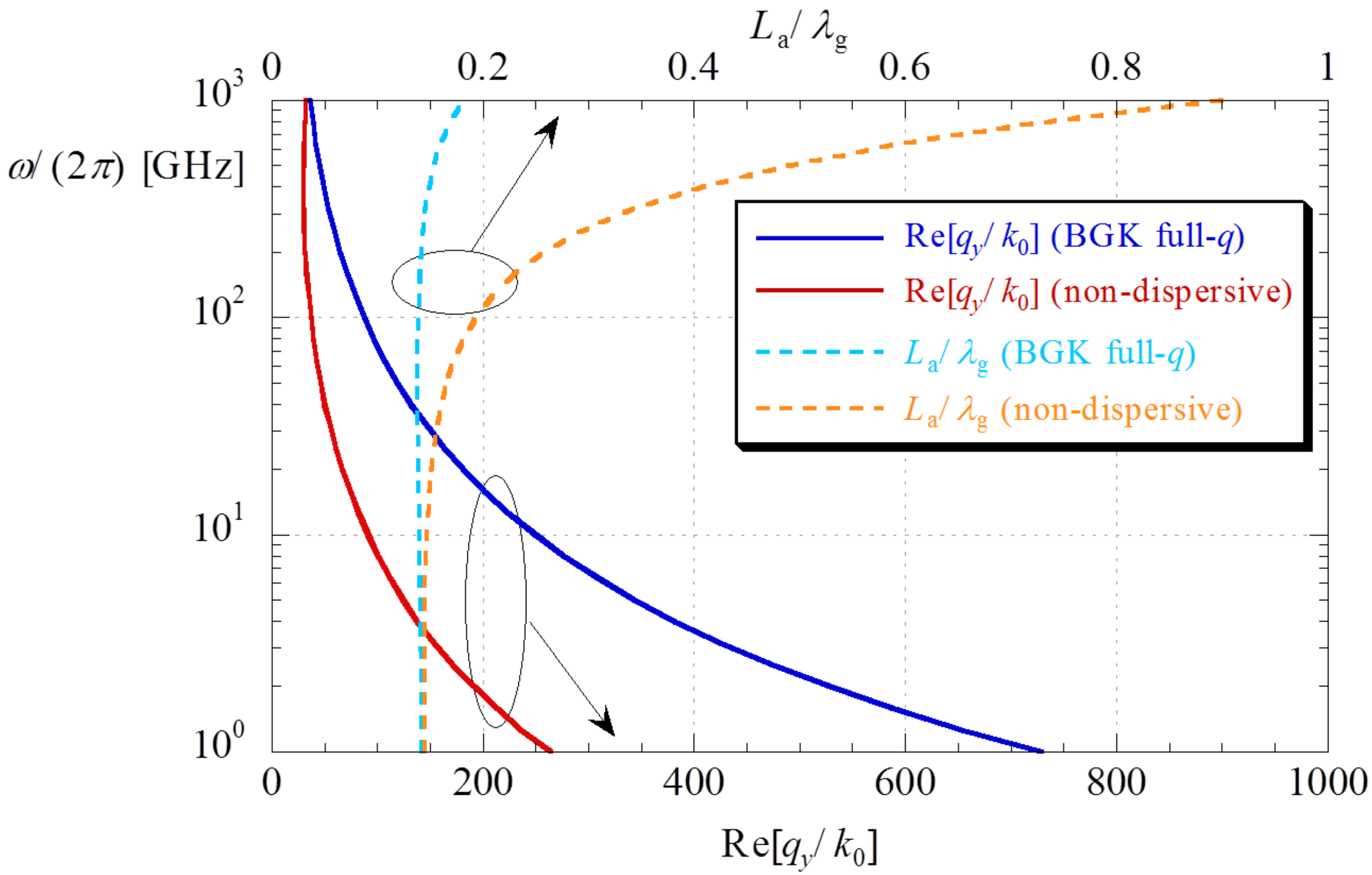
Graphene Nanoribbon (GNR) – no ground plane



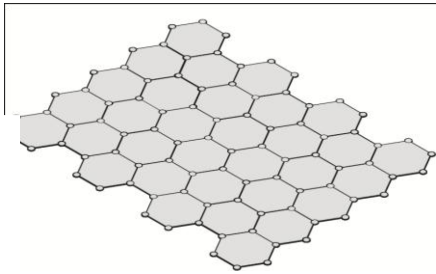


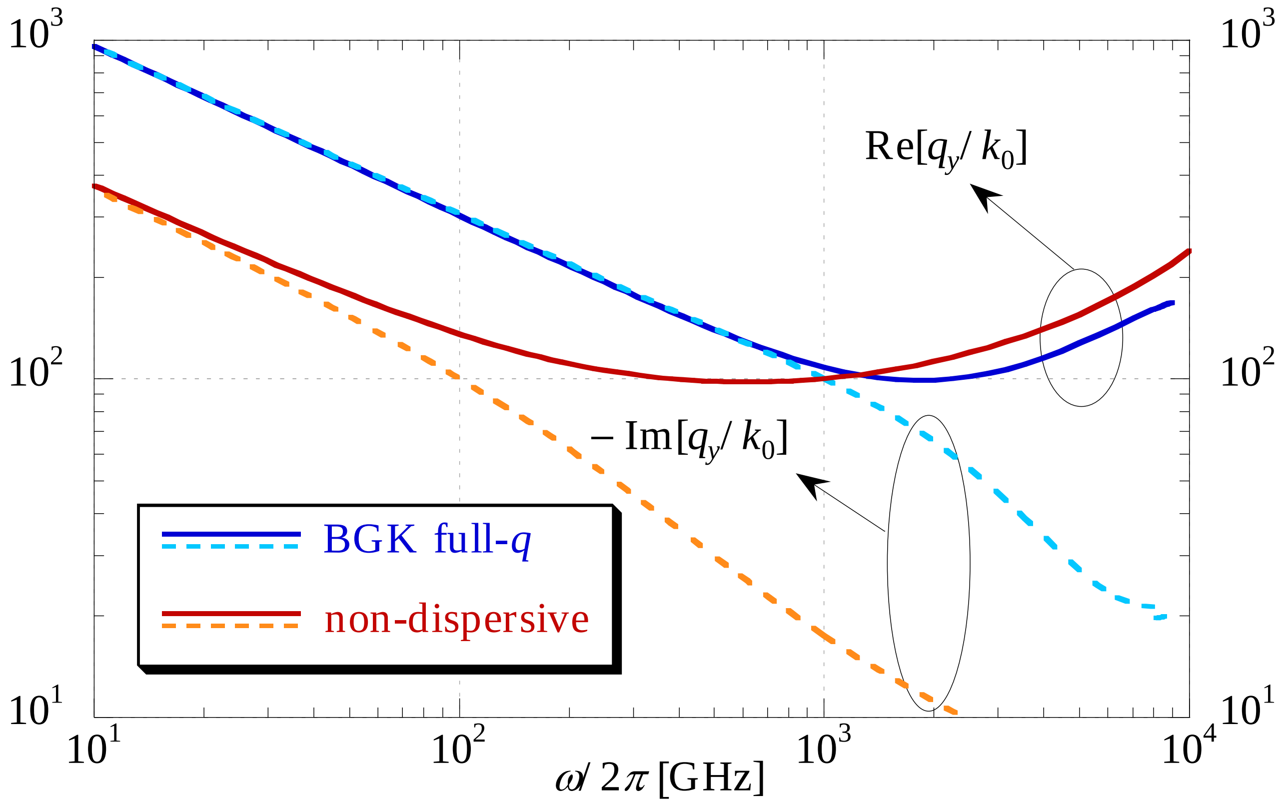
GNR – no ground plane



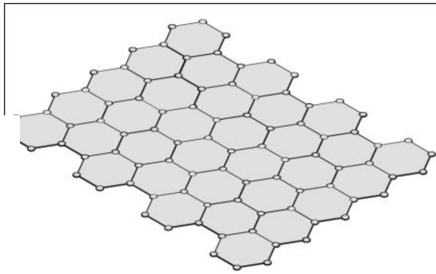


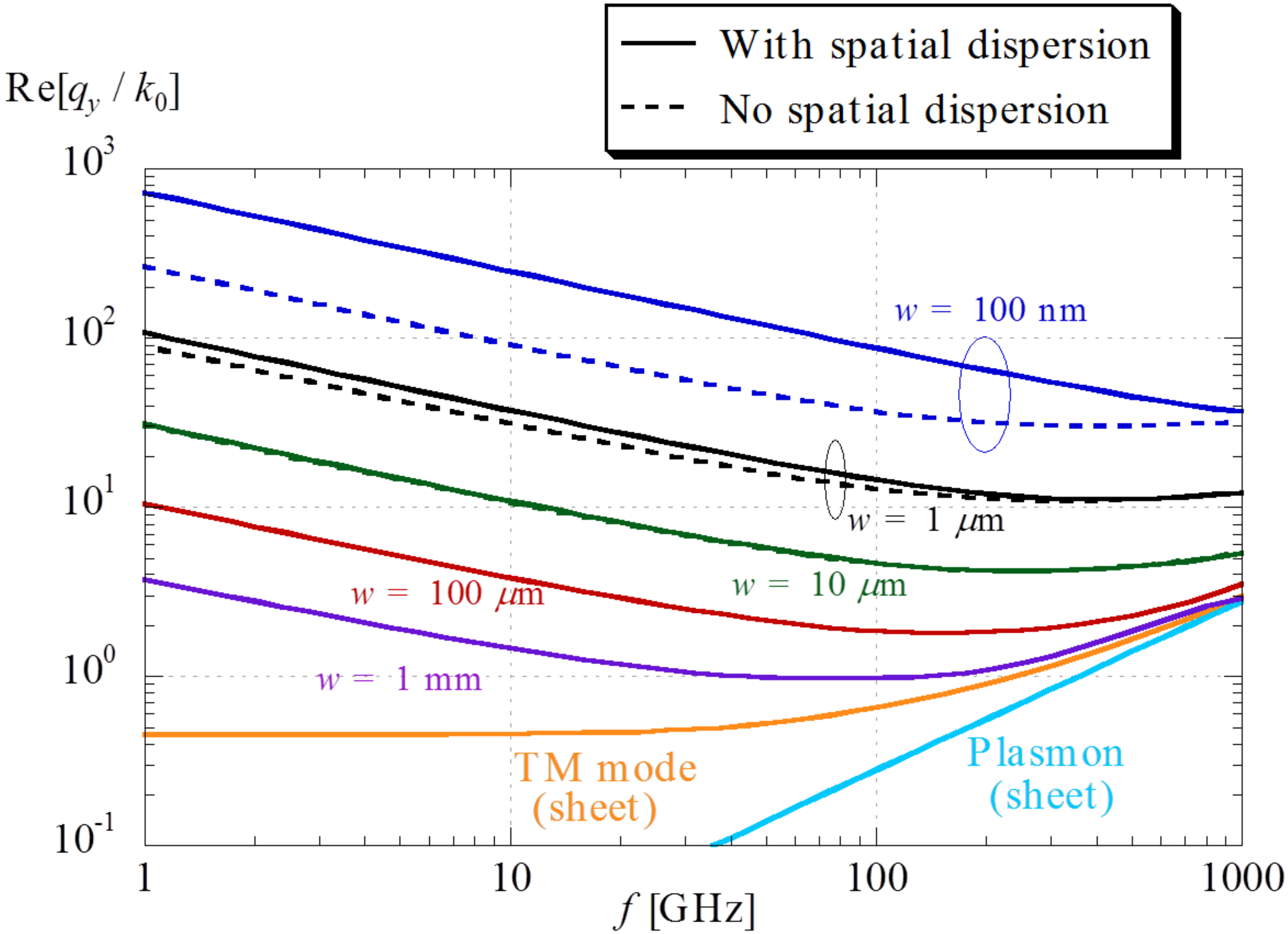
GNR – no ground plane

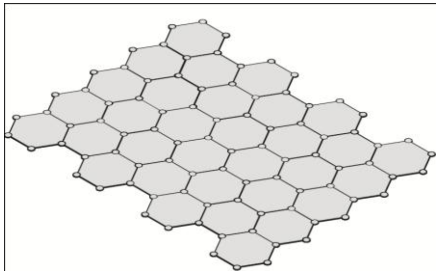




GNR – no ground plane







Measurements???

Conclusions

- Exact (within a tight-binding Boltzmann model) numerical results for the spatially-dispersive tensor conductivity of graphene have been presented.
- The tensor is given in analytical form for linear dispersion throughout the first BZ.
- For infinite graphene sheets spatial dispersion is not very important in many applications, but for GNRs spatial dispersion is quite important in some frequency ranges.

Thank You