



Collective excitations in graphene and the effect of electron-electron interaction

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Introduction

Which are the main features of the excitation spectrum of a two-dimensional (2D) electron?

- with/without strong magnetic field: $\mathbf{B}=B~\hat{\mathbf{z}}$
- with/without electron-electron interactions (RPA): $r_s = arepsilon_{int} / arepsilon_F$

- for a standard 2DEG versus doped graphene

	2DEG	(Doped) graphene	
$B = 0, r_s = 0$	Continuum PHES	(Intra-) & inter-band continuum PHES	
$B = 0, r_s \neq 0$	Continuum PHES + Plasmons	(Intra-) & inter-band continuum PHES + Plasmons	PHES = particle-hole excitation spectrum
$B \neq 0, r_s = 0$	Discretized PHES (magneto-excitons)	Discretized PHES (hints linear magneto-plasmons)	
$B \neq 0, r_s \neq 0$	Discretized PHES (ME) + upper hybrid mode	Discretized PHES (LMP) + upper hybrid mode	

+ Effect of disorder in the spectrum

π-band tight-binding model for graphene



π-band tight-binding model for graphene







• Scalar wave-functions

 Two-component (spinorial) wave-functions

Method: polarization function as a particle-hole pair propagator

$$\Pi^{0}(\mathbf{q},\omega) = \underset{\mathbf{q},\omega}{\overset{\mathbf{k}+\mathbf{q},\omega+\omega'}{\underset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\omega}{\overset{\mathbf{q},\om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 $\Pi(\mathbf{q},\omega)$ = dressed particle-hole pair propagator (e.g. in the RPA)

 $S(q,\omega) = -Im \prod(q,\omega)/\pi =$ spectral density of this propagator (a.k.a. dynamic structure factor)

Pole of $\Pi(\mathbf{q},\omega)$ = collective mode (coherent particle-hole excitation) \Rightarrow peak in S(\mathbf{q},ω):

whose position gives the dispersion relation of the collective mode whose width gives the damping (1/lifetime)

Therefore: we will look for peaks in $S(q,\omega)$

Particle-hole excitations in a standard 2DEG



Interacting 2DEG: RPA theory





PHES of undoped graphene in the Dirac cone approximation







Interacting graphene at B = 0: RPA theory



PHES of undoped graphene beyond the Dirac cone approximation

Kubo Formula

$$\Pi \left(\mathbf{q}, \omega \right) = \frac{i}{V} \int_{0}^{\infty} d\tau e^{i\omega\tau} \left\langle \left[\rho \left(\mathbf{q}, \tau \right), \rho \left(-\mathbf{q}, 0 \right) \right] \right\rangle$$
$$\rho \left(\mathbf{q} \right) = \sum_{i} c_{i}^{\dagger} c_{i} \exp \left(i\mathbf{q} \cdot \mathbf{r}_{i} \right)$$

$$\rho(\mathbf{q},\tau) = e^{iH\tau}\rho(\mathbf{q})e^{-iH\tau}$$

$$\Pi(\mathbf{q},\omega) = -\frac{2}{V} \int_0^\infty d\tau e^{i\omega\tau} \operatorname{Im} \langle \varphi | n_F(H) e^{iH\tau} \\ \times \rho(\mathbf{q}) e^{-iH\tau} [1 - n_F(H)] \rho(-\mathbf{q}) | \varphi \rangle$$

 $|\varphi\rangle = \sum_{i} a_{i} c_{i}^{\dagger} |0\rangle \qquad \sum_{i} |a_{i}|^{2} = 1$

Lindhard Function

$$\Pi(\mathbf{q},\omega) = -\frac{g_s}{(2\pi)^2} \int_{\mathrm{BZ}} d^2 \mathbf{k} \sum_{s,s'=\pm} f_{s\cdot s'}(\mathbf{k},\mathbf{q}) \frac{n_F[E^s(\mathbf{k})] - n_F[E^{s'}(\mathbf{k}+\mathbf{q})]}{E^s(\mathbf{k}) - E^{s'}(\mathbf{k}+\mathbf{q}) + \omega + i\delta}$$

$$E^{\pm}(\mathbf{k}) = \pm t |\phi_{\mathbf{k}}| - \mu$$

$$\phi_{\mathbf{k}} = 1 + 2e^{i3k_x a/2} \cos\left(\frac{\sqrt{3}}{2}k_y a\right)$$

$$f_{\pm}(\mathbf{k},\mathbf{q}) = \frac{1}{2} \left(1 \pm \operatorname{Re}\left[e^{iq_{x}a} \frac{\phi_{\mathbf{k}}}{|\phi_{\mathbf{k}}|} \frac{\phi_{\mathbf{k}+\mathbf{q}}^{*}}{|\phi_{\mathbf{k}+\mathbf{q}}|} \right] \right)$$

see also T. Stauber, J. Shliemann & N. M. R. Peres Phys. Rev. B **81**, 085409 (2010)

S. Yuan, H. De Raedt & M. I. Katsnelson. Phys. Rev. B 82, 115448 (2010)
S. Yuan, RR & M. I. Katsnelson. Phys. Rev. B 84, 035439 (2011)

PHES of undoped graphene beyond the Dirac cone approximation



High energy π-Plasmons



DOS and to zeros of the dielectric function...

High energy π-Plasmons



PHES of undoped graphene beyond the Dirac cone approximation





Effect of disordered in graphene: DOS with resonant impurites



Optical conductivity of disordered graphene: the effect of resonant impurites



Summary of the PHES with B=0

• High energy resonances (π-plasmons) associated to transitions between Van Hove singularities in undoped graphene. (No phase space for *classical* plasmon within the RPA).

- Theoretical results for the loss function compare well with EELS measurements.
- Effect of resonant scatterers (vacancies, adatoms, etc.) which leads to the creation of zero-energy impurity bands: Background contribution in the optical conductivity.
- Effect of disorder in antidot graphene lattices: stability of the gap

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$B \neq 0, r_s = 0$	Discretized PHES (hints magneto-excitons)	Discretized PHES (hints linear magneto-plasmons)
$B \neq 0, r_s \neq 0$	Discretized PHES (ME) + upper hybrid mode	Discretized PHES (LMP) + upper hybrid mode

S. Yuan, **RR** & M. I. Katsnelson *Phys. Rev. B* **84**, 035439 (2011)

S. Yuan, **RR**, H. De Raedt & M. I. Katsnelson *Phys. Rev. B* 84, 195418 (2011)

D. Makogon, R. van Gelderen, RR & C. Morais Smith Phys. Rev. B 84, 125404 (2011)

Graphene in a strong magnetic field

Tight-binding model at B≠0: Peierls subtitution



DOS in the ultra-high magnetic field limit



 Non-trivial Landau level quantization of the spectrum around the Van Hove singularity with two different sets of LLs that merge at the saddle point

S. Yuan, RR & M. I. Katsnelson, Solid State Comm. 152, 1446 (2012)



PHES of graphene in a magnetic field using a full π-band tight-binding model

• This problem has been first considered in graphene here... Plasma Excitations in Graphene: Their Spectral Intensity and Temperature Dependence in Magnetic Field

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PHES of graphene in a magnetic field using a full π-band tight-binding model



Loss function of graphene in a magnetic field using a full π-band tight-binding model

el-el interactions within the RPA





PHES of a standard 2DEG in a magnetic field



Interacting 2DEG in a magnetic field: RPA theory



- Interactions lead to a transfer of spectral weight from the long-wave length region of the PHES to the plasmon mode, modified by the magnetic field: known as upper hybrid (UH) mode in plasma phys.
- The magneto-excitons acquire a dispersion due to the inclusion of Coulomb interaction.



Particle-hole polarization in graphene: B≠0

$$\begin{split} & \text{Decomposition in inter-} \\ & \text{and intra-band contributions} \\ & \Pi_n^{\lambda}(\mathbf{q},\omega) = \sum_{\lambda'}^{n-1} \prod_{nn'}^{\lambda\lambda'}(\mathbf{q},\omega) \\ & \Pi^0(\mathbf{q},\omega) = \sum_{n=1}^{N_F} \prod_n^{\lambda_F}(\mathbf{q},\omega) + \Pi^{vac}(\mathbf{q},\omega) \\ & + \sum_{\lambda'} \sum_{n'=n+1}^{N_c} \prod_{nn'}^{\lambda\lambda'}(\mathbf{q},\omega) + \prod_{nn'}^{\lambda-\lambda}(\mathbf{q},\omega) \\ & \text{Vacuum (inter-band) contribution} \\ & \Pi^{vac}(\mathbf{q},\omega) \equiv -\sum_{n=1}^{N_c} \prod_n^{\lambda=1}(\mathbf{q},\omega) \\ & \Pi^{\lambda\lambda'}_{nn'}(\mathbf{q},\omega) \equiv \frac{\overline{\mathcal{F}}_{nn'}^{\lambda\lambda'}(\mathbf{q})}{\lambda\xi_n - \lambda'\xi_{n'} + \omega + i\delta \text{sgn}(\omega)} \\ & \Pi^{\lambda\lambda'}_{nn'}(\mathbf{q},\omega) \equiv \frac{\overline{\mathcal{F}}_{nn'}^{\lambda\lambda'}(\mathbf{q})}{\lambda\xi_n - \lambda'\xi_{n'} + \omega + i\delta \text{sgn}(\omega)} \\ & \text{Form factor of the polarization function at } \mathbf{B} \neq \mathbf{0} \\ & \overline{\mathcal{F}}_{nn'}^{\lambda\lambda'}(\mathbf{q}) = \frac{e^{-l_{n}^2g^2/2}}{2\pi l_B^2} \left(\frac{l_B^2g^2}{2}\right)^{n_s - n_c} \left\{\lambda l_{n+1n'}^{*1*} \sqrt{\frac{(n_c - 1)!}{(n_s - 1)!}} \left[L_{n_c - 1}^{n_s - n_c} \left(\frac{l_B^2g^2}{2}\right)\right] + \lambda' 2_n^* 2_{n'}^* \sqrt{\frac{n_c!}{n_s!}} \left[L_{n_c - n_c}^{n_s - n_c} \left(\frac{l_B^2g^2}{2}\right)\right] \right\}^2 \end{split}$$

PHES of graphene in a magnetic field



Interacting graphene in a magnetic field: RPA theory



- Interactions lead to a transfer of spectral weight from the PHES to the upper-hybrid mode
- Relatively weak renormalization of the intra-band region of the spectrum.
- The linear magneto-plasmons are clearly pronounced due to the inclusion of Coulomb interaction.

Zoom of the low energy PHES: Graphene vs. 2DEG



Structure of the PHES: 2DEG vs. Graphene



Structure of the PHES: 2DEG vs. Graphene



Effect of disorder: Landau level broadening



Effect of doping: Landau level filling



Hydrodynamics: upper hybrid mode (plasmon)

• Euler and continuity equations:

$$\frac{d}{dt} \left(\frac{\varepsilon_F}{v_F^2} \mathbf{J}(\mathbf{r}, t) \right) = e \nabla P(\mathbf{r}, t) + en(\mathbf{r}, t) \nabla \int d\mathbf{r}' \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} [n(\mathbf{r}', t) - n_0] - e \mathbf{J}(\mathbf{r}, t) \times \mathbf{B},$$

$$\frac{\partial n(\mathbf{r}, t)}{\partial t} = \frac{1}{e} \nabla \cdot [\mathbf{J}(\mathbf{r}, t)]$$
• Approximate dispersion relation:

$$\omega(q) \simeq \sqrt{\# v_F^2 q^2 + \frac{2\pi e^2 n_0 v_F^2}{\epsilon_b \varepsilon_F}} q + \omega_c(\varepsilon_F)^2} \tag{9}$$

 ql_B

-0.8

$$\# = \begin{cases} 1/2 & \text{Hydrodynamic} \\ 3/4 & - - - RPA \end{cases}$$

Dispersion of the plasmon and upper hybrid modes



Spin-flip & spin-wave modes in graphene

Time-dependent Hartree-Fock approximation



$$\Omega_{ME}(q) = E_{kin}^{(n_e,n_h)} + \Delta E^{(n_e,s_z^e;n_h,s_z^h)}(q)$$

$$\Omega_{SW}(q) = g\mu_B BS_z + \Delta E^{(n_e,s_z^e;n_h,s_z^h)}(q)$$

$$\Omega_{SF}(q) = E_{kin}^{(n_e,n_h)} + g\mu_B BS_z + \Delta E^{(n_e,s_z^e;n_h,s_z^h)}(q)$$

$$E_{kin}^{(n_e,n_h)} = \frac{v_F}{l_B} \sqrt{2} \left(\lambda_e \sqrt{n_e} - \lambda_h \sqrt{n_h}\right)$$

Includes:

- -Depolarization or exchange term (RPA)
- -Direct Coulomb interaction between electron and hole (vertex correction)

-Difference in exchange self-energy between electron and hole

A. Iyengar, J. Wang, H. A. Fertig, and L. Brey, *PRB* **75**, 125430 (2007); Y. A. Bychkov and G. Martinez, *PRB* **77**, 125417 (2008); RR, J.-N. Fuchs and M. O. Goerbig, *PRB* **82**, 205418 (2010)

Spin-flip & spin-wave modes in graphene



Bernstein modes (BMs): hybridization of a plasmon mode with inter-Landau level transitions



Phenomenological model for Bernstein modes in graphene

Hamiltonian for the plasmon (UH mode):

$$H_{\rm uh} = \sum_{\mathbf{q}} \omega_{\rm uh}(q, B) b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} \qquad b_{\mathbf{q}}^{(\dagger)} \propto \rho_{uh}(\mathbf{q})$$

Hamiltonian for coupling, via Coulomb interaction, between plasmon and inter-LL excitations:

$$H_{\text{coupl}} = \frac{1}{4} \sum_{\mathbf{q}} \frac{2\pi e^2}{\epsilon |\mathbf{q}|} \left[\rho(-\mathbf{q})\rho_{\text{uh}}(\mathbf{q}) + \rho_{\text{uh}}(-\mathbf{q})\rho(\mathbf{q}) \right]$$

Density components of inter-LL excitations:

$$\rho(\mathbf{q}) = \sum_{\lambda n, \lambda' n'} \mathcal{F}_{\lambda n, \lambda' n'}(\mathbf{q}) \sum_{m, m'} \langle m | e^{-i\mathbf{q} \cdot \mathbf{R}} | m' \rangle c^{\dagger}_{\lambda n, m} c_{\lambda' n', m'}$$



Phenomenological model for Bernstein modes in graphene

Dyson-type equation:

$$\left[\omega^2 - \omega_{\rm uh}^2\right] \left[\omega^2 - \Omega_{\lambda n, n'}^2\right] = \frac{g \mathcal{V}^2}{4} \omega_{\rm uh} \Omega_{\lambda n, n'}$$

$$\mathcal{V} \equiv (e^2 / \epsilon q l_B^2) |\mathcal{F}_{\lambda n, n'}(\mathbf{q})|^2$$

$$\Omega_{\lambda n,n'} = \frac{v_F}{l_B} \sqrt{2} (\sqrt{n'} - \lambda \sqrt{n})$$

The poles of the dressed propagator leads to the dispersions:

$$\omega_{\pm}^{2} = \frac{\omega_{\mathrm{uh}}(q)^{2} + \Omega_{\lambda n, n'}^{2}}{2}$$
$$\pm \sqrt{\frac{\left[\omega_{\mathrm{uh}}^{2} - \Omega_{\lambda n, n'}^{2}\right]^{2}}{4} + \frac{g\mathcal{V}^{2}}{4}\omega_{\mathrm{uh}}\Omega_{\lambda n, n'}}$$



Avoided level crossing dominated by resonant term: $\omega \simeq \omega_{\mathrm{uh}} \simeq \Omega_{\lambda n, n'}$

Phenomenological model for Bernstein modes in graphene



Experimental measurements of Bernstein modes in a 2DEG I: transmission spectroscopy



Experimental measurements of Bernstein modes in a 2DEG II: inelastic light scattering



Summary of the PHES with B≠0

• Study of the particle-hole excitation spectrum of graphene in a magnetic field as compared to the standard 2DEG.

• Landau level quantization yields *linear magneto-plasmon* modes in contrast to the 2DEG, where the equidistant LL structure leads to pronounced horizontal magneto-exciton modes.

• Inelastic (Raman) light scattering could be used to reveal the existence and measure the dispersion relation of the linear magneto-plasmons, as well as the Bernstein modes in graphene.

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RR, J.-N. Fuchs and M.O. Goerbig, *Phys. Rev. B* 80, 085408 (2009); *ibid* 82, 205418 (2010); *ibid* 83, 205406 (2011)
RR, M.O. Goerbig & J.-N. Fuchs, *Semicond. Sci. Technol.* 25, 034005 (2010) [short review paper]
S. Yuan, RR, & M. I. Katsnelson, *Solid State Comm.* 152, 1446 (2012)

Conclusion: linear magneto-plasmons rather than horizontal magneto-excitons







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...and to you for your attention

Tainan, July 2012

Happy Birthday Prof. Lin!!!

