Dynamical polarization of doped graphene

Bernhard Wunsch[1,2], T. Stauber[2], F. Sols[1], F. Guinea[2]

[1]Departamento de Física de Materiales, UCM,
[2]Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid

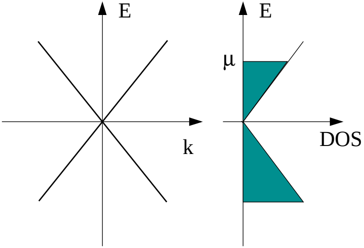
Electronic properties of graphene, Jan 07[1]

[1]New J. Phys. **8**, 318 (2006)

Outline

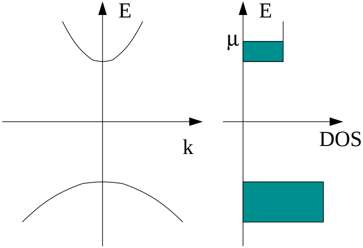
Comparison with 2DEG

Graphene



- $E(\mathbf{k}, \lambda) = \lambda\hbar\mathbf{v_F}\mathbf{k}$, no gap
- $DOS(E) := 1/A\partial N/\partial E \propto E$
- Two valleys *s* and spinor wavefunction (A,B)

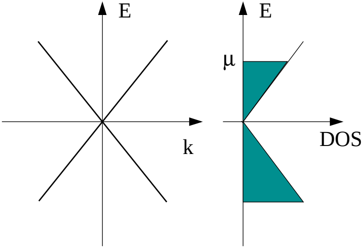
2DEG



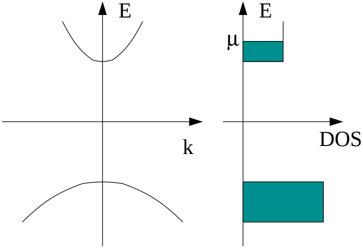
- $E(\mathbf{k}, \lambda) = \frac{\hbar^2\mathbf{k}^2}{2\mathbf{m}^*}$, gap (1.4 eV for GaAs)
- $DOS(E) = const$
- Eigenfunctions are plane waves

Comparison with 2DEG

Graphene



2DEG

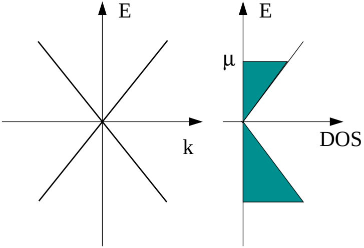


- $E(\mathbf{k},\lambda) = \lambda\hbar \mathbf{v_F k}$, no gap
- $DOS(E) := 1/A \partial N/\partial E \propto E$
- Two valleys *s* and spinor wavefunction (A,B)

- $E(\mathbf{k},\lambda) = \frac{\hbar^2 \mathbf{k}^2}{2\mathbf{m}^*}$, gap (1.4 eV for GaAs)
- $DOS(E) = const$
- Eigenfunctions are plane waves

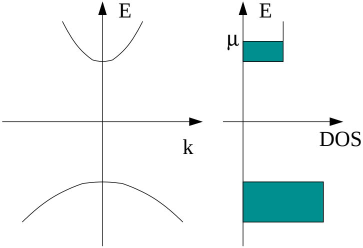
Comparison with 2DEG

Graphene



- $E(\mathbf{k},\lambda) = \lambda\hbar\mathbf{v_F k}$, no gap
- $DOS(E) := 1/A\partial N/\partial E \propto E$
- Two valleys *s* and spinor wavefunction (A,B)

2DEG



- $E(\mathbf{k},\lambda) = \frac{\hbar^2\mathbf{k}^2}{\mathbf{2m}^*}$, gap (1.4 eV for GaAs)
- $DOS(E) = const$
- Eigenfunctions are plane waves

Dielectric function and polarization in linear response

Dielectric function $\varepsilon(q,\omega)$ and polarization $\chi(q,\omega)$ describe internal el-el interaction as well as screening of an external potential $\phi_{ext}(q,\omega)$.

$$\phi_{tot}(q,\omega) = \frac{\phi_{ext}(q,\omega)}{\varepsilon(q,\omega)}; \quad \rho_{ind}(q,\omega) = -e\,\chi(q,\omega)\phi_{ext}(q,\omega)$$

$$\chi^0(q,i\omega_n) = -\frac{1}{A}\int_0^\beta d\tau e^{i\omega_n\tau}\langle T\rho(q,\tau)\rho(-q,0)\rangle$$

In RPA approximation electron-electron interaction treated self-consistently

$$\chi(q,\omega) \approx \frac{\chi^0(q,\omega)}{1-v_q\chi^0(q,\omega)} \Rightarrow \varepsilon(q,\omega) \approx 1 - v_q\chi^0(q,\omega)$$

v_q is in-plane Coulomb potential.

Mathematical expression

$$\chi^0(\mathbf{q}, i\omega_n) = \frac{g_S g_V}{(2\pi)^2} \int d^2k \sum_{\lambda,\lambda'=\pm} f^{\lambda\,\lambda'}(\boldsymbol{k}, \mathbf{q}) \frac{n_F(E^\lambda(\boldsymbol{k})) - n_F(E^{\lambda'}(\boldsymbol{k}+\boldsymbol{q}))}{E^\lambda(\boldsymbol{k}) - E^{\lambda'}(\boldsymbol{k}+\boldsymbol{q}) + i\hbar\omega_n}$$

$$f^{\lambda\,\lambda'}(\boldsymbol{k}, \mathbf{q}) = \frac{1}{2}\left(1 + \lambda\,\lambda' \frac{k + q\cos\varphi}{|\boldsymbol{k}+\mathbf{q}|}\right)$$

- Summation over bonding and anti-bonding bands λ, λ', $E^\lambda(\boldsymbol{k}) = \lambda\hbar v_F k$
- Wavefunction overlaps $f^{\lambda\,\lambda'}(\boldsymbol{k}, \mathbf{q})$
- Linear energy dispersion $E^\lambda(\boldsymbol{k}) = \lambda\hbar v_F$

We calculate at zero temperature (i.e. we assume $\mu/k_B \gg T$).

E. Hwang, S. Das Sarma, cond-mat/0610561; Shung *et al.* PRB **34** 934 (1986)

Mathematical expression

$$\chi^0(\mathbf{q}, i\omega_n) = \frac{g_S g_V}{(2\pi)^2} \int d^2k \sum_{\lambda,\lambda'=\pm} f^{\lambda\,\lambda'}(\boldsymbol{k}, \mathbf{q}) \frac{n_F(E^\lambda(\boldsymbol{k})) - n_F(E^{\lambda'}(\boldsymbol{k}+\boldsymbol{q}))}{E^\lambda(\boldsymbol{k}) - E^{\lambda'}(\boldsymbol{k}+\boldsymbol{q}) + i\hbar\omega_n}$$

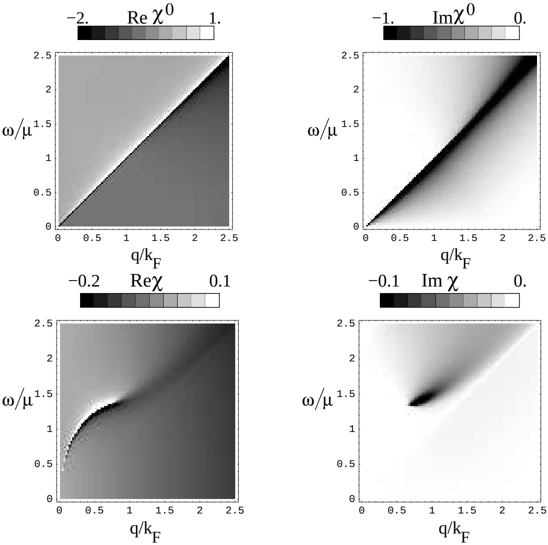
$$f^{\lambda\,\lambda'}(\boldsymbol{k}, \mathbf{q}) = \frac{1}{2}\left(1 + \lambda\,\lambda' \frac{k + q\cos\varphi}{|\boldsymbol{k}+\mathbf{q}|}\right)$$

- Summation over bonding and anti-bonding bands λ, λ', $E^\lambda(\boldsymbol{k}) = \lambda\hbar v_F k$
- Wavefunction overlaps $f^{\lambda\,\lambda'}(\boldsymbol{k}, \mathbf{q})$
- Linear energy dispersion $E^\lambda(\boldsymbol{k}) = \lambda\hbar v_F$

We calculate at zero temperature (i.e. we assume $\mu/k_B \gg T$).

E. Hwang, S. Das Sarma, cond-mat/0610561; Shung *et al.* PRB **34** 934 (1986)

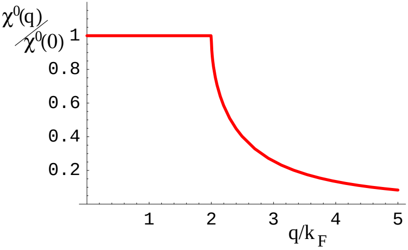
General characteristics of RPA Polarization



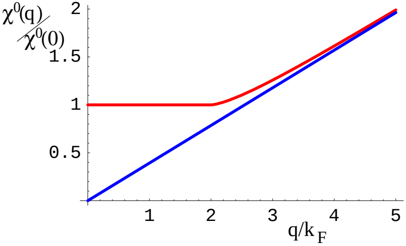
- Singularity of $\chi^0(q, \omega)$ at limit of intraband SPE.
- Singularity of $\chi(q, \omega)$ reflects plasmon

Static polarization $\omega = 0$

2DEG



Graphene

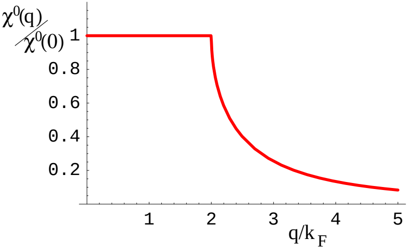


- Polarization is constant ($-DOS(\mu)$) for $q < 2k_F$, however for $q > 2k_F$ the polarization increases linear in q for graphene and falls of quadratically for the 2DEG.
- At $q = 2k_F$ the polarization is non-analytical with a discontinuous second (first) derivative for graphene (2DEG).

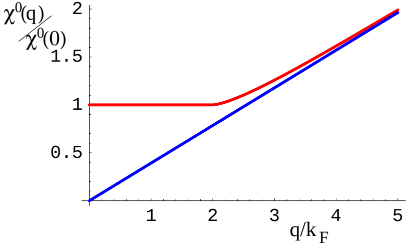
Gorbar *et al* PRB **66**, 045108 (2002); Ando, J. Phys. Soc. Jpn **75**, 074716 (2006).

Static polarization $\omega = 0$

2DEG



Graphene

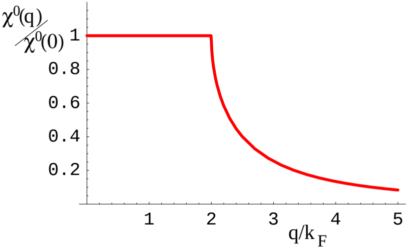


- Polarization is constant ($-DOS(\mu)$) for $q < 2k_F$, however for $q > 2k_F$ the polarization increases linear in q for graphene and falls of quadratically for the 2DEG.
- At $q = 2k_F$ the polarization is non-analytical with a discontinuous second (first) derivative for graphene (2DEG).

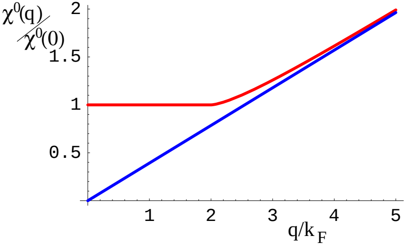
Gorbar *et al* PRB **66**, 045108 (2002); Ando, J. Phys. Soc. Jpn **75**, 074716 (2006).

Static polarization $\omega = 0$

2DEG



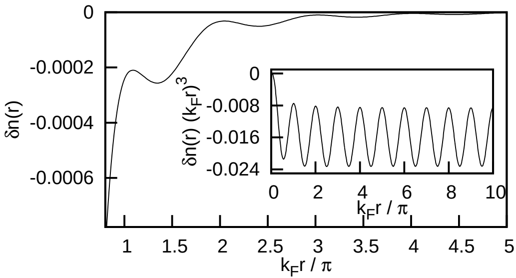
Graphene



- Polarization is constant $(-DOS(\mu))$ for $q < 2k_F$, however for $q > 2k_F$ the polarization increases linear in q for graphene and falls of quadratically for the 2DEG.
- At $q = 2k_F$ the polarization is non-analytical with a discontinuous second (first) derivative for graphene (2DEG).

Gorbar *et al* PRB **66**, 045108 (2002); Ando, J. Phys. Soc. Jpn **75**, 074716 (2006).

Screening of charged impurities in doped graphene



$$\delta n(r) = \frac{e}{(2\pi)^2} \int d^2q \left(\frac{1}{\epsilon(q,0)} - 1\right) e^{i\mathbf{q}\cdot\mathbf{r}} = n_{TF}(r) + n_{osc}(r)$$

$$n_{TF}(r) \propto \frac{1}{k_F r^3}\ ; \quad \mathbf{n_{osc}(r)} \propto \frac{\cos(2\mathbf{k_F r})}{\mathbf{k_F r^3}}\ ; \quad \mathbf{n_{osc}^{2DEG}(r)} \propto \frac{\cos(2\mathbf{k_F r})}{\mathbf{r^2}}$$

In graphene $n_{TF}(r) > n_{osc}(r)$, so that $\delta n(r)$ has always same sign.

V. V. Cheianov, V. Fal'ko PRL **97**, 226801 (2006).

Screening of charged impurities in undoped graphene

- Static polarization is linear in q,
  $\chi^0(q,0) = -\frac{q}{4\hbar v_F}$.
  Since it is analytic, there is no oscillating contribution to the induced charge or potential.
- The static dielectric function is constant,
  $\varepsilon(q,0) = 1 - v_q \chi^0(q,0) = const.$
  The total potential and the total charge density are reduced by a constant with respect to the external ones.
- This screening behavior is typical for an insulator.

Screening of charged impurities in undoped graphene

- Static polarization is linear in q,
  $\chi^0(q,0) = -\frac{q}{4\hbar v_F}$.
  Since it is analytic, there is no oscillating contribution to the induced charge or potential.
- The static dielectric function is constant,
  $\varepsilon(q,0) = 1 - v_q \chi^0(q,0) = const$.
  The total potential and the total charge density are reduced by a constant with respect to the external ones.
- This screening behavior is typical for an insulator.

Screening of charged impurities in undoped graphene

- Static polarization is linear in q,
  $\chi^0(q,0) = -\frac{q}{4\hbar v_F}$.
  Since it is analytic, there is no oscillating contribution to the induced charge or potential.
- The static dielectric function is constant,
  $\varepsilon(q,0) = 1 - v_q\chi^0(q,0) = const.$
  The total potential and the total charge density are reduced by a constant with respect to the external ones.
- This screening behavior is typical for an insulator.

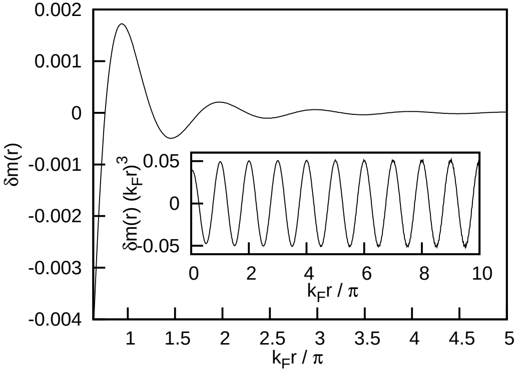
RKKY interaction

Effective interaction between magnetic imp. or induced spin density

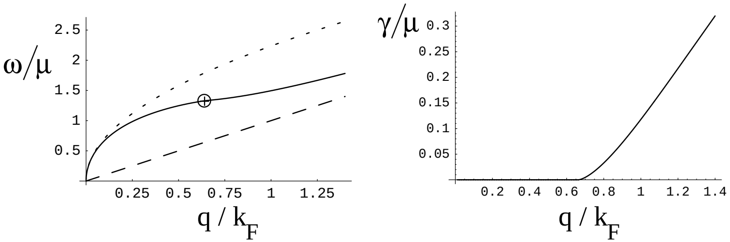
$$\delta m(\mathbf{r}) \quad \propto \chi^0(\mathbf{r})$$
$$\delta m^{2DEG}(\mathbf{r}) \quad \sim \frac{\cos(2k_F r)}{r^2}$$
$$\delta m^{Graph}(\mathbf{r}) \quad \sim \frac{\cos(2k_F r)}{r^3}$$

However if spin impurities replace single carbon atoms sublattice-symmetry is broken: $\delta m^{Graph}(\mathbf{r}) \sim r^{-2}$

V. V. Cheianov, V. Fal'ko PRL **97**, 226801 (2006).



Plasmon in graphene

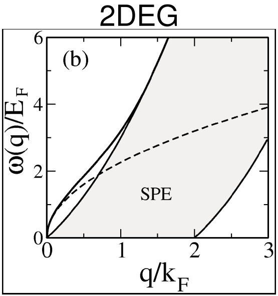


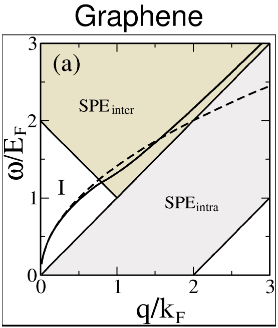
Dispersion $\omega_P(q)$ and decay rate $\gamma(\mathbf{q})$ determined by $\varepsilon(q, \omega_P - i\gamma) = 0$, with $\varepsilon(q,\omega) = 1 - v_q\chi^0(q,\omega)$

- As in 2DEG we obtain for $q \to 0$: $\omega_P^2(q) \propto \mu q$.
- Different dependence on electron concentration since $\mu \propto n^{1/2}$ ($\mu \propto n$) in graphene (2DEG).[2]

[2] E. Hwang, S. Das Sarma, cond-mat/0610561

Plasmons in 2DEG and in graphene





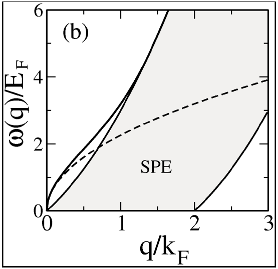
E. Hwang, S. Das Sarma, cond-mat/0610561

- Damping due to interband excitations absent in 2DEG. Stability regime increases proportional to doping μ. For $\mu = T = 0$ plasmons are always unstable, however not at T>0[3]

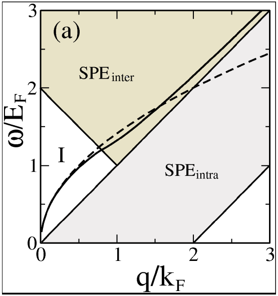
[3] O. Vafek, PRL **97**, 266406 (2006)

Plasmons in 2DEG and in graphene

2DEG



Graphene



E. Hwang, S. Das Sarma, cond-mat/0610561

- Damping due to interband excitations absent in 2DEG. Stability regime increases proportional to doping μ. For $\mu = T = 0$ plasmons are always unstable, however not at T>0[3]

[3] O. Vafek, PRL **97**, 266406 (2006)

Acoustical phonons in graphene

- Screening of the ion-ion interaction by conduction electrons determines phonon dispersion.
- Following Ashcraft and Mermin phonon dispersion is estimated by:

$$\omega_{AP}^2(k) \sim \frac{\Omega_P^2(k)}{\epsilon(k)},$$

  with $\Omega_P(k)$ is ion plasma frequency
- For $k \to 0$ one obtains $\omega_{AP}(k) = v_S k$ with the sound velocity:
  In 2DEG: $v_S \approx \sqrt{m/2M}\, v_F$ (Bohm-Staver relation).
  In graphene: $v_S = v_F \sqrt{\frac{\pi E_0}{\mu}}$ with $E_0 = \hbar^2/MA_C \approx 0.1$ meV.

Acoustical phonons in graphene

- Screening of the ion-ion interaction by conduction electrons determines phonon dispersion.
- Following Ashcraft and Mermin phonon dispersion is estimated by:

$$\omega_{AP}^2(k) \sim \frac{\Omega_P^2(k)}{\epsilon(k)},$$

with $\Omega_P(k)$ is ion plasma frequency

- For $k \to 0$ one obtains $\omega_{AP}(k) = v_S k$ with the sound velocity:
  In 2DEG: $v_S \approx \sqrt{m/2M}\, v_F$ (Bohm-Staver relation).
  In graphene: $v_S = v_F \sqrt{\frac{\pi E_0}{\mu}}$ with $E_0 = \hbar^2/MA_C \approx 0.1$ meV.

Acoustical phonons in graphene

- Screening of the ion-ion interaction by conduction electrons determines phonon dispersion.
- Following Ashcraft and Mermin phonon dispersion is estimated by:

$$\omega_{AP}^2(k) \sim \frac{\Omega_P^2(k)}{\epsilon(k)},$$

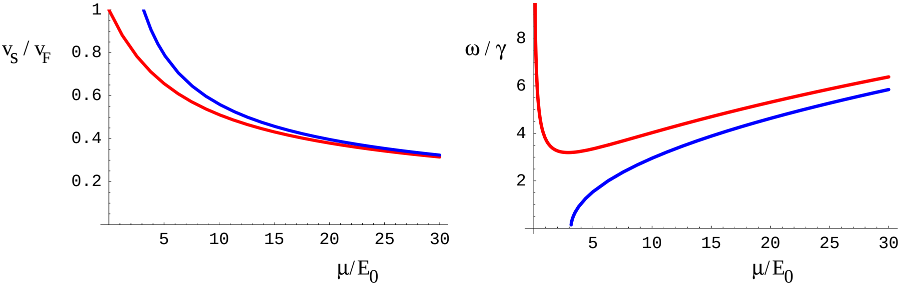
  with $\Omega_P(k)$ is ion plasma frequency
- For $k \to 0$ one obtains $\omega_{AP}(k) = v_S k$ with the sound velocity:
  In 2DEG: $v_S \approx \sqrt{m/2M}\, v_F$ (Bohm-Staver relation).
  In graphene: $v_S = v_F \sqrt{\frac{\pi E_0}{\mu}}$ with $E_0 = \hbar^2/MA_C \approx 0.1$ meV.

Acoustical phonons in graphene

Phonon dispersion and decay rate given by roots of $\varepsilon_{\rm tot}(k, \omega + i\gamma)$:

$$0 = \varepsilon_{\rm tot}(k, \omega) = \varepsilon_{\rm el}(k, \omega) + \varepsilon_{\rm ion}(k, \omega) - 1$$

with $\varepsilon_{\rm ion}(k, \omega) = 1 - \frac{\Omega_P^2(k)}{\omega^2}$ dielectric function of ion plasma.



Outlook and summary

- Analytic expression of RPA polarization at arbitrary k and ω.
- Reduced static screening in comparison to 2DEG and no sign change in induced density.
- Plasma dispersion and decay rate.
- Expected: Tunable and huge sound velocity. $v_S \propto \sqrt{1/\mu}$

Outlook and summary

- Analytic expression of RPA polarization at arbitrary k and ω.
- Reduced static screening in comparison to 2DEG and no sign change in induced density.
- Plasma dispersion and decay rate.
- Expected: Tunable and huge sound velocity. $v_S \propto \sqrt{1/\mu}$

Outlook and summary

- Analytic expression of RPA polarization at arbitrary k and ω.
- Reduced static screening in comparison to 2DEG and no sign change in induced density.
- Plasma dispersion and decay rate.
- Expected: Tunable and huge sound velocity. $v_S \propto \sqrt{1/\mu}$

Outlook and summary

- Analytic expression of RPA polarization at arbitrary k and ω.
- Reduced static screening in comparison to 2DEG and no sign change in induced density.
- Plasma dispersion and decay rate.
- Expected: Tunable and huge sound velocity. $v_S \propto \sqrt{1/\mu}$

Minimal conductivity at Dirac point

Conductivity and polarization are related due to continuity equation/ charge conservation

$$\begin{aligned} \mathrm{Re}(\sigma(q,\omega)) &= -\frac{e^2\omega}{q^2}\mathrm{Im}(\chi(q,\omega)) \\ \sigma_0 &:= \lim_{\omega\to 0}\lim_{q\to 0}\mathrm{Re}(\sigma(q,\omega)) = \frac{\pi}{2}\frac{e^2}{h} \end{aligned}$$

Finite conductivity at Dirac-point. Value of conductivity is unaffected by Coulomb interaction, since same result for $\chi = \chi_0$ or $\chi = \chi_0/(1 - v_q\chi_0)$. Small deviation from Landauer formula which results in $\sigma_0 = 4/\pi\, e^2/h$

A. Ludwig *et al.* PRB 50, 7526 (1994), cond-mat/0610598.

Katsnelson Eur. Phys. J. B **51**, 157 (2006).