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

E. H. Hwang and S. Das Sarma
Phys. Rev. B 75, 205418

Ajinkya Werulkar
Nitish Ujjwal
Chaitrali Duse
Guru Kalyan Jayasingh
Vedant Motamarri

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

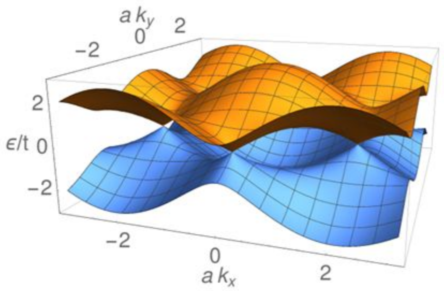
Dielectric function, screening, and plasmons in two-dimensional graphene

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)

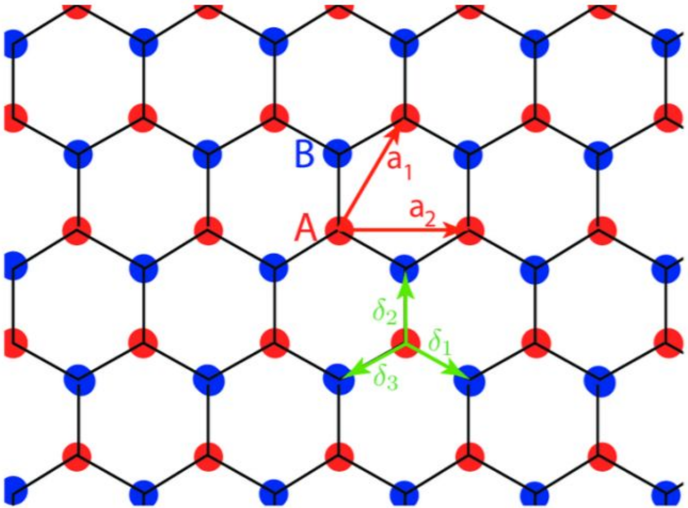
The dynamical dielectric function of two-dimensional graphene at arbitrary wave vector q and frequency ω, $\epsilon(q,\omega)$, is calculated in the self-consistent-field approximation. The results are used to find the dispersion of the plasmon mode and the electrostatic screening of the Coulomb interaction in two-dimensional (2D) graphene layer within the random-phase approximation. At long wavelengths ($q\rightarrow 0$), the plasmon dispersion shows the local classical behavior $\omega_{cl}=\omega_0\sqrt{q}$, but the density dependence of the plasma frequency ($\omega_0 \propto n^{1/4}$) is different from the usual 2D electron system ($\omega_0 \propto n^{1/2}$). The wave-vector-dependent plasmon dispersion and the static screening function show very different behavior than the usual 2D case. We show that the intrinsic interband contributions to static graphene screening can be effectively absorbed in a background dielectric constant.

DOI: 10.1103/PhysRevB.75.205418 PACS number(s): 73.21.−b, 71.10.−w, 73.43.Lp

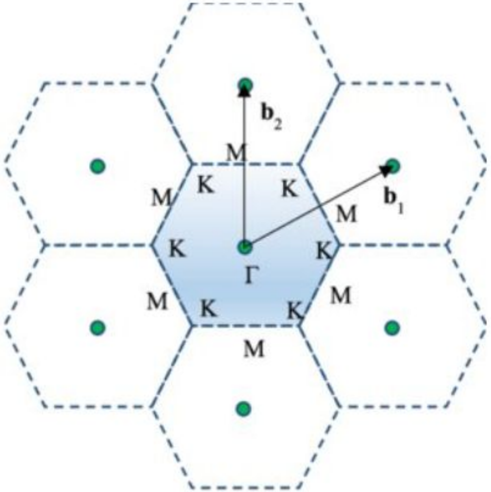
Graphene



(Ref. 1)

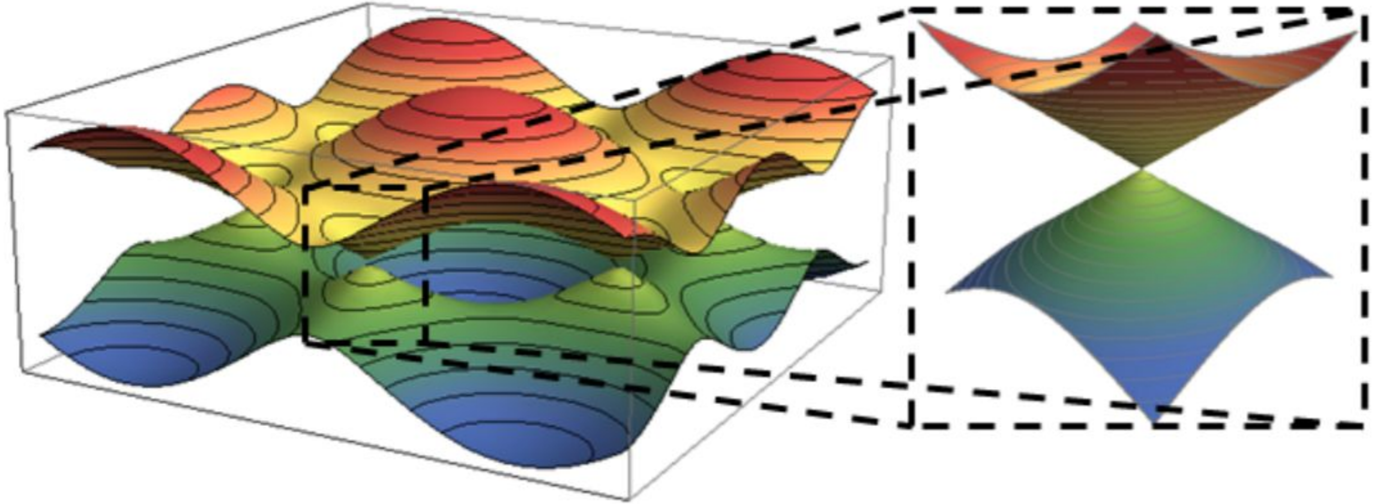


Honeycomb lattice of graphene. The primitive cell of the lattice consists of two carbon atoms labeled A and B, each of which is bonded to three nearest neighbors of the other type. (Ref. 2)



Reciprocal space structure of graphene. (Ref. 2)

Band structure of Graphene



(Ref. 2)

$$\varepsilon_{c/v}(\mathrm{k}) = \pm t\sqrt{1 + 4\cos^2\frac{k_x a\sqrt{3}}{2} + 4\cos\frac{k_x a\sqrt{3}}{2}\cos\frac{3ak_y}{2}}$$

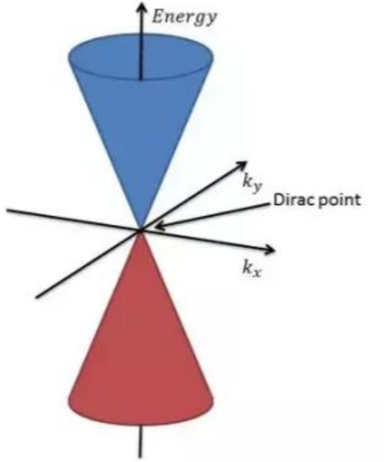
Linear dispersion for Graphene

Nearest-Neighbour Tight binding Hamiltonian:

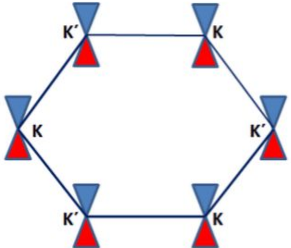
$$\tilde{H}(\mathrm{k}) = \frac{3at}{2}\begin{pmatrix} 0 & \mp k'_x + ik'_y \\ \mp k'_x - ik'_y & 0 \end{pmatrix} + O(k'^2)$$

$$= \mp\frac{3at}{2}k'_x\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \frac{3at}{2}k'_y\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + O(k'^2)$$

$$= \mp v_F k'_x \sigma_x - v_F k'_y \sigma_y + O(k'^2),$$



Pair of Dirac cones centered at a Dirac point. (Ref. 1)



(Ref .2)

$$\tilde{H}(\mathrm{k}) \approx -v_F \boldsymbol{\sigma}\cdot\mathrm{k} \qquad \text{near } K,$$

$$\tilde{H}(\mathrm{k}) \approx v_F \boldsymbol{\sigma}^T\cdot\mathrm{k} \qquad \text{near } K',$$

$$\varepsilon_{c/v}(\mathrm{k}) \approx \pm\frac{3at}{2}\sqrt{k'^2_x + k'^2_y}$$

Some important quantities and notations

$\hbar = 1$

Kinetic Energy of Graphene: $\epsilon_{s\mathbf{k}} = s\gamma|\mathbf{k}|$; $s = \pm 1$; γ is a band parameter

Density of States (DOS): $D(\epsilon) = g_s g_v |\epsilon| / (2\pi\gamma^2)$ $g_s = 2$ and $g_v = 2$

Fermi Momentum: $k_F = (4\pi n / g_s g_v)^{1/2}$

Fermi Energy: $E_F = \gamma k_F$

$$n = g_s g_v \int_{|\mathbf{q}|\leq k_F} \frac{d\mathbf{q}}{(2\pi)^2} \rightarrow k_F = \sqrt{\frac{4\pi n}{g_s g_v}}$$

	E_F	$D(E)$	$D_0 = D(E_F)$
MLG	$\hbar v_F \sqrt{\frac{4\pi n}{g_s g_v}}$	$\frac{g_s g_v E}{2\pi(\hbar v_F)^2}$	$\frac{\sqrt{g_s g_v n}}{\sqrt{\pi}\hbar v_F}$
BLG/2DEG	$\frac{2\pi\hbar^2 n}{m g_s g_v}$	$\frac{g_s g_v m}{2\pi\hbar^2}$	$\frac{g_s g_v m}{2\pi\hbar^2}$

(Table from Ref. 1)

Wigner-Seitz Radius (r_s)

Measures the ratio of potential to kinetic energy: $r_s = (e^2/\kappa\gamma)(4/g_s g_v)^{1/2}$

κ is the background lattice dielectric constant

For 3DEG (as done in class): $\frac{E_{el\text{-}el}}{E^{(0)}} \propto \frac{1}{n^{1/3}} \longrightarrow 0$ as $n \to \infty$

3D $(r_s \sim n^{-1/3})$

2D $(r_s \sim n^{-1/2})$

	r_s
MLG	$\frac{e^2}{\kappa\hbar v_F}\frac{\sqrt{g_s g_v}}{2}$
BLG/2DEG	$\frac{me^2}{2\kappa\hbar^2}\frac{g_s g_v}{\sqrt{\pi n}}$

(Table from Ref. 1)

For 2D Graphene monolayer, r_s is a constant! So interactions effects do not scale with carrier density.

RPA (Random Phase Approximation)

- A first order perturbative treatment of the problem.
- A valid approximation for weakly interacting system.

$$\phi^{ext}(\mathbf{q}) = \epsilon(\mathbf{q})\phi(\mathbf{q}), \qquad \rho^{ind}(\mathbf{q}) = \chi(\mathbf{q})\phi(\mathbf{q}).$$

$$\boxed{\epsilon(\mathbf{q}) = 1 - \frac{4\pi}{q^2}\chi(\mathbf{q})}$$

- The quantities are related only to the corresponding q. The contribution from the other q's are assumed to average out.

Lindhard Equation

- We consider a perturbative potential eV. We get H = H_o + eV. We then look into the induced charge density arising due to the perturbative potential.

$$i\hbar\partial_t\rho = [H, \rho].$$

$$i\hbar\partial_t\rho_0 + i\hbar\partial_t\rho_1 = [H_0 + eV, \rho_0 + \rho_1] = [H_0, \rho_0] + [H_0, \rho_1] + [eV, \rho_0] + [eV, \rho_1].$$

$$i\hbar\partial_t\rho_1 = [H_0, \rho_1] + [eV, \rho_0],$$

$$\langle k|\rho_1|k+q\rangle = \frac{f_{k+q} - f_k}{\epsilon_{k+q} - \epsilon_k - \hbar\omega} eV_0(q),$$

Contd.

With the induced charge, we now calculate the screening potential caused by it.

$$\nabla^2 V(\vec{x}) = -4\pi e n(\vec{x}),$$

$$n_s(\vec{x}) = \mathrm{Tr}\{\rho_1(\vec{x},\vec{x})\} = \mathrm{Tr}\{\langle\vec{x}|\rho_1|\vec{x}\rangle\} =$$
$$= \int dk \int dk' \langle x|k\rangle\langle k|\rho_1|k'\rangle\langle k'|x\rangle = \int dk \int dk' e^{i(k-k')x}\langle k|\rho_1|k'\rangle.$$

$$n_s(\vec{q}) \quad = \int dk \langle k|\rho_1|k+q\rangle.$$

Solving for screening potential, we get

$$V_s(q) = \frac{4\pi e^2}{q^2}\sum_k \frac{f_{k+q}-f_k}{\epsilon_{k+q}-\epsilon_k-\hbar\omega}V_0(q).$$

$$\epsilon^{3d}(q,\omega) = 1 + \frac{4\pi e^2}{q^2}\sum_k \frac{f_{k+q}-f_k}{\epsilon_{k+q}-\epsilon_k-\hbar\omega}$$

Dielectric function

$$\varepsilon(q,\omega) = 1 + \upsilon_c(q)\Pi(q,\omega),$$

$\upsilon_c(q) = 1/q^2\kappa\varepsilon_o$ for 3D gas

$\upsilon_c(q) = 1/2q\kappa\varepsilon_o$ for 2D gas

$$\Pi(q,\omega) = -\frac{g_s g_v}{L^2}\sum_{\mathbf{k}ss'}\frac{f_{s\mathbf{k}} - f_{s'\mathbf{k}'}}{\omega + \epsilon_{s\mathbf{k}} - \epsilon_{s'\mathbf{k}'} + i\eta}F_{ss'}(\mathbf{k},\mathbf{k}'),$$

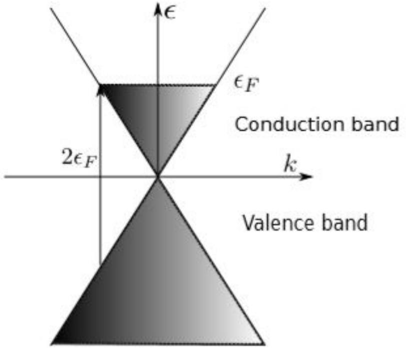
$$F_{ss'}(\mathbf{k},\mathbf{k}') = (1 + ss'\cos\theta)/2,$$

$$\cdot|\langle\mathbf{k}'l'|e^{i\mathbf{q}\cdot r}|\mathbf{k}l\rangle|^2$$

Contd.

$$\Pi(q,\omega) = \Pi^{+}(q,\omega) + \Pi^{-}(q,\omega),$$

$$\Pi^{+}(q,\omega) = -\frac{g_s g_v}{2L^2}\sum_{k}\left[\frac{[f_{\mathbf{k}+} - f_{\mathbf{k}'+}](1+\cos\theta_{kk'})}{\omega + \epsilon_{\mathbf{k}+} - \epsilon_{\mathbf{k}'+} + i\eta} + \frac{f_{\mathbf{k}+}(1-\cos\theta_{kk'})}{\omega + \epsilon_{\mathbf{k}+} - \epsilon_{\mathbf{k}'-} + i\eta} - \frac{f_{\mathbf{k}'+}(1-\cos\theta_{kk'})}{\omega + \epsilon_{\mathbf{k}-} - \epsilon_{\mathbf{k}'+} + i\eta}\right]$$



$$\Pi^{-}(q,\omega) = -\frac{g_s g_v}{2L^2}\sum_{k}\left[\frac{[f_{\mathbf{k}-} - f_{\mathbf{k}'-}](1+\cos\theta_{kk'})}{\omega + \epsilon_{\mathbf{k}-} - \epsilon_{\mathbf{k}'-} + i\eta} + \frac{f_{\mathbf{k}-}(1-\cos\theta_{kk'})}{\omega + \epsilon_{\mathbf{k}-} - \epsilon_{\mathbf{k}'+} + i\eta} - \frac{f_{\mathbf{k}'-}(1-\cos\theta_{kk'})}{\omega + \epsilon_{\mathbf{k}+} - \epsilon_{\mathbf{k}'-} + i\eta}\right].$$

Interband and
Intraband contributions
(Valley - Valley transitions are
ignored)

Plasmons

Long wavelength limit:

$$\Pi(q,\omega) \approx \begin{cases} \dfrac{D_0\gamma^2 q^2}{2\omega^2}[1-(\omega^2/4E_F^2)], & \gamma q < \omega < 2E_F \\ D_0[1+i(\omega/\gamma q)], & \omega < \gamma q \end{cases}$$

$$\epsilon(\mathbf{q},\omega) = 1 - v(q)\Pi(\mathbf{q},\omega)$$

In 2D, $v(q) = \dfrac{2\pi e^2}{\kappa q}$

$$V_{ext}(q,\omega) = \epsilon(q,\omega)V_{tot}(q,\omega)$$

Setting ε = 0 gives plasmon dispersion relation

$$\left(\frac{D_0\gamma^2 q^2}{2\omega^2}\right)\left(\frac{2\pi e^2}{\kappa q}\right) = 1 \qquad \Rightarrow \omega \propto \sqrt{q}$$

	2D Graphene	2D (parabolic dispersion)
Dispersion	$\omega_{cl} = \omega_0 \sqrt{q}$	$\omega_{cl} = \omega_0 \sqrt{q}$
	$\omega_0 = \sqrt{\frac{g_s g_v e^2 E_F}{2\kappa}} = \sqrt{\frac{e^2 \gamma \sqrt{\pi n g_s g_v}}{\kappa}}$	$\omega_0 = \sqrt{\frac{2\pi n e^2}{m\kappa}}$
Density Dependence	$\omega_0 \propto n^{1/4}$	$\omega_0 \propto n^{1/2}$
Non-local Effects	decrease in plasma frequency $\omega_p = \omega_{cl}(1 - \frac{q_0 q}{8k_F^2})$	increase in plasma frequency $\omega_p = \omega_{cl}(1 + \frac{3}{4}\frac{q}{q_{TF}})$

Bilayer Graphene

Optical plasmon (in-phase mode) $\omega_+(q) \approx \omega_0\sqrt{2q}$

Acoustic plasmon (out-of-phase mode) $\omega_-(q) \approx 2\omega_0\sqrt{dq}$

layer separation

Interlayer hopping in tight-binding?

»optical: similar

»acoustic: depolarization shift at long wavelengths

$$\omega_+ \ll \omega_-$$

$$\omega_-(q \rightarrow 0) = (2t_\perp)^2(1+q_0 d)$$

Plasmon dispersion

- Plasmon to e-hole conversion

$$\varepsilon_{\boldsymbol{l}+\boldsymbol{k}} - \varepsilon_{\boldsymbol{l}} = \frac{\hbar^2}{m}\left(\boldsymbol{l}\cdot\boldsymbol{k} + \frac{|\boldsymbol{k}|^2}{2}\right)$$

$$|\boldsymbol{l}+\boldsymbol{k}| > k_F \quad , \quad |\boldsymbol{l}| < k_F$$

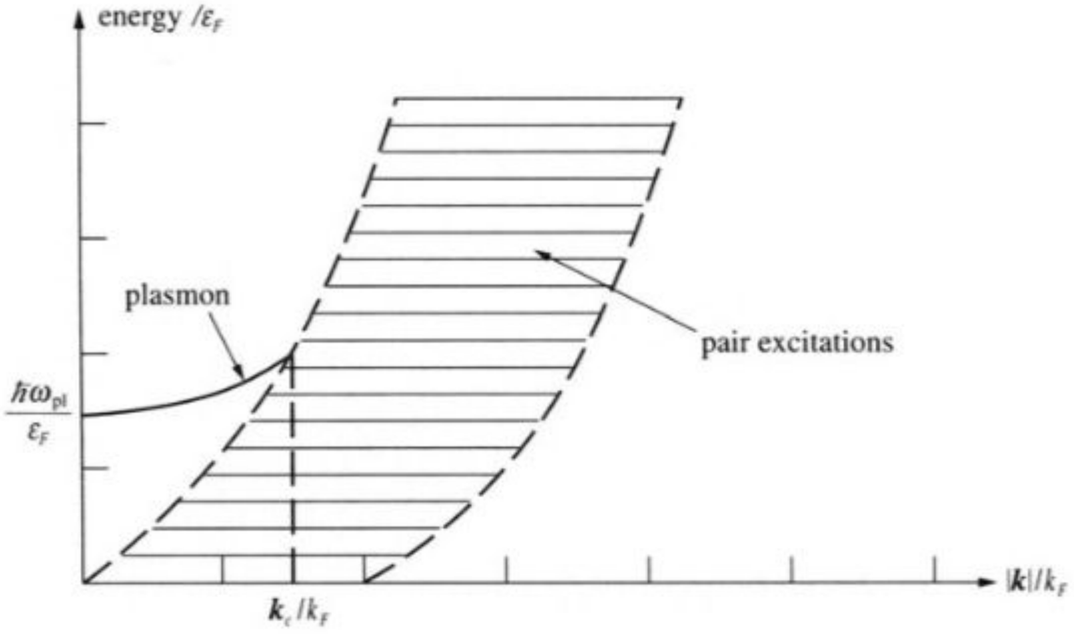


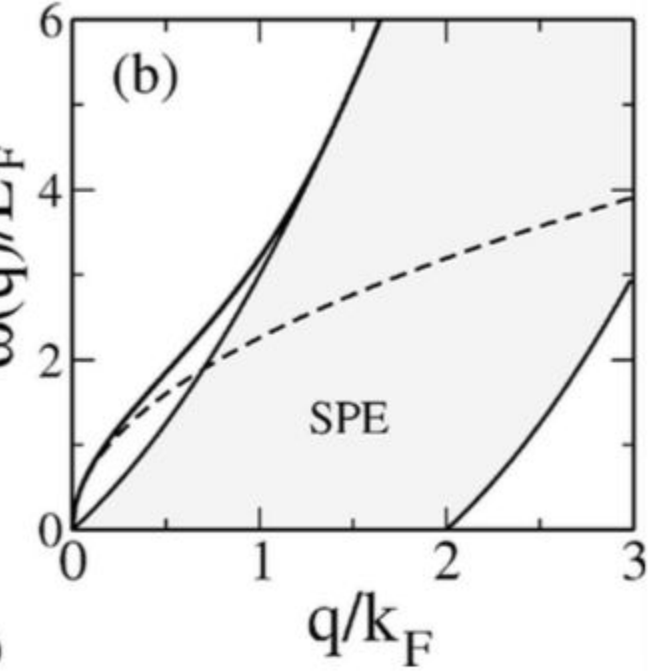
Fig taken from "Many body physics and quantum field theory"
By Martin et al.

$$\epsilon(\vec{k}, \omega(\vec{k})) = 0$$

$$for\ \vec{k} \neq 0$$

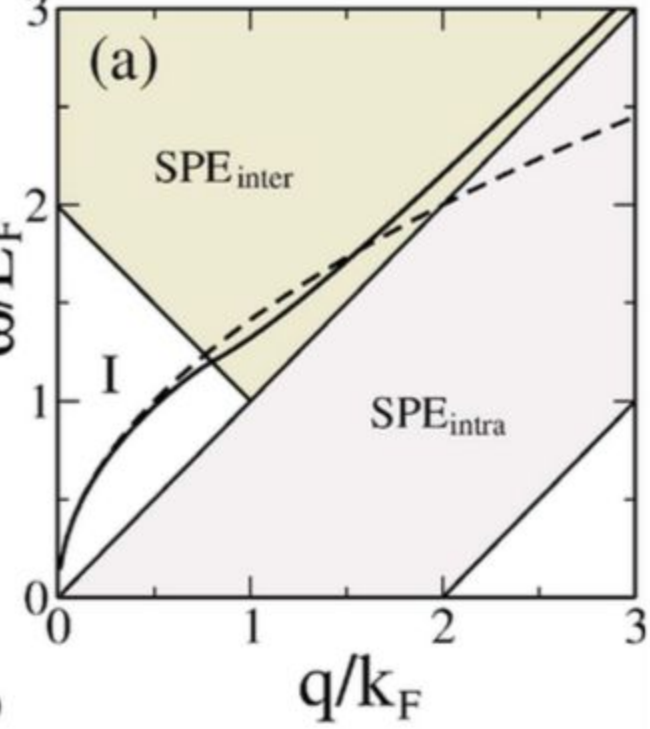
$$\omega(k) \ = \ \omega_1(k) + i\omega_2(k)$$

$$\tau \sim \frac{1}{\omega_2}$$



(b)

2DEG



(a)

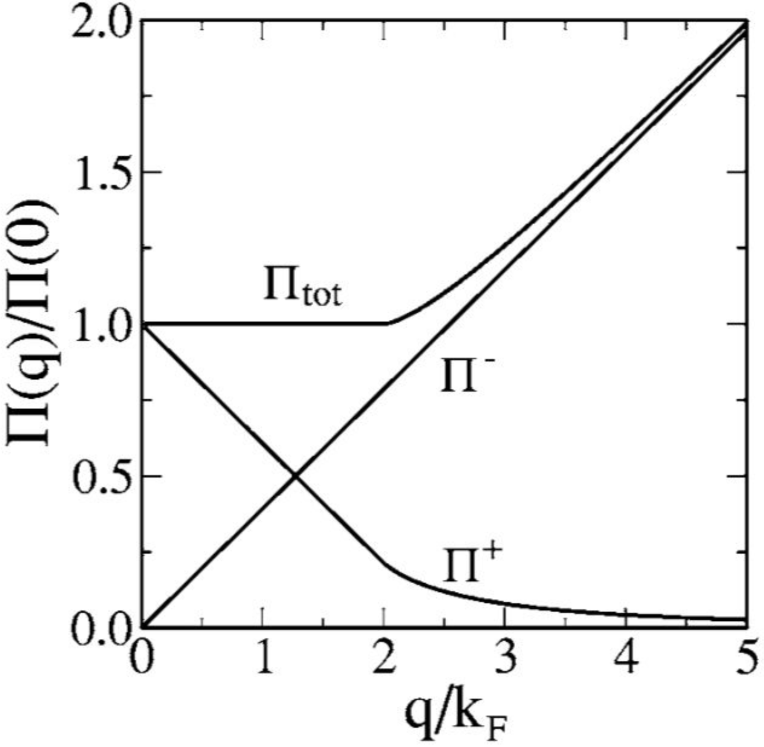
Graphene

Static screening (ω = 0)

$$\Pi(q,0) \;=\; \Pi^{-}(q,0)+\Pi^{+}(q,0)$$

$$\tilde{\Pi}^{-}(q)=\pi q/8k_F$$

$$\tilde{\Pi}^{+}(q)=\begin{cases} 1-\dfrac{\pi q}{8k_F}, & q\le 2k_F \\ 1-\dfrac{1}{2}\sqrt{1-\dfrac{4k_F^2}{q^2}}-\dfrac{q}{4k_F}\sin^{-1}\dfrac{2k_F}{q}, & q>2k_F, \end{cases}$$



Plot of Polarizability vs scaled momenta

$$For\ q \le 2k_F$$

$$\Pi(q,0) = \Pi^+ + \Pi^- = D(E_F)$$

$$= constant$$

$\Pi(\vec{q})\ vs\ \vec{q}$ for Graphene

Small Q

$$\Pi(\vec{q}) = D(E_F)$$

$$\Pi^+ + \Pi^- = const$$

Present in doped

Large Q

$$\Pi(\vec{q}) \propto q$$

Dominant: Π^-

Present always (intrinsic)

Vis a Vis 2DEG: Large q

$$q \geq 2k_F$$

2DEG

Graphene

Π Tends to 0 for large q

Π Goes linearly as q

$$\epsilon = 1 + v_q \Pi(q) \to 1$$

$$\epsilon \to 1 + v_q \Pi(q) = 1 + \frac{1}{q} \cdot q \cdot \alpha$$
$$= 1 + \beta = constant$$

$$V_{total} = \frac{V_{ext}}{\epsilon} \sim V_{ext}$$

$$V_{total} = \frac{V_{ext}}{\epsilon} \sim \frac{V_{ext}}{\epsilon'}$$

"Effective dielectric constant"

Check with 3DEG

- For large q, $\chi(q,0)$ decays

- Subsequently $\epsilon(q,0)$ tends to

  1

Plot of
Dielectric constant
And susceptibility vs
momenta

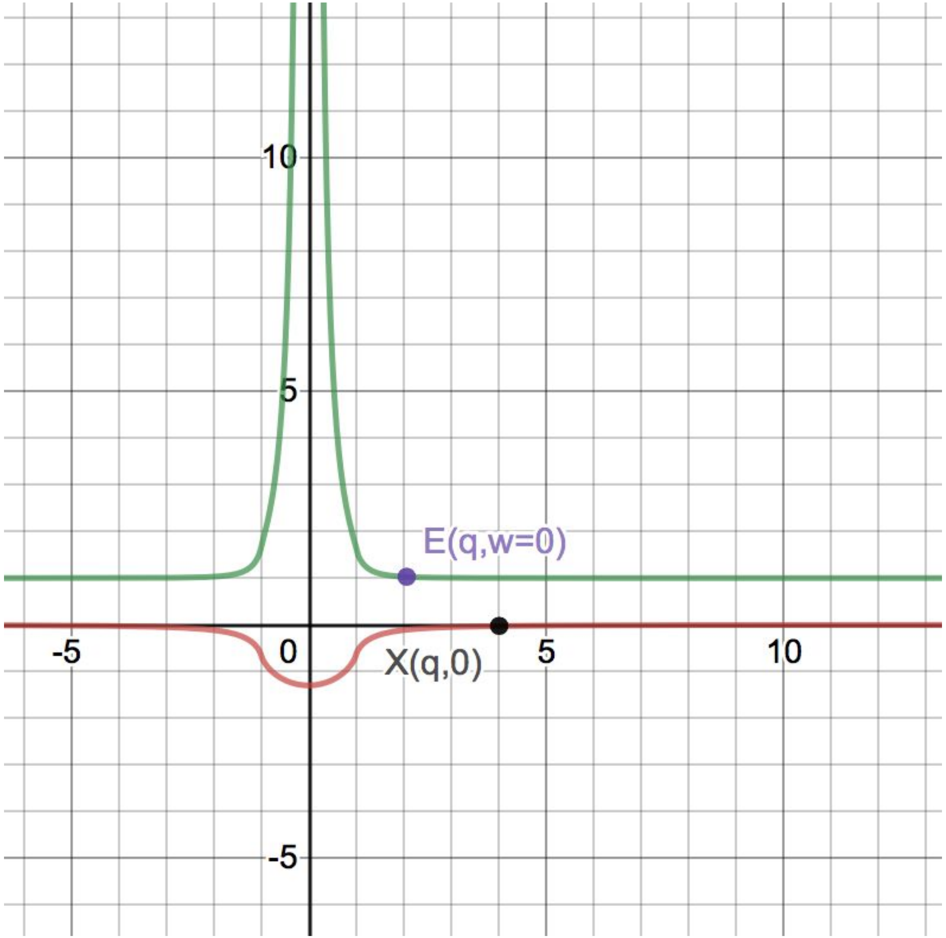


Fig: Desmos Graphing calculator

Vis a Vis 2DEG: Small q

$$\epsilon = 1 + \frac{1}{q} \cdot \Pi \sim 1 + \frac{k_s}{q}$$

2DEG

Graphene

$$q_s = q_{TF} = g_s g_v m e^2 / \kappa$$

$$q_s = g_s g_v e^2 k_F / \kappa\gamma$$

Constant, independent of density

$$\propto \sqrt{n}$$

Screening summary

Graphene

Small q

Dominant:

Typical of a 2DEG (metallic)

Doped

Large q

Dominant: Π^{-}

Typical of a dielectric (insulating)

Intrinsic (undoped)

Effective dielectric constant

We have

$$\epsilon(q) = 1 + \frac{2\pi e^2}{\kappa q}[\Pi^-(q) + \Pi^+(q)].$$

We get

$$\epsilon(q) = 1 + \frac{g_s g_v \pi}{8} r_s + v_c(q)\Pi^+(q)$$

Using

$$\Pi^-(q) = D(E_F)\pi q/8k_F$$

and

$$D(E_F) = g_s g_v k_F/2\pi\gamma.$$

Introduce an effective dielectric constant

$$\epsilon(q) = \kappa^*\left[1 + \frac{2\pi e^2}{\kappa\kappa^* q}\Pi^+(q)\right].$$

where

$$\kappa^* = 1 + g_s g_v \pi r_s/8$$

Free carrier screening

Free carrier screening function

$$\epsilon^{+}(q) = 1 + \frac{2\pi e^2}{\kappa\kappa^{*} q}\Pi^{+}(q)$$

with

$$\epsilon(q) \equiv \kappa^{*}\epsilon^{+}(q)$$

\Kappa is the background lattice dielectric constant arising from insulating substrate
For. e.g for graphene on silicon substrate

$$\kappa = (1+\kappa_{SiO_2})/2 \approx 2.5$$

$$\kappa^{*} = 1 + g_s g_v \pi r_s/8 \approx 2.3$$

$$\kappa\kappa^{*} \approx 6$$

Effective background dielectric constant

Short wavelength behaviour & Suspended graphene

Short wavelength behaviour

$$\epsilon(q \to \infty) \to \kappa^* = 1 + g_s g_v \pi r_s / 8,$$

~ Constant i.e. insulating behaviour

Screened Coulomb potential in 2D

$$2\pi e^2 / \kappa\kappa^* q.$$

Intrinsic graphene has a dielectric constant of 4 due to interband transitions

$$r_s = e^2 / \hbar\gamma \text{ (since } \kappa = 1)$$

$$\kappa^* \approx 4.$$

Thomas- Fermi screening

For small q

$$\epsilon_{TF}(q) = 1 + q_{TF}/q$$

Screening vector

$$q_{TF} \equiv q_s = g_s g_v e^2 k_F / \kappa \gamma.$$

Effective TF screening function

$$\epsilon^{+}_{TF}(q) = 1 + q^{*}_{TF}/q$$

where $q^{*}_{TF} = q_{TF}/\kappa^{*}.$

References

1. *Electronic transport in two dimensional graphene*, S. Das Sarma, Shaffique Adam, E. H. Hwang , and Enrico Rossi, 2010
2. Courtesy Prof. Alok Shukla's slides for PH 565 - Semiconductor Physics
3. https://thiscondensedlife.files.wordpress.com/2015/07/random-phase-approximation.pdf
4. *Electronic properties of two-dimensional systems*, Tsuneya Ando, Alan B. Fowler, and Frank Stern (https://journals.aps.org/rmp/pdf/10.1103/RevModPhys.54.437)
5. https://arxiv.org/pdf/1003.4731.pdf
6. https://www.weizmann.ac.il/condmat/oreg/sites/condmat.oreg/files/uploads/2015/tutorial_1.pdf
7. *Plasmon modes of spatially separated double-layer graphene*, E. H. Hwang and S. Das Sarma, Physical Review B 80, 205405 (2009)

Thank You!