Graphene

Dielectric Function, Screening and Plasmons

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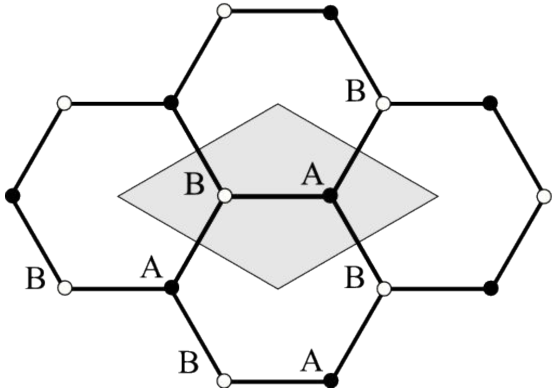
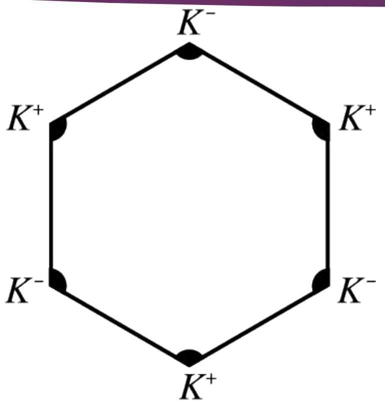
Graphene



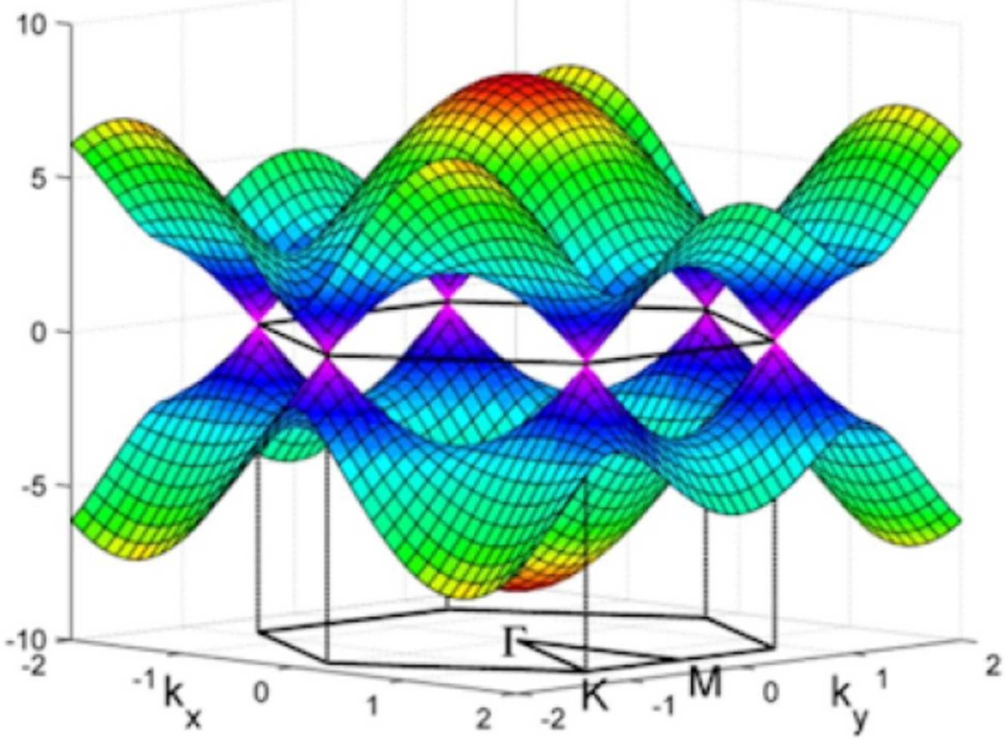


$$h = \begin{pmatrix} 0 & f(\vec{k}) \\ f^*(\vec{k}) & 0 \end{pmatrix}$$

$$H = \sum_{\vec{k}} \psi^\dagger(\vec{k}) h(\vec{k}) \psi(\vec{k}), \qquad \psi(\vec{k}) = \left(A(\vec{k}), B(\vec{k})\right)^T$$

$$f(\vec{k}) = -t\left(e^{-ik_x a} + 2e^{ik_x a/2}\cos\left(\frac{k_y a\sqrt{3}}{2}\right)\right)$$

$$\varepsilon_{\pm} = \pm\left|f(\vec{k})\right| = \pm t\sqrt{3 + 2\cos\left(\sqrt{3}k_y a\right) + 4\cos\left(\sqrt{3}k_y a/2\right)\cos\left(3k_x a/2\right)}.$$



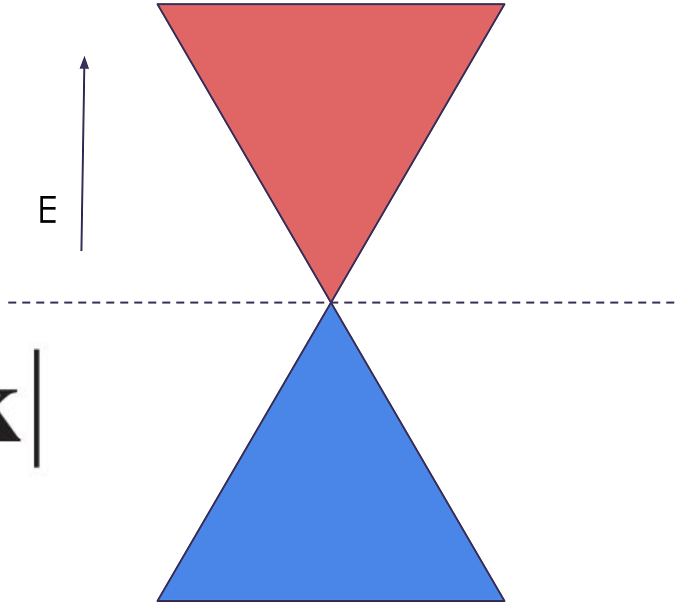
Dirac Physics in Graphene

$$h(K' + \mathbf{q}) = -\frac{3ta}{2}\begin{pmatrix} 0 & e^{-\frac{2\pi i}{3}}(q_y + iq_x) \\ e^{\frac{2\pi i}{3}}(q_y - iq_x) & 0 \end{pmatrix}.$$

$$h(\vec{K}' + \vec{q}) = \hbar v_F \vec{q}\cdot\vec{\sigma},$$

$$E = \pm\hbar v_F\,|\vec{q}|\,, \psi_\pm = \frac{1}{\sqrt{2}}(\ e^{i\theta_{\mathbf{q}}/2} \quad , \pm e^{-i\theta_{\mathbf{q}}/2}\ )^T.$$

$$\epsilon_{s\mathbf{k}} = s\gamma|\mathbf{k}|$$



$$D(\epsilon) = g_s g_v|\epsilon|/(2\pi\gamma^2)$$

$$r_s = (e^2/\kappa\gamma)(4/g_s g_v)^{1/2}$$

$$r_s \sim 0.5$$

Refs: 1) Mod.Phys.Lett. A31 (2016) no.40, 1630047

Lindhard equation

1. We consider an electron gas with a perturbation of the following form:

$$\delta U(\vec{r}, t) = \lim_{\alpha \to 0} \left(U\, e^{i\vec{q}\cdot\vec{r}}\, e^{-i\omega t}\, e^{\alpha t} + U\, e^{-i\vec{q}\cdot\vec{r}}\, e^{i\omega t}\, e^{\alpha t} \right)$$

2. Then we consider a perturbative solution of the w.f. To first order (wigner seitz radius being much lesser than 1)

$$|f\rangle = \sum_{k'} c_{k'} \left|\vec{k}'\right\rangle$$

$$\approx \lim_{\alpha \to 0} \sum_{k'} \left(\delta_{\vec{k},\vec{k}'} + \delta_{k',k+q} \frac{U/\hbar}{(\omega - \omega_{\mathrm{fi}} + i\alpha)} + \delta_{k',k-q} \frac{U/\hbar}{(-\omega - \omega_{\mathrm{fi}} + i\alpha)} \right) \left|\vec{k}'\right\rangle$$

$$= \left|\vec{k}'\right\rangle + \lim_{\alpha \to 0} \frac{U}{\left(E(\vec{k}) - E(\vec{k}+\vec{q}) + \hbar\omega + i\alpha\right)} \left|\vec{k}+\vec{q}\right\rangle + \lim_{\alpha \to 0} \frac{U}{\left(E(\vec{k}) - E(\vec{k}-\vec{q}) - \hbar\omega + i\alpha\right)} \left|\vec{k}-\vec{q}\right\rangle$$

3. We see that the final state is a superposition over states |k + q> and |k - q>. We then use this to calculate the charge density. The deviation in the charge density comes out to be:-

$$\delta\rho(\vec{r}, t) = \frac{eU}{V} \lim_{\alpha \to 0} \sum_{k} \left\{ \left(\frac{f^0(\vec{k}) - f^0(\vec{k}+\vec{q})}{E(\vec{k}) - E(\vec{k}+\vec{q}) - \hbar\omega + i\alpha} \right) e^{i\vec{q}\cdot\vec{r}} + c.c \right\}$$

4. We then use the poisson equation to find the deviation in the potential energy.

$$\vec{\nabla}^2 \phi(\vec{r}, t) = \frac{-e\,\delta\rho(\vec{r}, t)}{\epsilon_0}$$

Which leads to…..

$$\phi = \left(\frac{e^2}{\epsilon_0\, \vec{q}^{\,2}} \frac{1}{V} \lim_{\alpha \to 0} \sum_k \frac{f^0(\vec{k}) - f^0(\vec{k} + \vec{q})}{E(\vec{k}) - E(\vec{k} + \vec{q}) - \hbar\omega + i\alpha} \right) U$$

5. The total potential energy is

$$U_{\text{tot}}(\vec{r}, t) = U_{\text{ext}}(\vec{r}, t) + \phi(\vec{r}, t)$$

Which gives the dielectric function as:-

$$\boxed{\epsilon(\vec{q}, \omega) = 1 + \frac{e^2}{\epsilon_0\, \vec{q}^{\,2}} \frac{1}{V} \lim_{\alpha \to 0} \sum_k \frac{f^0(\vec{k}) - f^0(\vec{k} + \vec{q})}{E(\vec{k} + \vec{q}) - E(\vec{k}) - \hbar\omega + i\alpha}}$$

Polarisation

$$\varepsilon(q,\omega) = 1 + v_c(q)\Pi(q,\omega)$$ (dynamical screening function)

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

$$\boxed{(1+ss'\cos\theta)/2.}$$

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

Polarisation

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

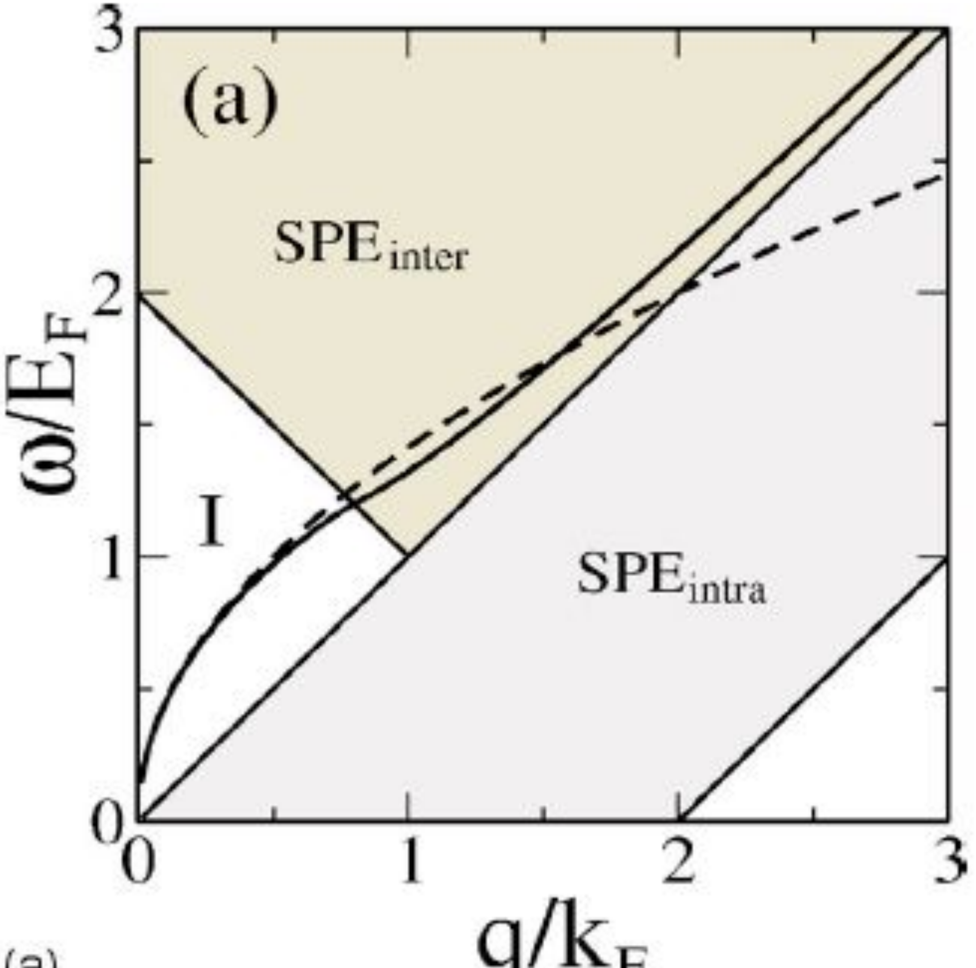
Upper band

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

Lower band

Plasmons in RPA

Graphene	2D Plasmons
Plasmon frequency for $q \to 0: \; w = w_0 q^{1/2}$ $w \sim q^{1/2}$	$w \sim q^{1/2}$
$w_0 \sim n^{1/4}$ because of different E_F , n, k_F dependence	$w_0 \sim n^{1/2}$
$[\omega_p(q)/\omega_{cl} = 1 - q_0 q/8k_F^2]$	$1+(3/4)(q/q_{TF})$



(a)

Static Screening ($\omega = 0$)

This limit gives us the transport properties (scattering by impurities of charge carriers)

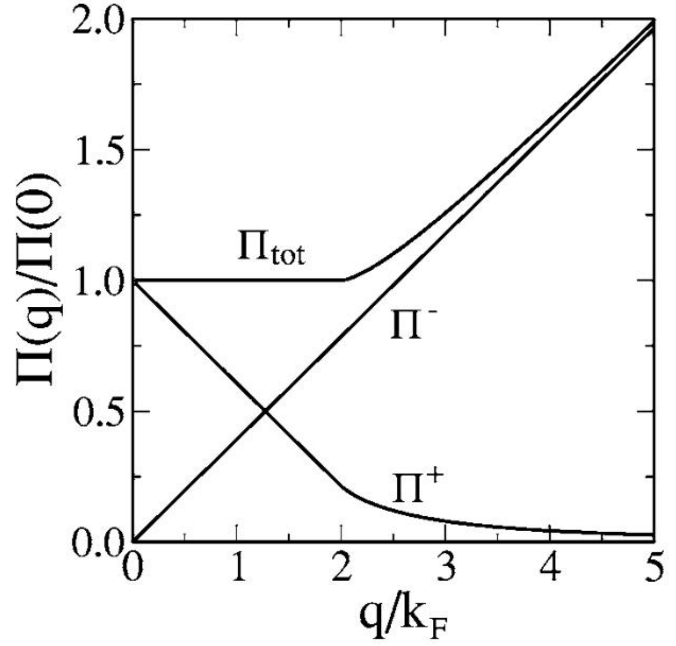
$$\tilde{\Pi}^{+}(q) = \begin{cases} 1 - \dfrac{\pi q}{8k_F}, & q \leq 2k_F \\ 1 - \dfrac{1}{2}\sqrt{1 - \dfrac{4k_F^2}{q^2}} - \dfrac{q}{4k_F}\sin^{-1}\dfrac{2k_F}{q}, & q > 2k_F, \end{cases}$$

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

Static Screening

$$For \quad q \le 2k_F$$

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



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Screening Wave Vector

$$\nabla.(\kappa\nabla\phi) = -4\pi(\rho_{ext} + \rho_{ind})$$

$$\rho_{ind}(r) = -e[N_s(\phi) - N_s(0)]\delta(z)$$

$$\nabla\cdot(\kappa\nabla\phi) - 2\bar{\kappa}\bar{q}_s\bar{\phi}(\mathbf{r})\delta(z) = -4\pi\rho_{\mathrm{ext}} ,$$

$$\bar{q}_s = \frac{2\pi e^2}{\bar{\kappa}}\frac{dN_s}{dE_F} ,$$

Screening Wave Vector

$$q \leq 2k_F$$

Normal 2D

$$q_s = g_s g_v \frac{me^2}{k}$$

Graphene

$$q_s = \frac{g_s g_v e^2 k_F}{k\gamma} \propto n^{1/2}$$

Screening Wave Vector

$$q > 2k_F$$

Normal 2D

Graphene

Falls of rapidly with q.

ıncreases linearly with q due to interband transition.

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

In this limit interaction decreases with q which is typical of insulators

$$\Pi$$

Intrinsic

$$\Pi^{-}$$

Insulating

Because of Doping

$$\Pi^{+}$$

Metalic

Screening - Effects of Extrinsic Carriers

Screening in Graphene

Intrinsic

Interband Transitions

Π^{-}

Absorb in Dielectric Constant

Because of Doping

Intraband Transitions

Π^{+}

Consider only this part in effective dielectric function

Screening - Effects of Extrinsic Carriers

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

$$v_c(q)\Pi^-(q) = \frac{g_s g_v \pi}{8}\frac{e^2}{\kappa\gamma} = \frac{g_s g_v \pi}{8} r_s.$$

$$\epsilon(q) = \kappa^+ \epsilon^+(q)$$

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

$$\kappa^* = \kappa\kappa^+$$

Effective Dielectric Constant

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

Effective Dielectric function for free carriers

Background lattice dielectric constant

For pure Graphene, $\kappa = 1$

Experimentally, κ **is the dielectric constant arising out of substrate.**

Usually, SiO_2 **is used.** $\kappa = (1 + \kappa_{SiO_2})/2 \approx 2.5$

suspended 2D graphene

No Substrate, $\kappa = 1 \qquad r_s \approx 2.2$

$$\kappa^* \approx 4$$

background static lattice dielectric constant of intrinsic graphene due to interband transitions

Thomas-Fermi Screening

Transport properties of Graphene $\Longrightarrow$ Charged Impurity Scattering

At long Wavelength, we need Thomas Fermi Theory.

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

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

We can absorb interband Screening effects

$$\epsilon^+_{TF} = 1 + \frac{q^+_{TF}}{q}$$

$$q^+_{TF} = \frac{q_{TF}}{\kappa^+}$$

Conclusions

Relations Obtained: polarizability, dielectric function, plasmon dispersion, and static screening properties for doped graphene

Deviations: $w_p \sim n^{1/4}$ as to $n^{1/2}$

Justification: Zero band gap, linear E-K relation

Validity: $T_F \sim 1300K(n \sim 10^{12})$, r_s is constant throughout (<1) ⇒ RPA valid

- **The study was primarily on extrinsic grpahene (gated or doped)**

References

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