



The Abdus Salam
International Centre for Theoretical Physics



1960-17

ICTP Conference Graphene Week 2008

25 - 29 August 2008

Spectral properties of doped graphene

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Spectral properties of doped graphene

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Yafis Barlas, Tami Pereg-Barnea, and Allan H. MacDonald
(U. Texas, Austin)



Trieste, August 27th 2008



Outline

➊ Introduction and motivations

- ✓ Why is it interesting to study the impact of e-e interactions in graphene?
- ✓ Experimental results (ARPES)

➋ Theory of quasiparticle properties in doped graphene

- ✓ A quick note on Landau parameters (quasiparticle velocity, compressibility, etc)
- ✓ Numerical results for the GW quasiparticle self-energy
- ✓ Discussion of the main features

➌ Theory vs experiment

- ✓ Spectral function and quasiparticle decay
- ✓ Comments on the role of beyond-RPA physics, disorder, nearby layers, etc
- ✓ Conclusions and future perspectives

Related literature (very rough list)

• Electron-electron interactions in graphene

- ✓ Guinea's group
- ✓ Castro Neto's group
- ✓ Das Sarma's group
- ✓ ...

• Impact of electron-electron interactions on 1-particle properties

- ✓ E.W. Hwang and S. Das Sarma, PRB 77, 0801412(R) (2008)

• Very recent works on 1-particle properties based on ab initio GW

- ✓ P.E. Trevisanutto et al., arXiv:0806.3365v1
- ✓ C. Attaccalite et al., arXiv:0808.0786v1

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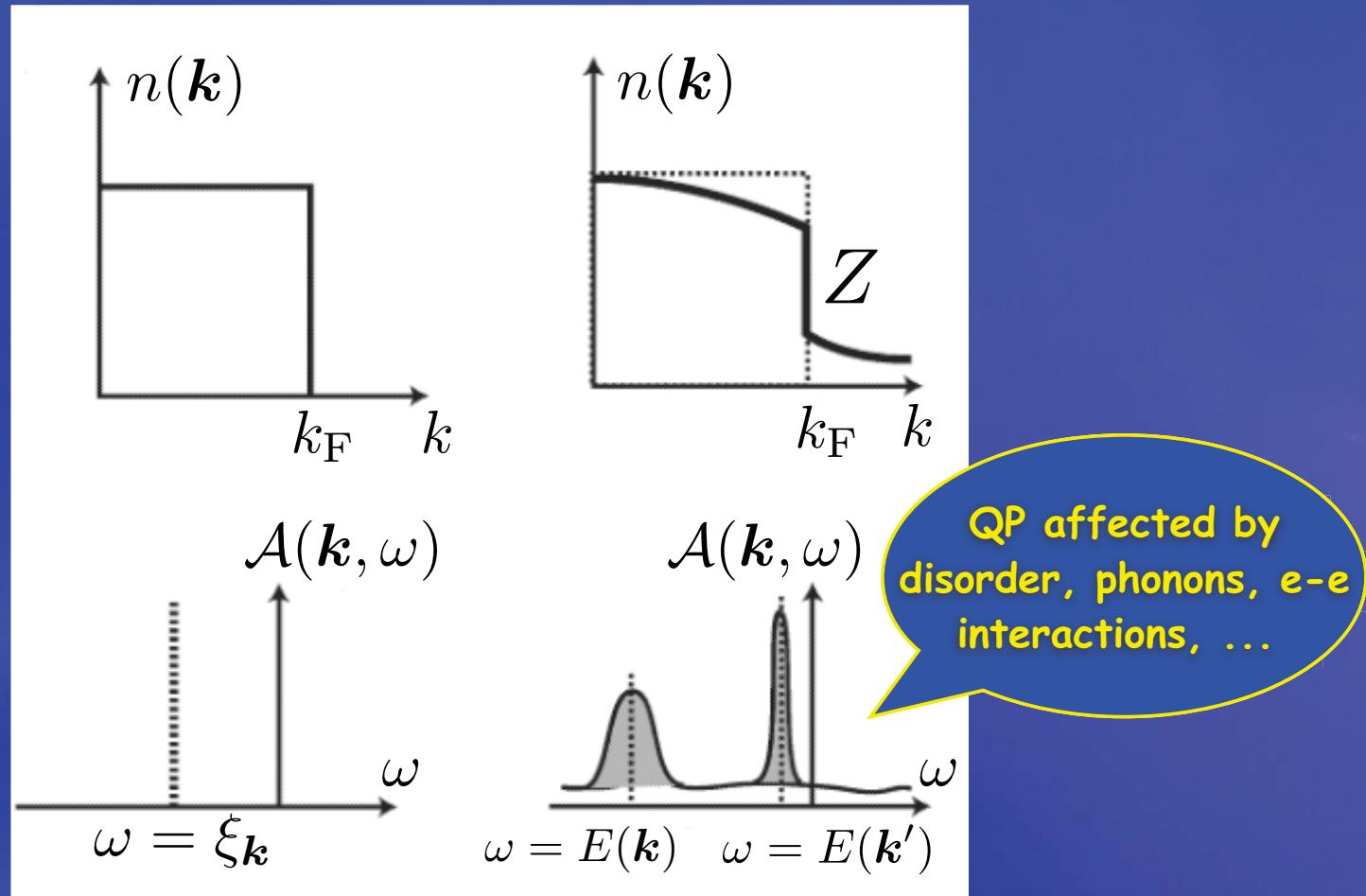
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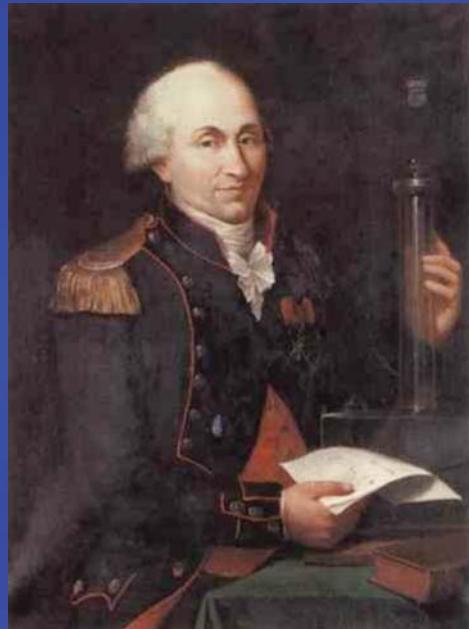
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Landau theory of normal Fermi liquids



Our objective is to study the impact of electron-electron interactions

e-e interactions in graphene: I



Charles Augustin de Coulomb
1736 - 1806

A diagram showing two spherical charges: one black and one red. They are separated by a horizontal green double-headed arrow, representing the interaction between them.

$$v(r) = \frac{e^2}{\epsilon r}$$

$$\mathcal{H}_{\text{band}} = v(\sigma \cdot p)$$

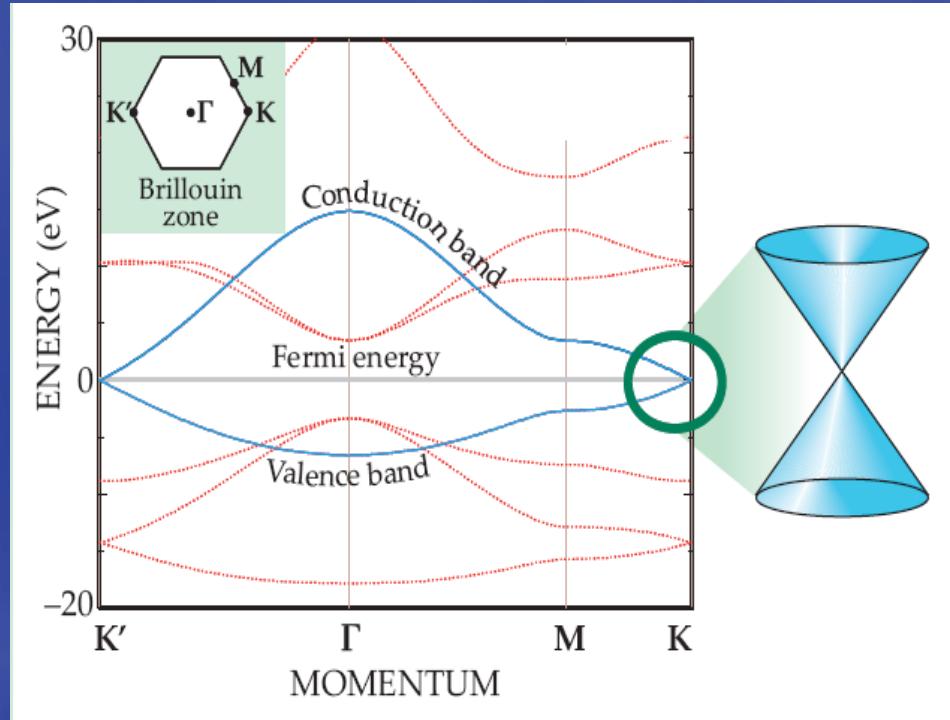
also scales with inverse distance!

$$\frac{\langle \mathcal{H}_{\text{int}} \rangle \sim e^2 k_{\text{F}} / \epsilon}{\langle \mathcal{H}_{\text{band}} \rangle \sim \hbar v k_{\text{F}}}$$

$$\alpha_{\text{ee}} = \frac{e^2}{\epsilon \hbar v} \sim 0.5 \quad (\text{graphene on } \text{SiO}_2) \quad \alpha_{\text{gr}} = g \alpha_{\text{ee}} \sim 2$$

coupling parameter is independent of density....BUT....

$e\text{-}e$ interactions in graphene: II



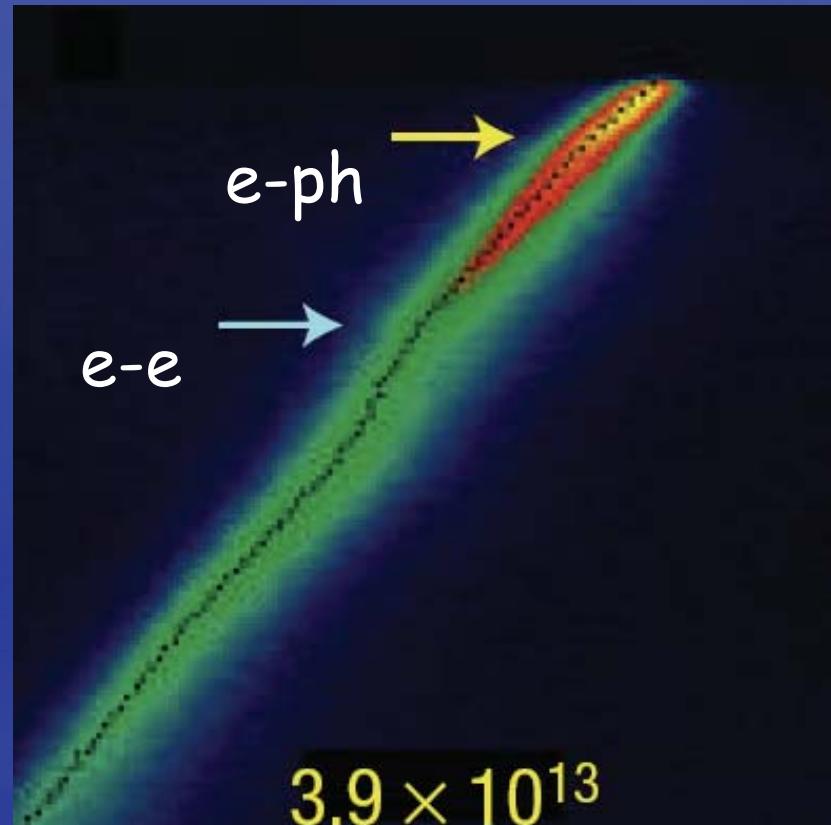
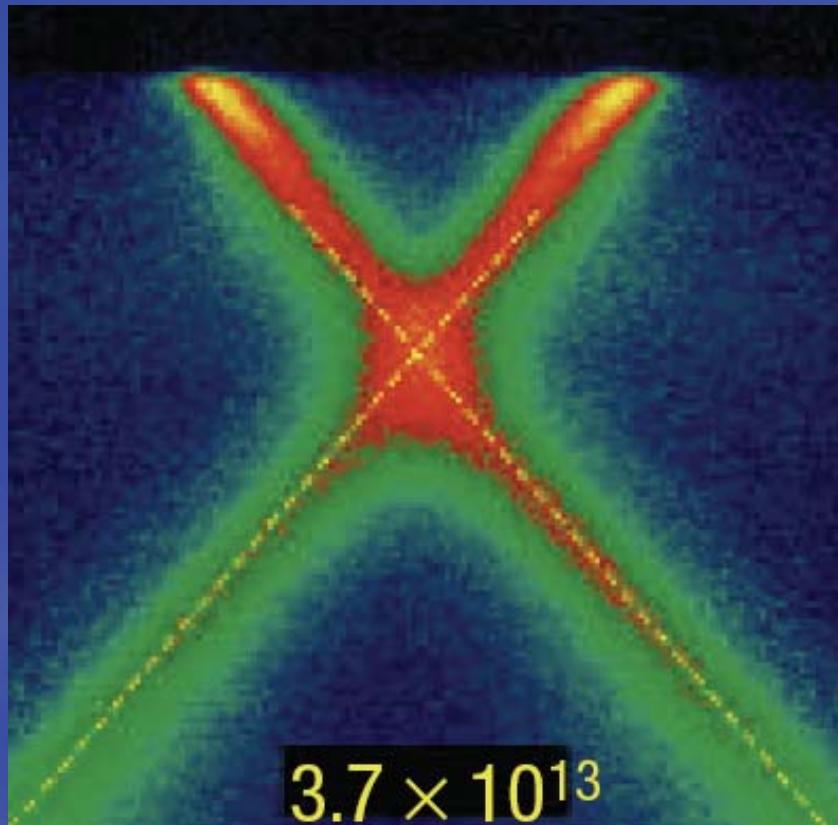
Introduce an ultraviolet cutoff: $\int \frac{d^2 q}{(2\pi)^2} \rightarrow \int_0^{k_c} \frac{qdq}{2\pi}$

$$\Lambda = \frac{k_c}{k_F} \gg 1 \quad \Lambda(n) = \frac{2}{\sqrt{n \mathcal{A}_0}}$$

density

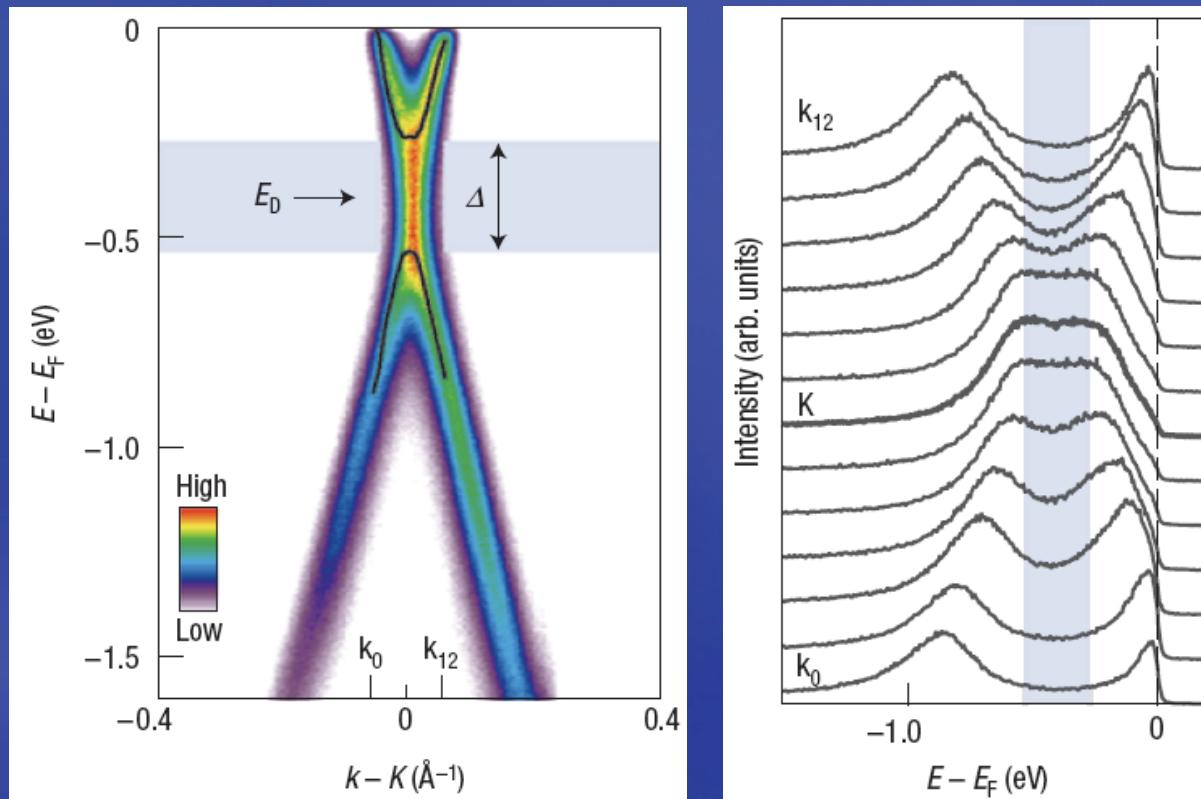
no problems:
screening

ARPES spectra on epitaxial graphene: I



A. Bostwick, T. Ohta, T. Seyller, K. Horn, and E. Rotenberg, Nature Physics (2007)

ARPES spectra on epitaxial graphene: II



Band-gap opening in epitaxial graphene
A gap (partly) due to many-body effects ???
Or only due to substrate ???

S.Y. Zhou, G.-H. Gweon, A.V. Fedorov, P.N. First, W.A. de Heer, D.-H. Lee, F. Guinea, A.H. Castro Neto,
and A. Lanzara, Nature Materials (2007)

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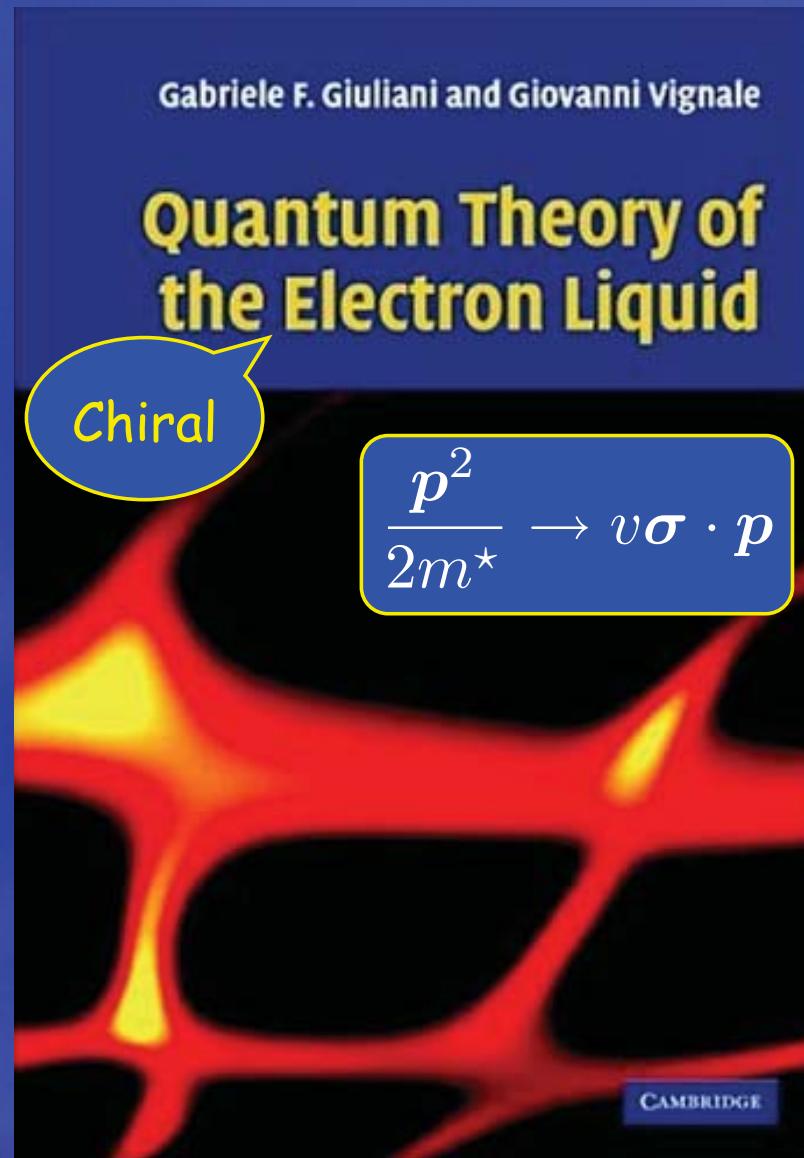
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The electron gas Bible



Main message

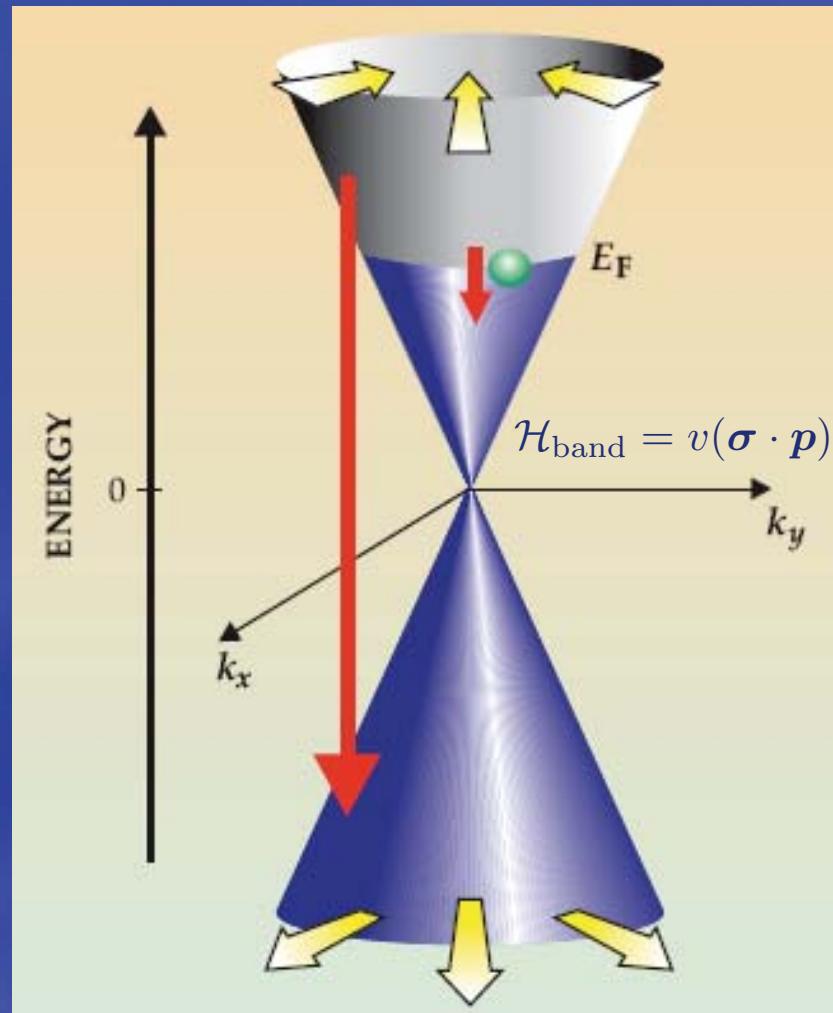
Doped graphene is a 2D electron gas like ordinary 2D EG in ordinary semiconductors in many ways but with interesting new features because of

- i) interband electron-hole excitations and interband exchange interactions
- ii) (sublattice pseudospin) chirality of eigenstates

Most important consequences:

- i) Quasiparticle velocity is enhanced rather than suppressed
- ii) Charge and spin susceptibilities are suppressed rather than enhanced
- iii) xc effects favor *homogeneous* phases and enhance screening
- iv) stronger plasmon features

Chirality and e-e interaction physics



A.K. Geim and A.H. MacDonald, Physics Today (2007)

GW theory for 1-particle properties

Quasiparticle self-energy

$$\Sigma_s(\mathbf{k}, i\omega_n) = -\frac{1}{\beta} \sum_{s'} \int \frac{d^2\mathbf{q}}{(2\pi)^2} \sum_{m=-\infty}^{+\infty} W(\mathbf{q}, i\Omega_m) \frac{1 + ss' \cos(\theta_{\mathbf{k}, \mathbf{k}+\mathbf{q}})}{2} G_{s'}^{(0)}(\mathbf{k} + \mathbf{q}, i\omega_n + i\Omega_m)$$

Dynamically screened interaction

$$W(\mathbf{q}, i\Omega) = \frac{v_q}{\varepsilon(\mathbf{q}, i\Omega)}$$

RPA

Single-particle Green's function

$$G_s^{(0)}(\mathbf{k}, i\omega) = \frac{1}{i\omega - \xi_s(\mathbf{k})}$$

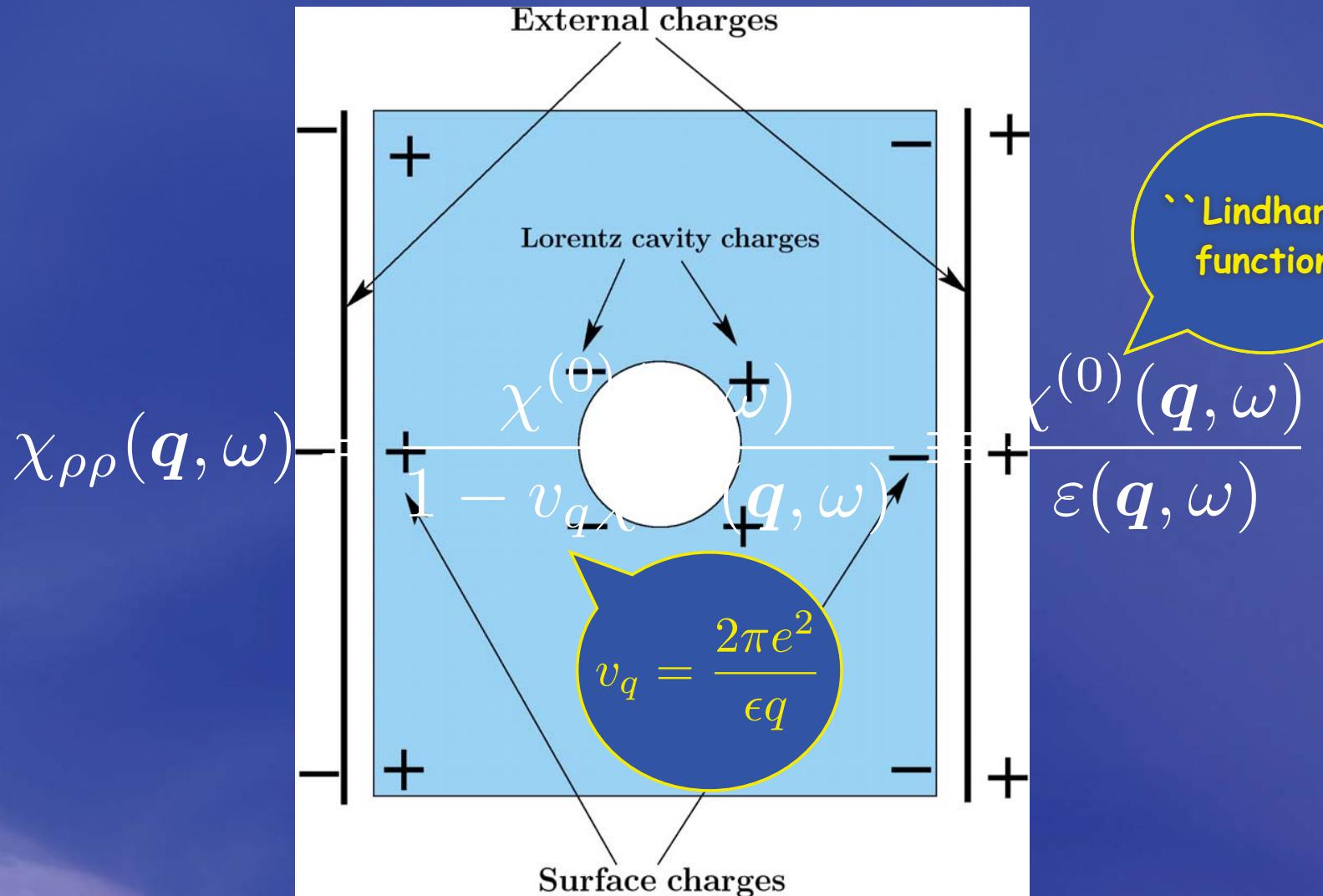
$$\xi_s(\mathbf{k}) = svk - \varepsilon_F$$

Why RPA ?

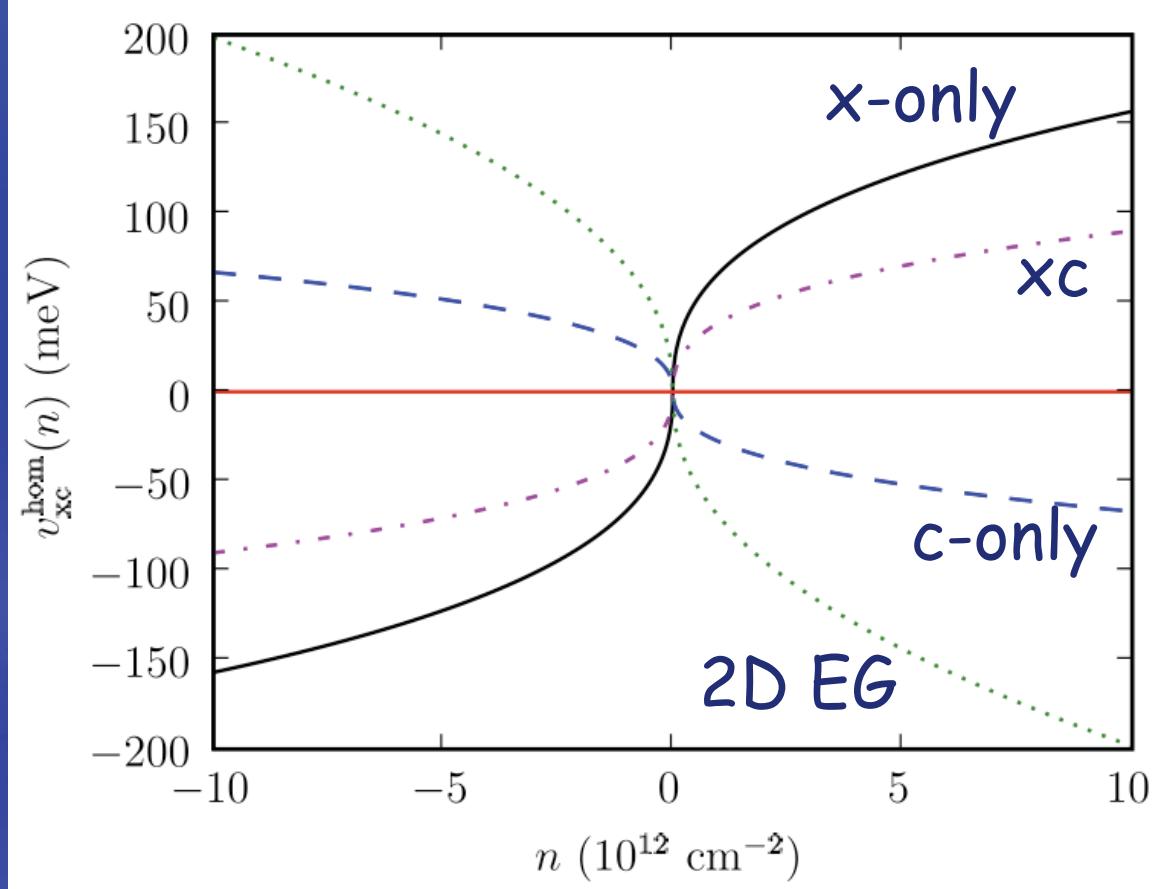
- i) It is easy
- ii) It captures dynamical screening, which is essential in doped systems
- iii) It is believed to be rigorously justified in the *doped* case in the weak coupling limit (see e.g. comments by Mishchenko and Das Sarma on this point)



Random Phase Approximation

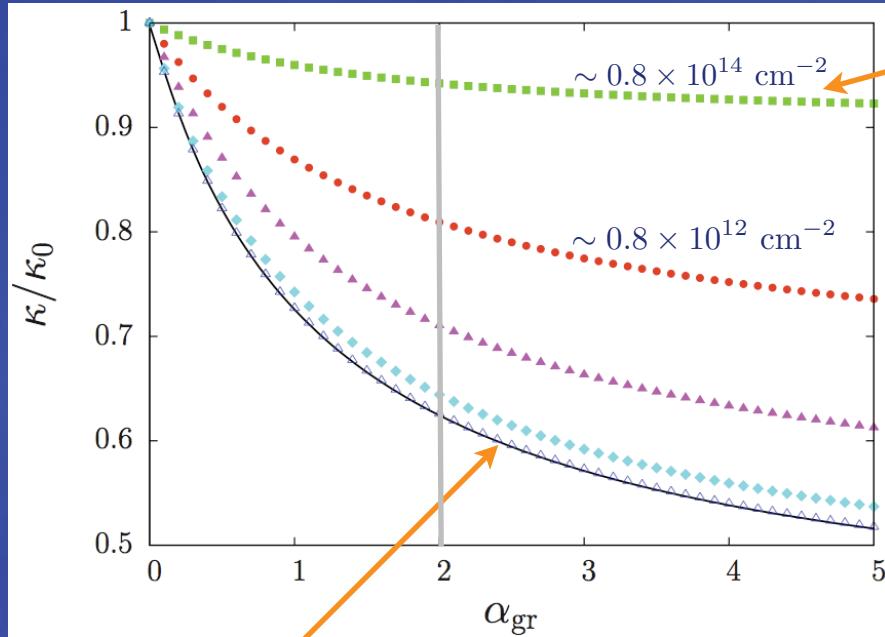


xc effects and non-linear screening in graphene



$$[v\boldsymbol{\sigma} \cdot \boldsymbol{p} + \mathbb{I}_\sigma V_{\text{KS}}(\boldsymbol{r})] \Phi_\lambda(\boldsymbol{r}) = \varepsilon_\lambda \Phi_\lambda(\boldsymbol{r})$$

Compressibility and spin susceptibility

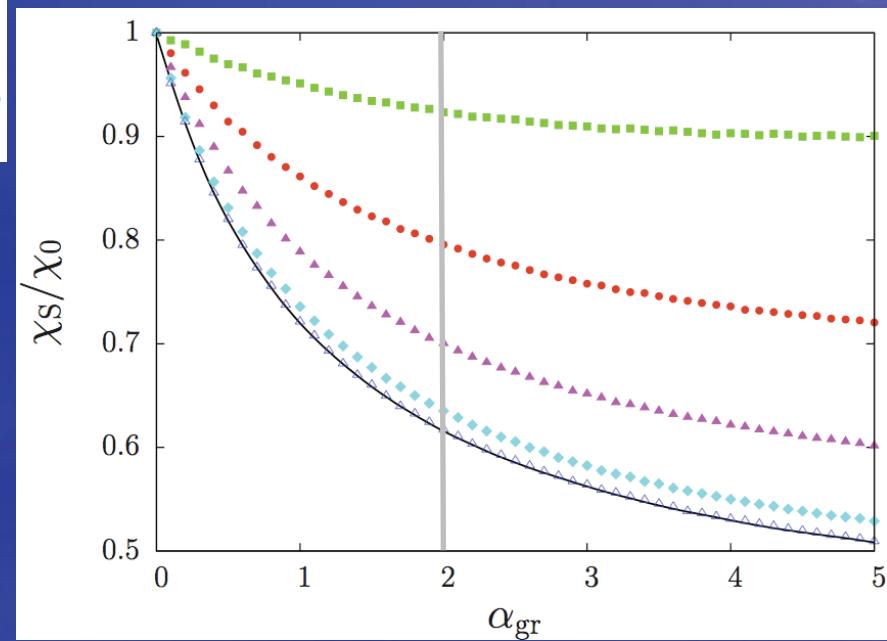


high density

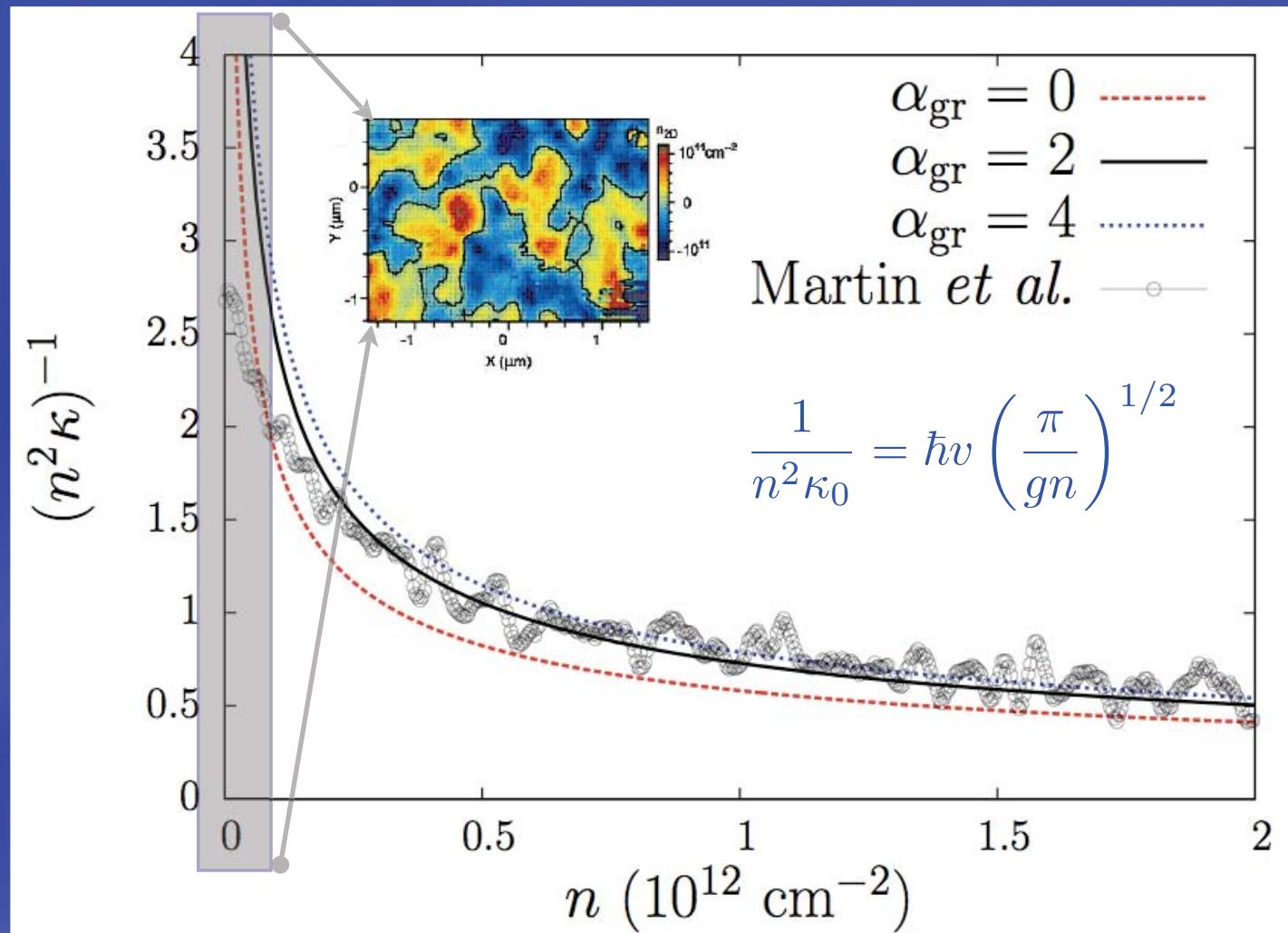
$$\frac{\kappa}{\kappa_0} < 1$$

low density

$$\frac{\chi_S}{\chi_0} < 1$$



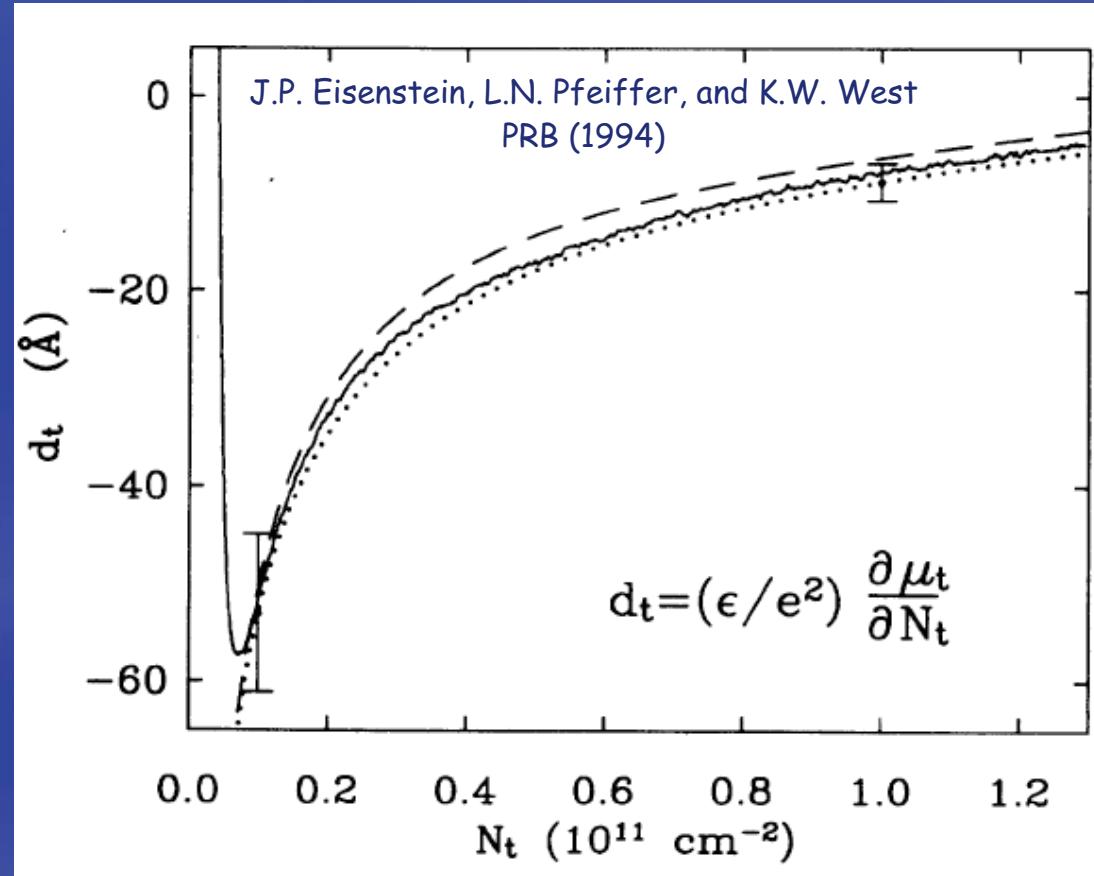
Compressibility: theory vs experiment



Theory: Y. Barlas, T. Pereg-Barnea, MP, R. Asgari, and A.H. MacDonald, Phys. Rev. Lett. **98**, 236601 (2007)

Experiment: J. Martin, N. Akerman, G. Ulbricht, T. Lohmann, J.H. Smet, K. von Klitzing, and A. Yacoby, Nature Phys. **4**, 144 (2008)

Compressibility of parabolic-band electron liquids



Dotted curve: 2D exchange + finite thickness

Main message: exchange enhances κ correlation enhances κ

Self-energy and Fermi liquid parameters

Quasiparticle renormalization factor

$$Z = \frac{1}{1 - \partial_\omega \Re e \Sigma_+^{\text{ret}}(\mathbf{k}, \omega) \Big|_{k=k_F, \omega=0}}$$

Renormalized velocity

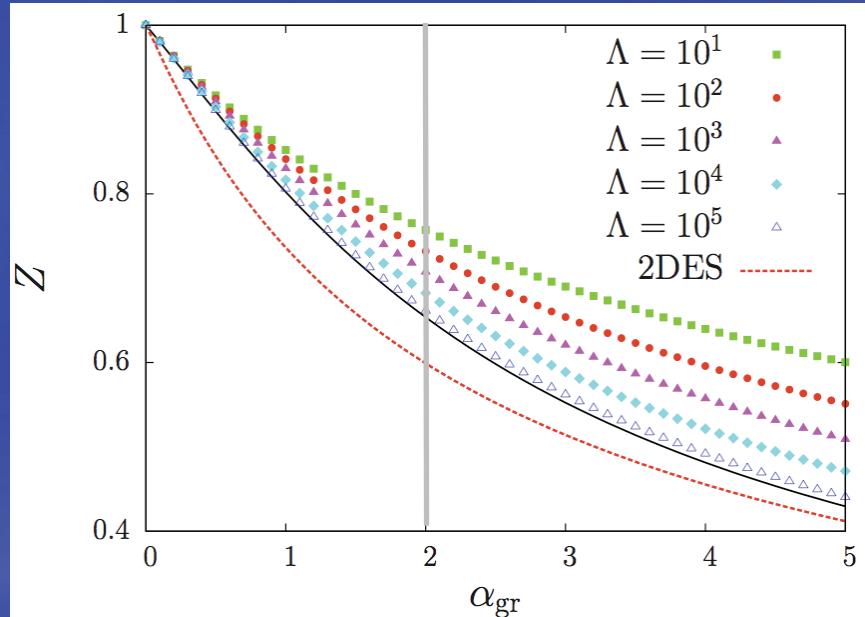
$$\frac{v^*}{v} = \frac{1 + (v)^{-1} \partial_k \Re e \Sigma_+^{\text{ret}}(\mathbf{k}, \omega) \Big|_{k=k_F, \omega=0}}{1 - \partial_\omega \Re e \Sigma_+^{\text{ret}}(\mathbf{k}, \omega) \Big|_{k=k_F, \omega=0}}$$

Compressibility and spin susceptibility

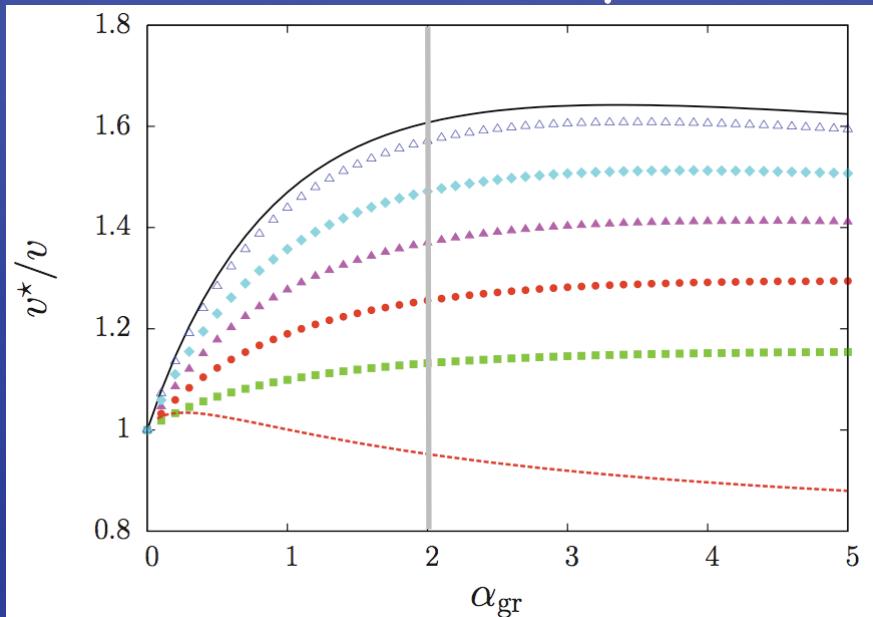
$$\frac{\kappa}{\kappa_0} = \frac{v/v^*}{1 + F_0^s} \quad \frac{\chi_S}{\chi_0} = \frac{v/v^*}{1 + F_0^a}$$

Renormalization factor and velocity enhancement

QP Z factor



QP velocity



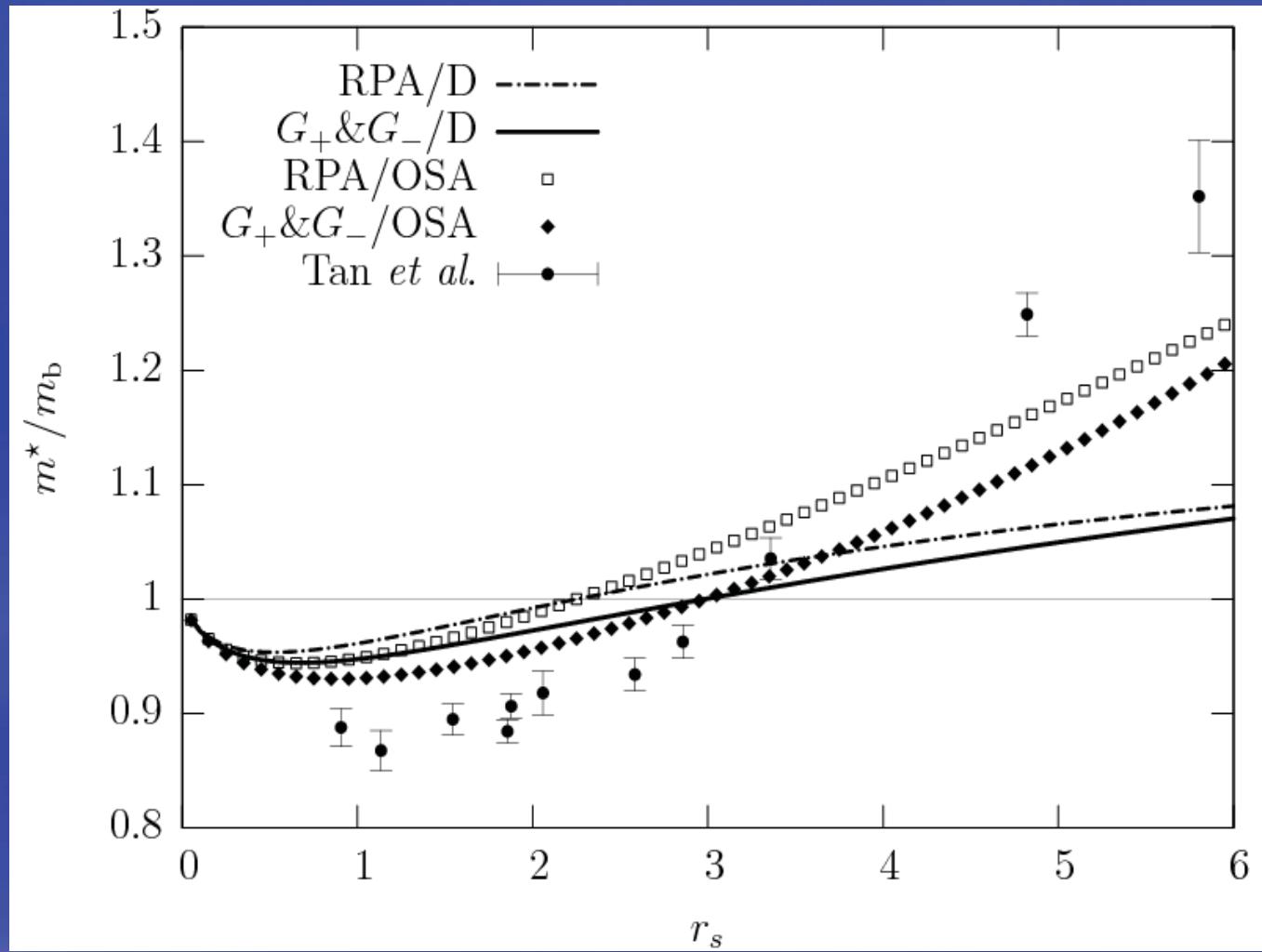
$$Z^{-1} = 1 + \frac{\alpha_{\text{gr}} \lambda(\alpha_{\text{gr}})}{6g} \ln(\Lambda) + \text{regular terms}$$

$$\lambda(\alpha_{\text{gr}}) = \frac{1}{4}\alpha_{\text{gr}} - \frac{3\pi^2}{256}\alpha_{\text{gr}}^2 + \dots$$

$$\frac{v^*}{v} = 1 + \frac{\alpha_{\text{gr}}[1 - \alpha_{\text{gr}}\xi(\alpha_{\text{gr}})]}{4g} \ln(\Lambda) + \text{regular terms}$$

$$\xi(\alpha_{\text{gr}}) = \frac{1}{3} - \frac{3\pi^2}{256}\alpha_{\text{gr}} + \dots$$

Quality of GW for semiconductors



Theory: R. Asgari, B. Davoudi, MP, G.F. Giuliani, M.P. Tosi, and G. Vignale, PRB (2005)

Experimental Results: Y.-W. Tan, J. Zhu, H.L. Stormer, L.N. Pfeiffer, K.W. Baldwin, and K.W. West, PRL (2005)

Exchange and quantum fluctuations (Hedin 1965)

$$\Sigma_s^{\text{SX}}(\mathbf{k}, \omega) = - \sum_{s'} \int \frac{d^2\mathbf{q}}{(2\pi)^2} \frac{v_q}{\varepsilon(\mathbf{q}, \omega - \xi_{s'}(\mathbf{k} + \mathbf{q}))} \frac{1 + ss' \cos(\theta_{\mathbf{k}, \mathbf{k} + \mathbf{q}})}{2} \Theta(-\xi_{s'}(\mathbf{k} + \mathbf{q}))$$

exchange interaction with
occupied states
in the static Fermi sea

$$\Sigma_s^{\text{CH}}(\mathbf{k}, \omega) = - \sum_{s'} \int \frac{d^2\mathbf{q}}{(2\pi)^2} v_q^2 \frac{1 + ss' \cos(\theta_{\mathbf{k}, \mathbf{k} + \mathbf{q}})}{2} \int_0^{+\infty} \frac{d\omega'}{\pi} \frac{\Im m \chi_{\rho\rho}(\mathbf{q}, \omega')}{\omega - \omega' - \xi_{s'}(\mathbf{k} + \mathbf{q}) + i\epsilon}$$

correlation contribution due
to quantum fluctuations of
the Fermi sea

Line and residue (Quinn-Ferrell 1958)

$$\Sigma_s^{\text{line}}(\mathbf{k}, \omega) = - \sum_{s'} \int \frac{d^2\mathbf{q}}{(2\pi)^2} v_q \frac{1 + ss' \cos(\theta_{\mathbf{k}, \mathbf{k}+\mathbf{q}})}{2} \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi} \frac{1}{\varepsilon(\mathbf{q}, i\Omega)} \frac{1}{\omega + i\Omega - \xi_{s'}(\mathbf{k} + \mathbf{q})}$$

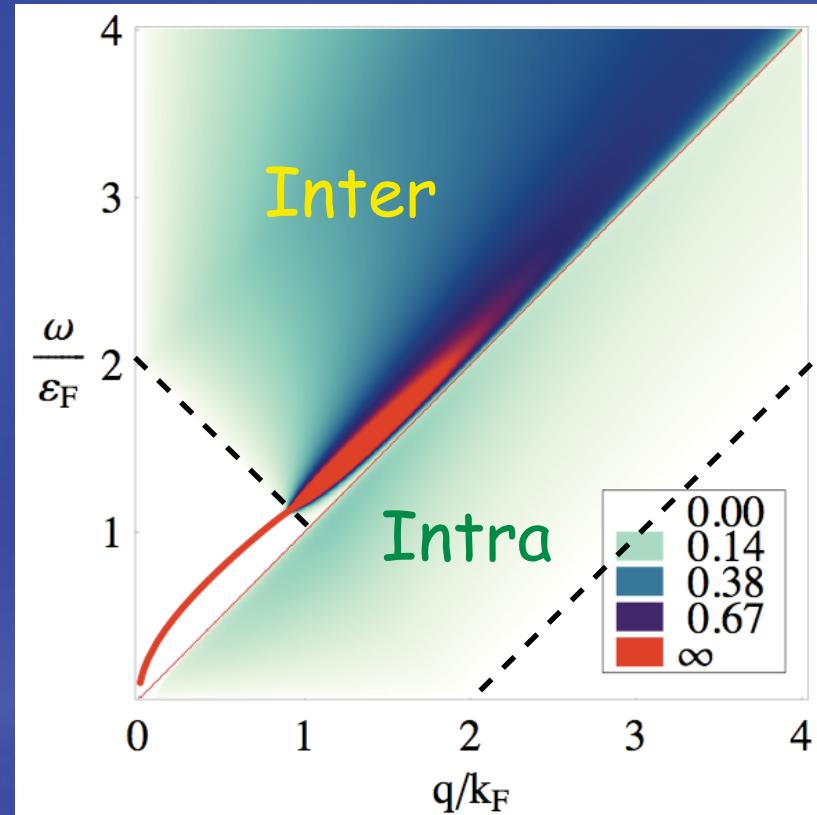
- i) requires ultraviolet cut-off
- ii) describes interaction of electrons at the Fermi energy with electrons far away in energy
- iii) velocity enhancement

$$\begin{aligned} \Sigma_s^{\text{res}}(\mathbf{k}, \omega) &= \sum_{s'} \int \frac{d^2\mathbf{q}}{(2\pi)^2} \frac{v_q}{\varepsilon(\mathbf{q}, \omega - \xi_{s'}(\mathbf{k} + \mathbf{q}))} \frac{1 + ss' \cos(\theta_{\mathbf{k}, \mathbf{k}+\mathbf{q}})}{2} \\ &\times [\Theta(\omega - \xi_{s'}(\mathbf{k} + \mathbf{q})) - \Theta(-\xi_{s'}(\mathbf{k} + \mathbf{q}))] \end{aligned}$$

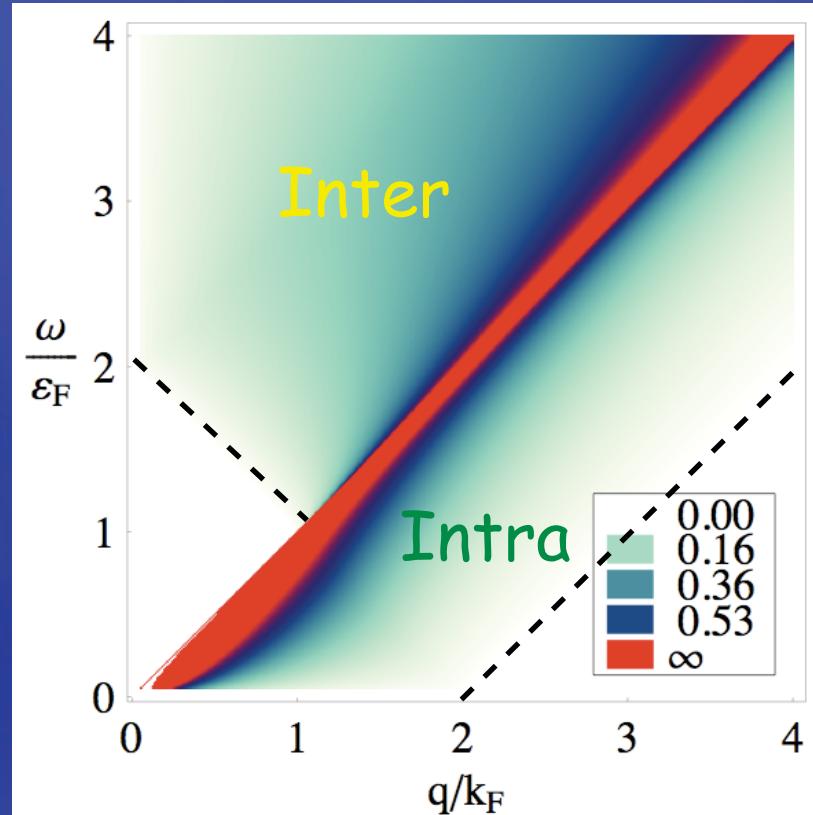
- i) no ultraviolet cut-off
- ii) describes quasiparticle decay
- iii) strong plasmon features below Fermi energy

Plasmons

$$-\Im m [1/\varepsilon(\mathbf{q}, \omega)]$$



$$-v_q \Im m [\chi^{(0)}(\mathbf{q}, \omega)]$$

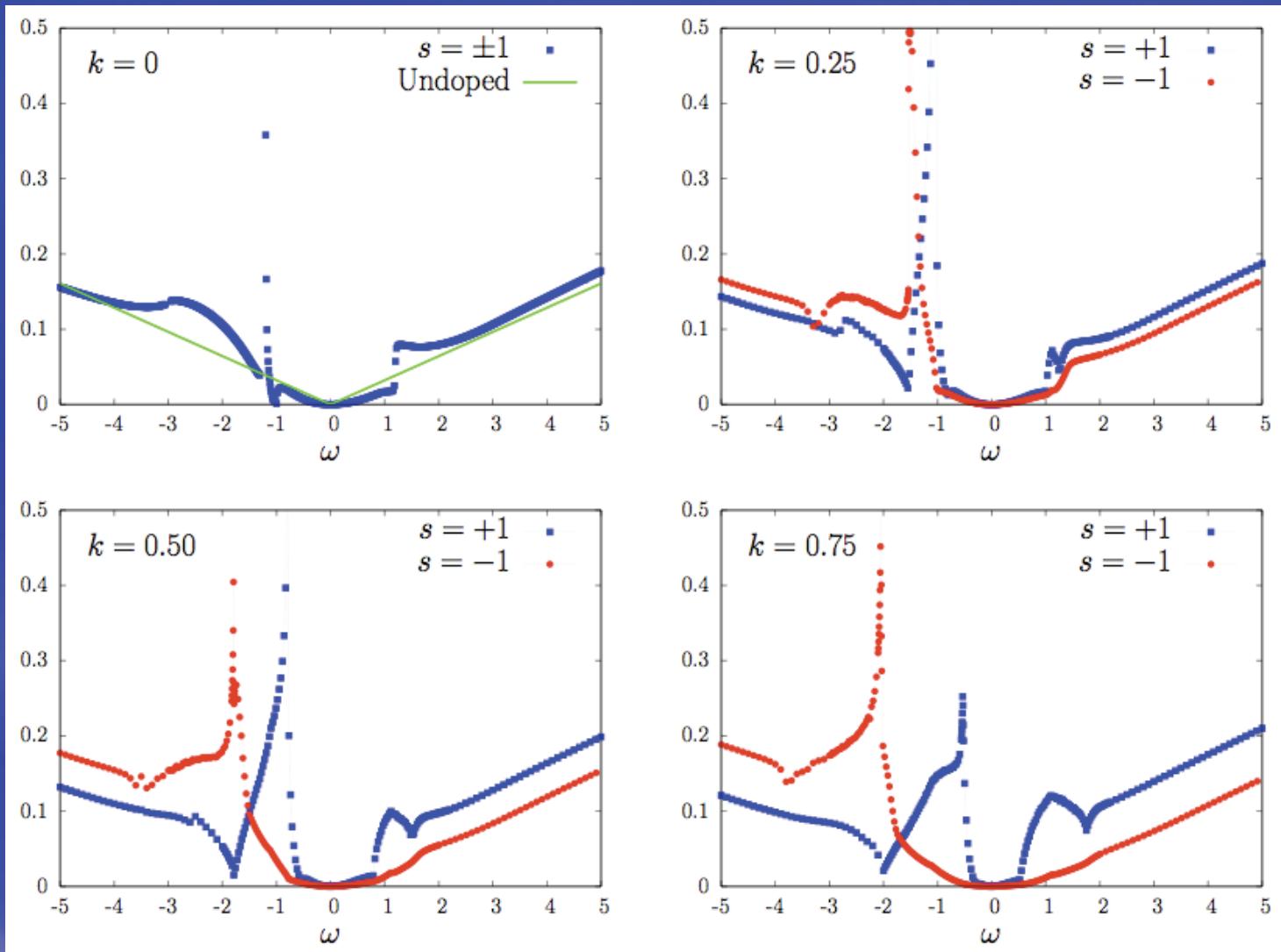


$$\omega_{\text{pl}}(q \rightarrow 0) = \varepsilon_F \sqrt{\frac{\alpha_{\text{gr}}}{2}} \sqrt{\frac{q}{k_F}}$$

$$\frac{1 \pm \cos(\theta_{\mathbf{k}, \mathbf{k}+q})}{2}$$

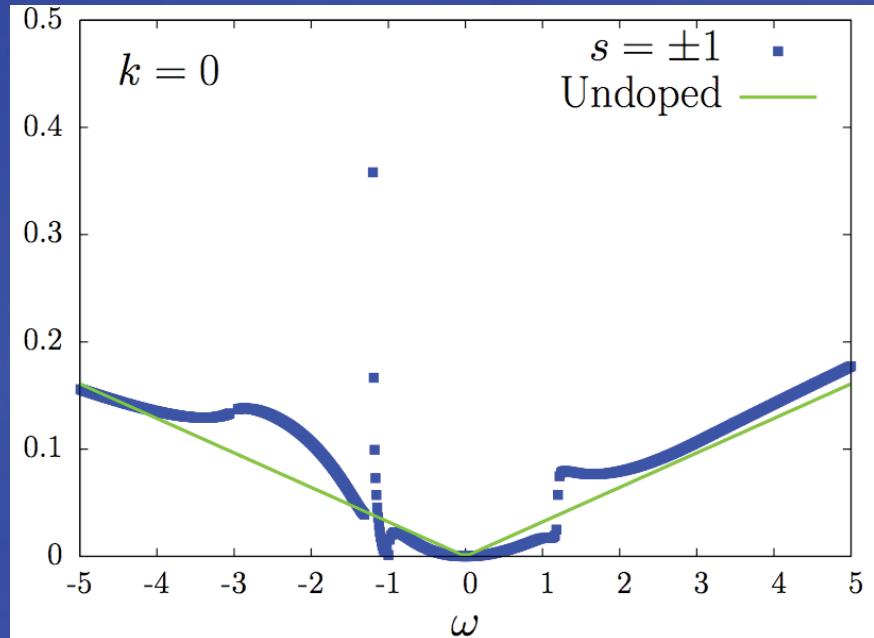
MP, R. Asgari, G. Borghi, Y. Barlas, T. Pereg-Barnea, and A.H. MacDonald, Phys. Rev. B **77**, 081411(R) (2008)

Quasiparticle decay



M.P., R. Asgari, G. Borghi, Y. Barlas, T. Pereg-Barnea, and A.H. MacDonald, Phys. Rev. B **77**, 081411(R) (2008)
see also E.W. Hwang and S. Das Sarma, PRB **77**, 0801412(R) (2008)

Main features: I



$$\omega > 0$$

$$\Im m \Sigma_s(\mathbf{k}, \omega)$$

represents electron scattering

$$\mathbf{k}, \omega \rightarrow \mathbf{k} + \mathbf{q}, \xi_{s'}(\mathbf{k} + \mathbf{q})$$

$$\omega < 0$$

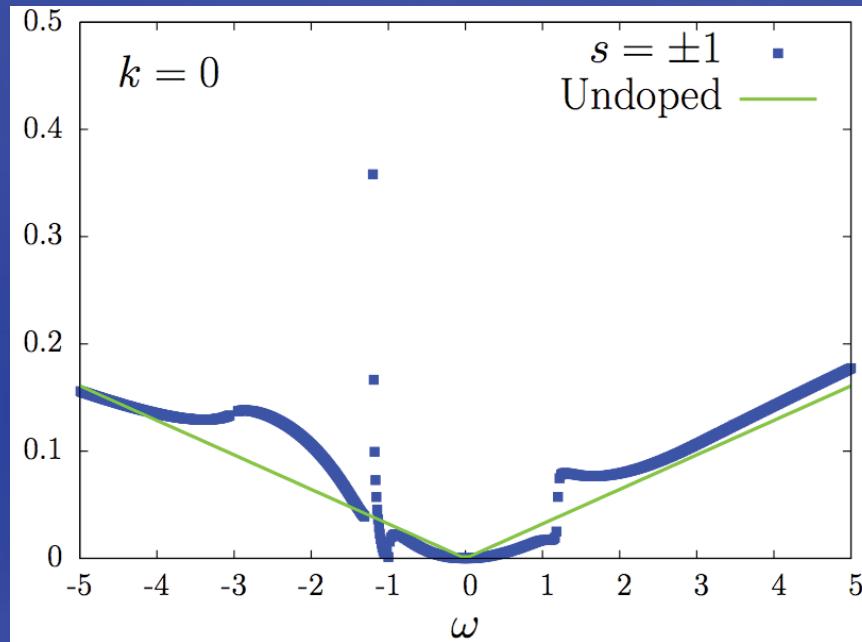
$$\Im m \Sigma_s(\mathbf{k}, \omega)$$

represents hole scattering

Only $\omega < 0$ relevant for ARPES in *n-doped* samples

$\Sigma_s(\mathbf{k}, \omega)$ in an n-doped system is identical to $\Sigma_{-s}(\mathbf{k}, -\omega)$
in a p-doped system

Main features: II



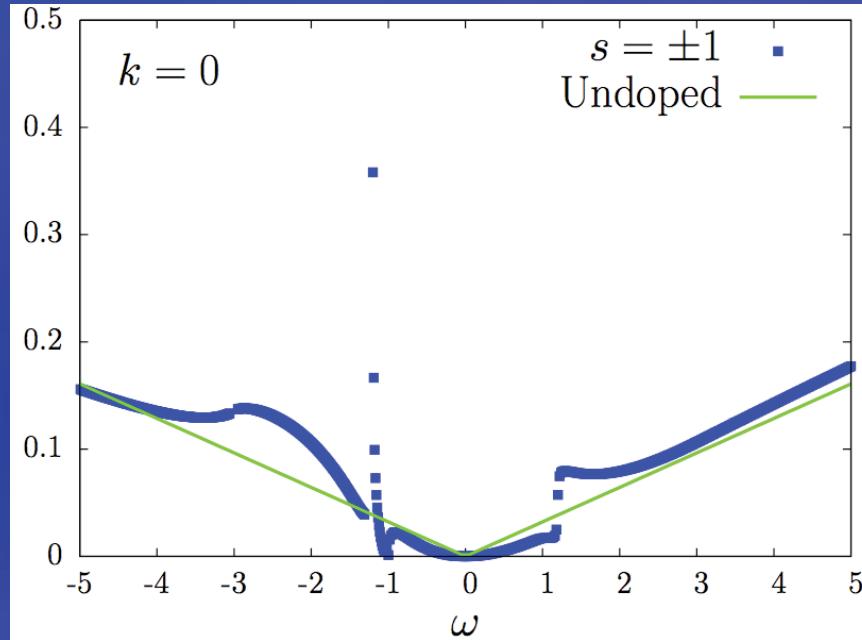
Undoped limit reached only very far away from the Fermi energy

$$\Im m[\Sigma_s(\mathbf{k}, \omega)] = \varepsilon_F F(\omega/\varepsilon_F, k/k_F)$$

$$F(x \rightarrow \infty, y = 0) \rightarrow -\pi \alpha_{\text{gr}}^2 \ell(\alpha_{\text{gr}}) |x| / (64g)$$

Standard Fermi liquid behavior $\Im m[\Sigma_s(\mathbf{k}, \omega \rightarrow 0)] \propto \omega^2$

Main features: III



Behavior below the Dirac point

final state in valence band

$$\frac{\Im m \Sigma_+(\mathbf{k} = 0, \omega)}{\varepsilon_F} = \frac{\alpha_{\text{gr}}}{2g} \int_0^1 d\bar{q} \Im m \left[\frac{1}{\varepsilon(\bar{q}, |\bar{\omega}| - 1 + \bar{q})} \right] + \frac{\alpha_{\text{gr}}}{2g} \int_0^{-(\bar{\omega}+1)} d\bar{q} \Im m \left[\frac{1}{\varepsilon(\bar{q}, |\bar{\omega}| - 1 - \bar{q})} \right]$$

final state in conduction band

$$\Omega(q) = |\omega| - 1 + s'q \quad \text{excitation energy}$$

Plasmon emission occurs when $\Omega(q) = \omega_{\text{pl}}(q)$

Plasmarons in graphene

Density-of-states
factor

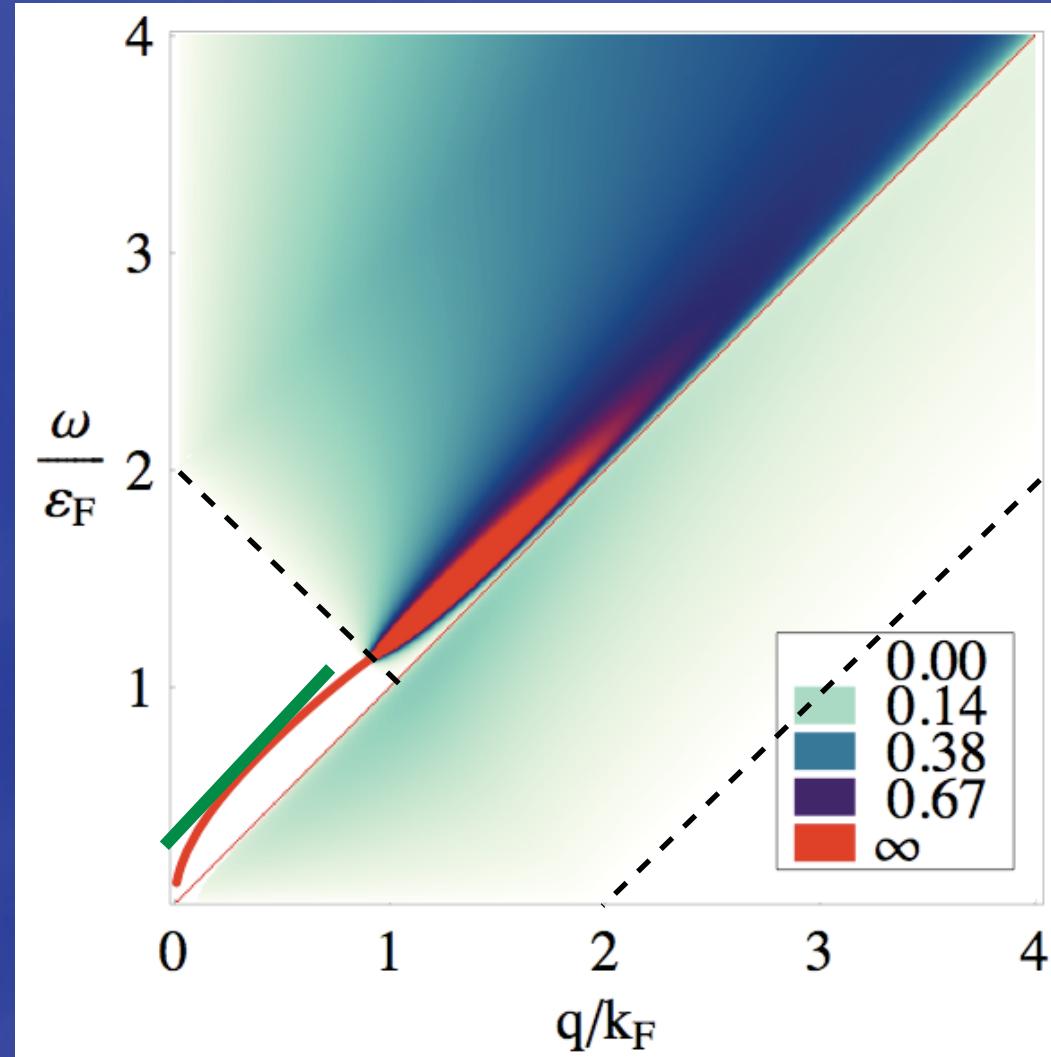
$$|s' - d\omega_{\text{pl}}/dq|^{-1}$$

$$s' = +1$$

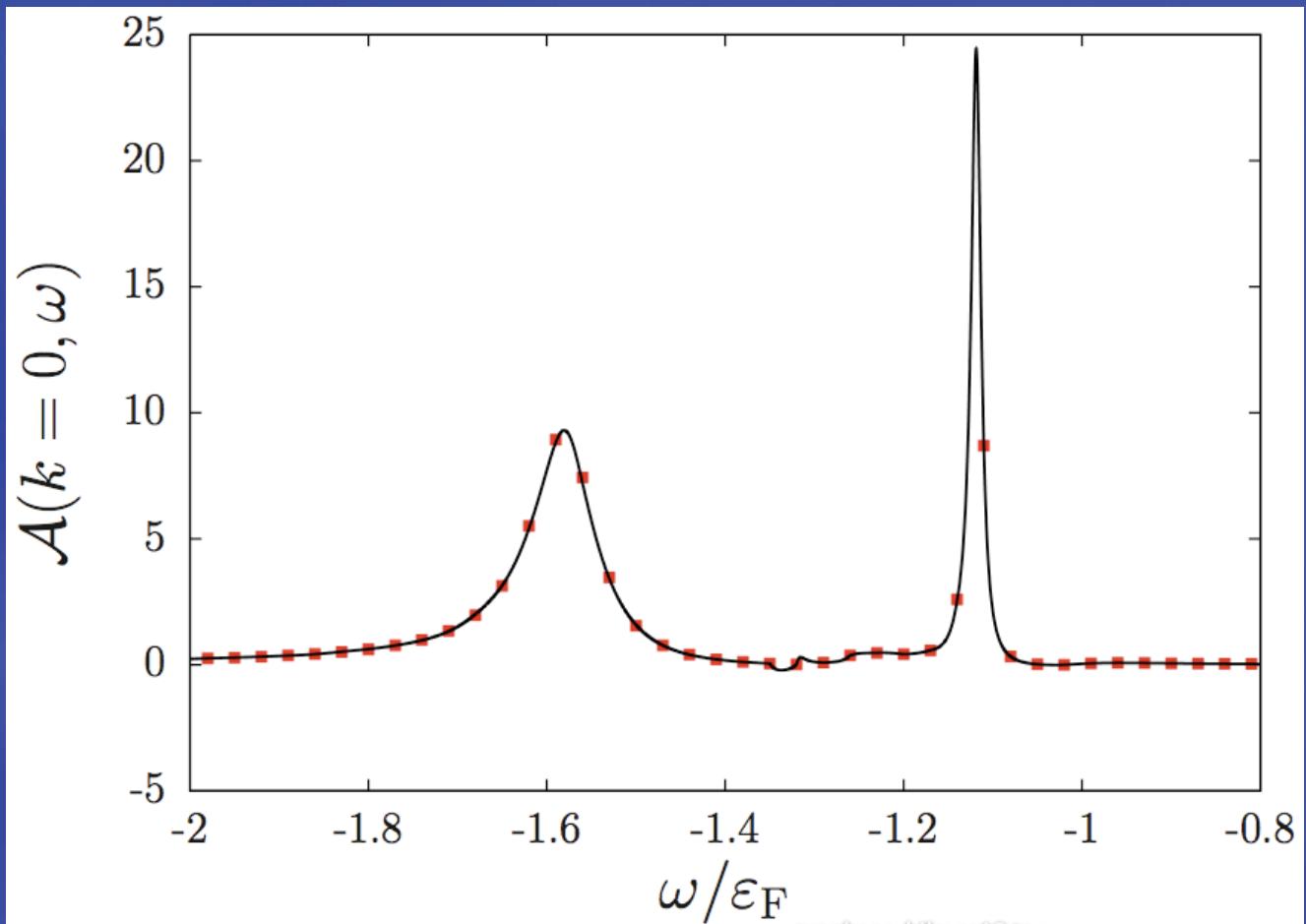
diverges

$$s' = -1$$

cannot diverge

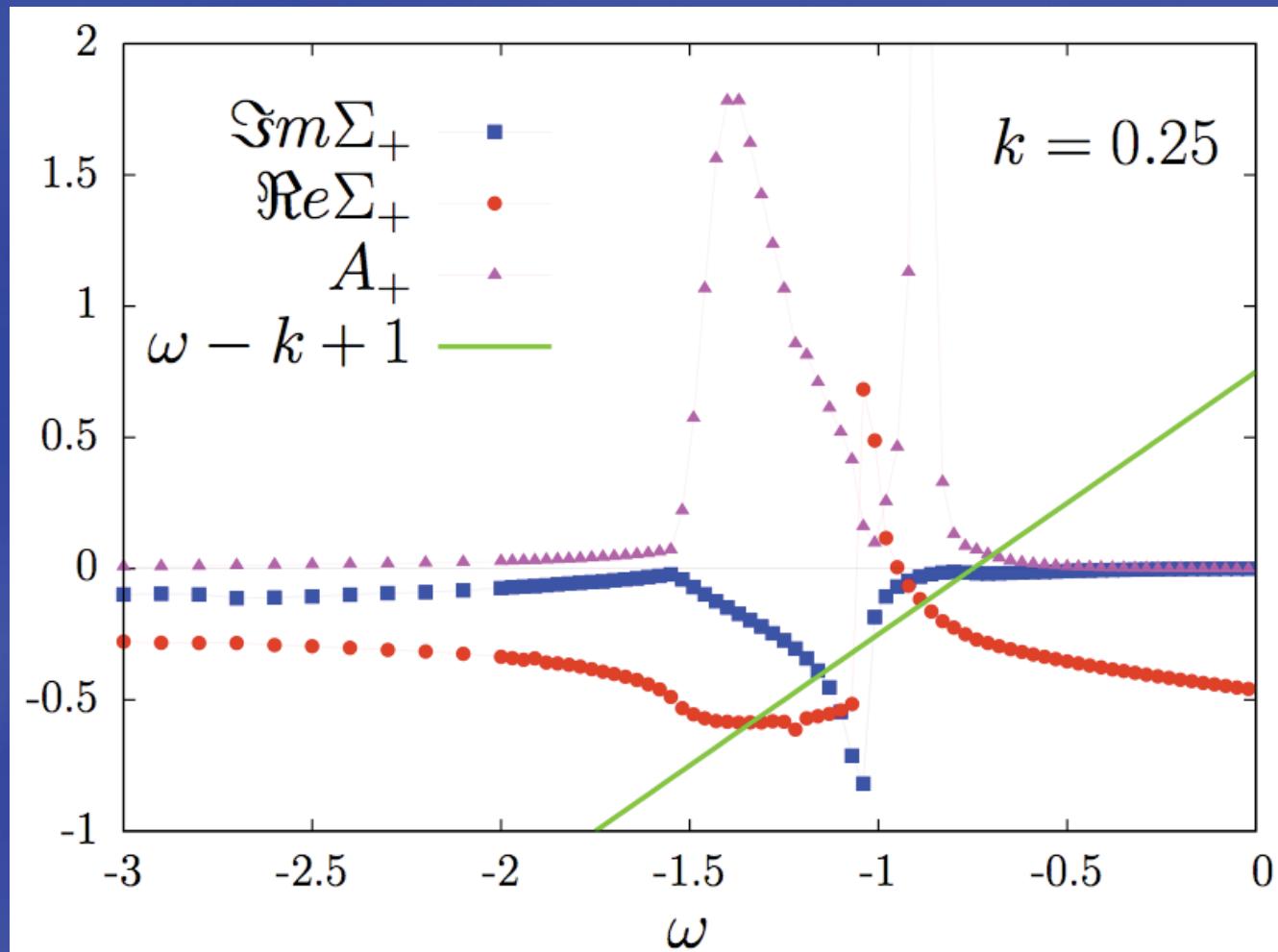


The spectral function at $\mathbf{k}=0$



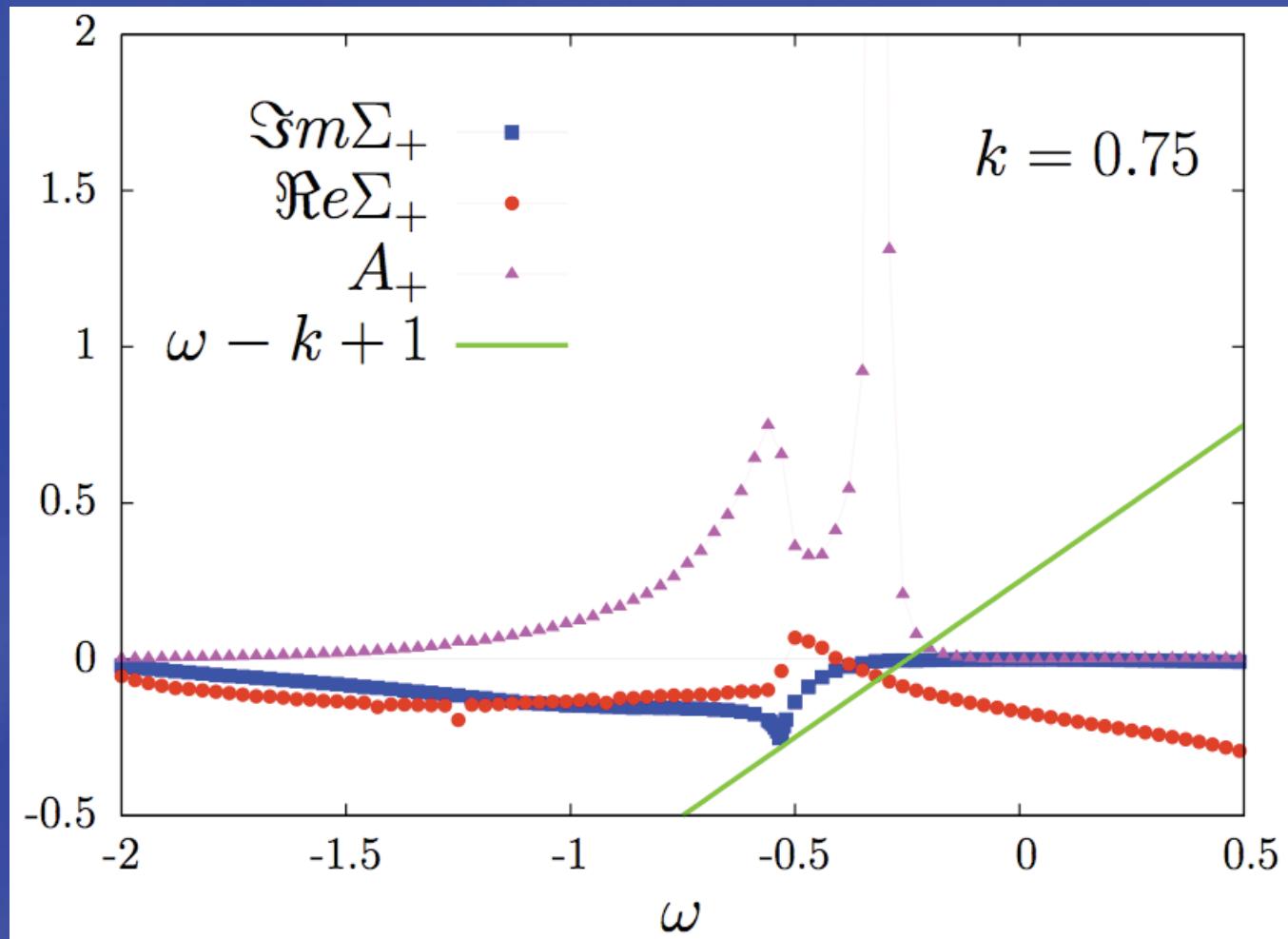
$$\mathcal{A}_s(\mathbf{k}, \omega) = \frac{1}{\pi} \frac{|\Im m \Sigma_s(\mathbf{k}, \omega)|}{[\omega - \xi_s(\mathbf{k}) - \Re e \Sigma_s(\mathbf{k}, \omega)]^2 + [\Im m \Sigma_s(\mathbf{k}, \omega)]^2}$$

Spectral function: small k



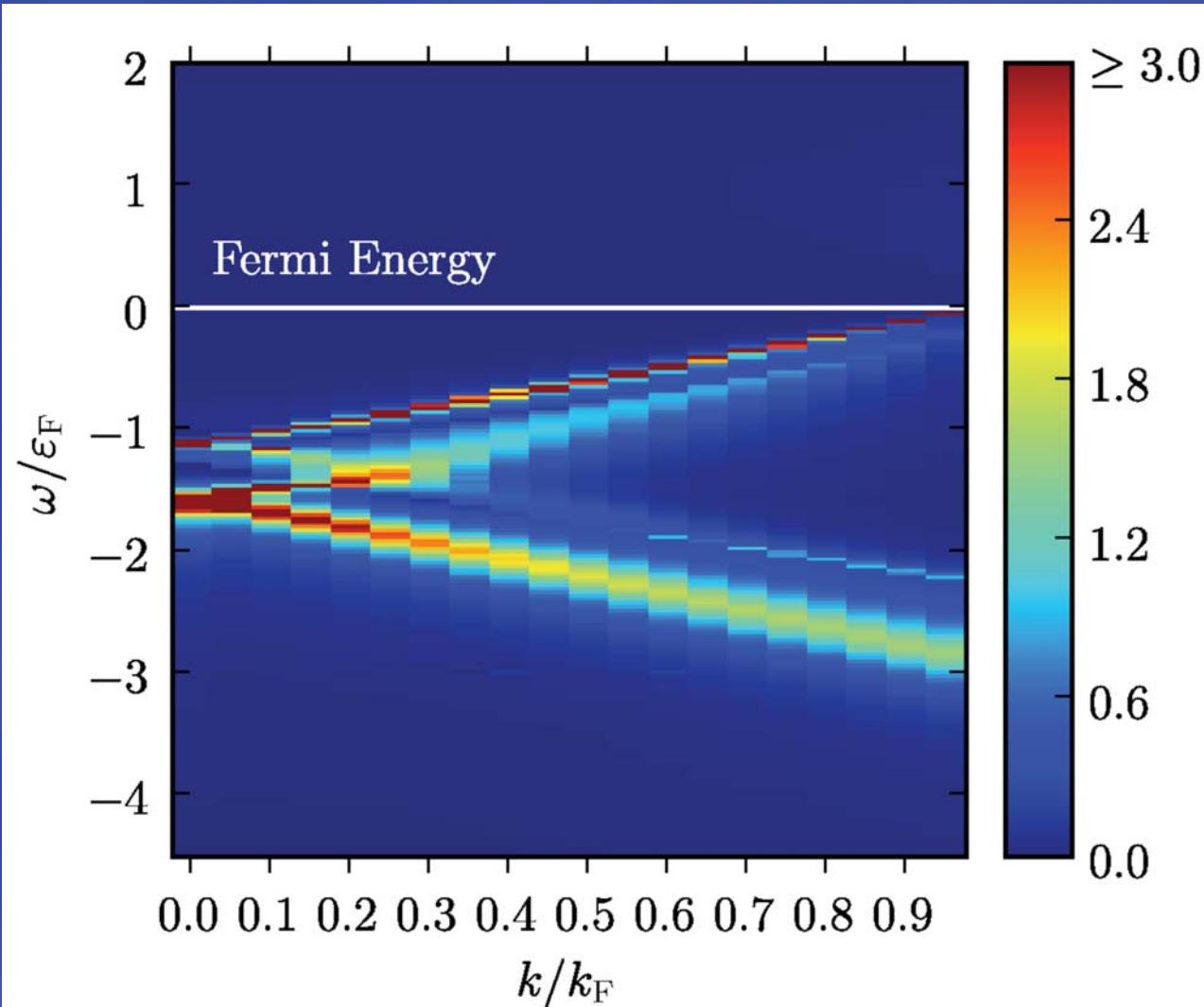
MP, R. Asgari, G. Borghi, Y. Barlas, T. Pereg-Barnea, and A.H. MacDonald, Phys. Rev. B 77, 081411(R) (2008)

Spectral function: large k



MP, R. Asgari, G. Borghi, Y. Barlas, T. Pereg-Barnea, and A.H. MacDonald, Phys. Rev. B 77, 081411(R) (2008)

Spectral function



MP, R. Asgari, G. Borghi, Y. Barlas, T. Pereg-Barnea, and A.H. MacDonald, Phys. Rev. B 77, 081411(R) (2008)

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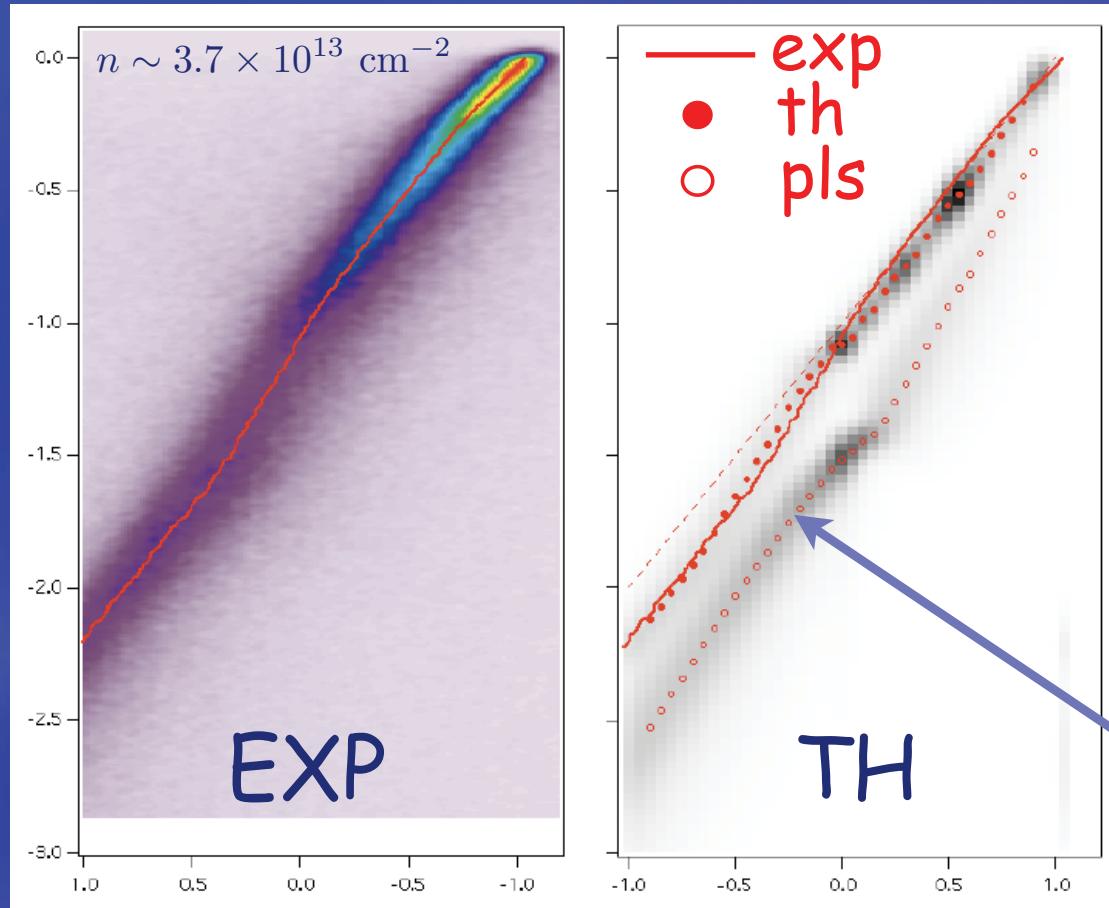
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Theory vs experiment: E(k)

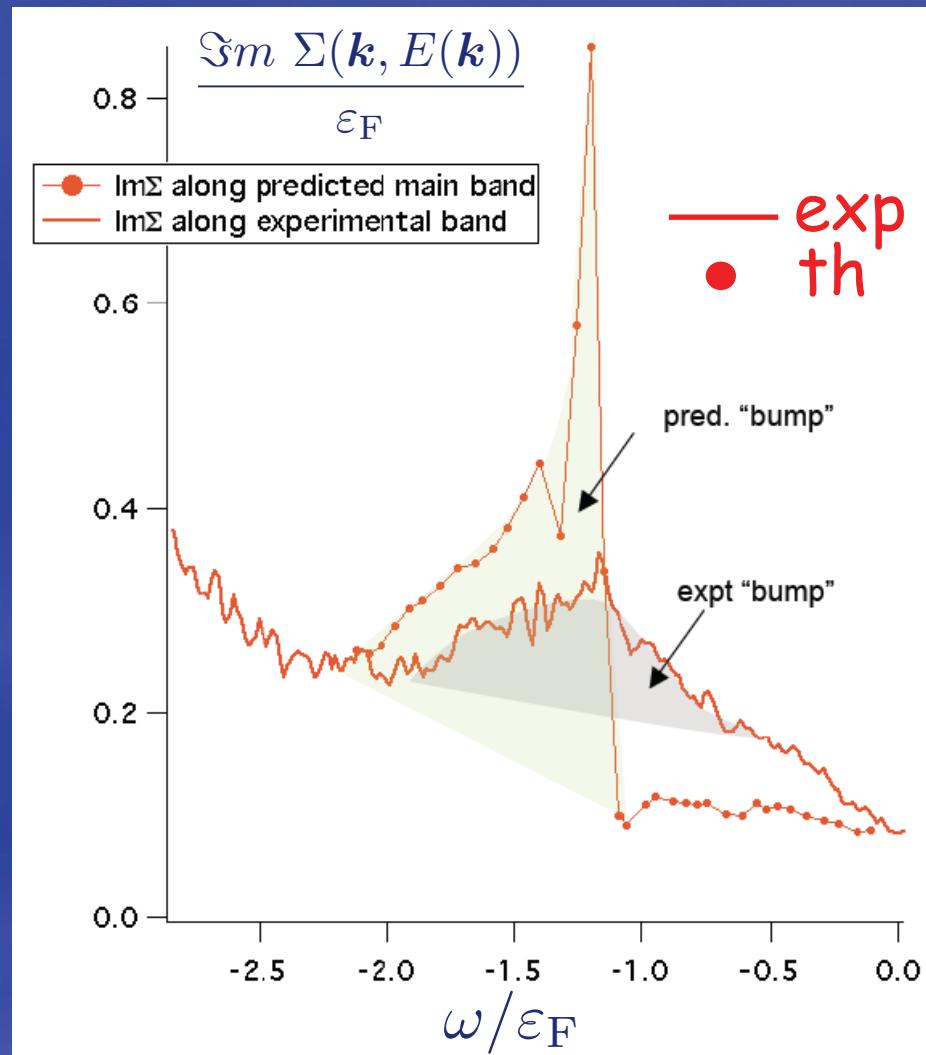
ω/ε_F



k/k_F

from Eli Rotenberg

Theory vs experiment: QP decay



from Eli Rotenberg

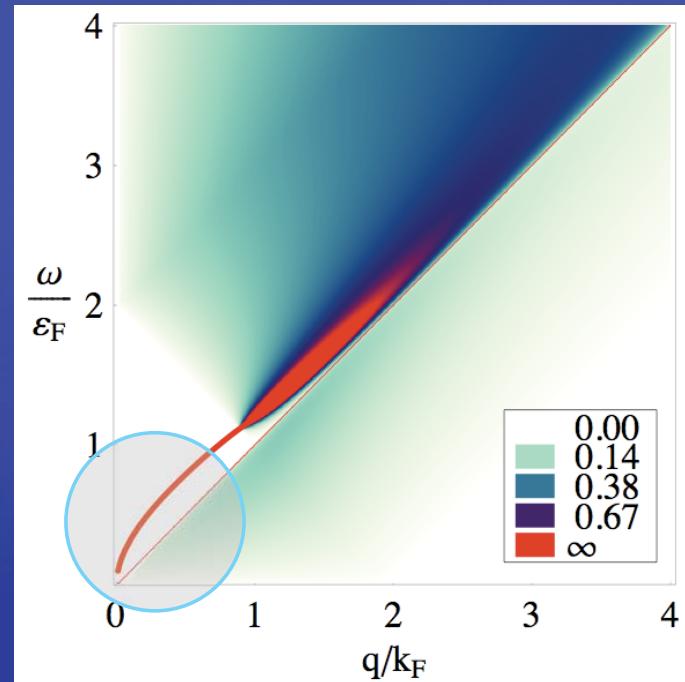
Satellite band not seen in experiments: why?

Maybe many-body effects beyond RPA ?

Plasmon damping

$$\chi_{\rho\rho}(q, \omega) = \frac{1}{S} \langle \langle \hat{\rho}_{\mathbf{q}}; \hat{\rho}_{-\mathbf{q}} \rangle \rangle_{\omega}$$

$$\langle \langle \hat{A}; \hat{B} \rangle \rangle_{\omega} = -i \lim_{\epsilon \rightarrow 0^+} \int_0^{+\infty} dt e^{i\omega t} e^{-\epsilon t} \langle \Psi_{\text{GS}} | [\hat{A}(t), \hat{B}(0)] | \Psi_{\text{GS}} \rangle$$



$$\langle \langle \hat{A}; \hat{B} \rangle \rangle_{\omega} = \frac{1}{\omega} \langle [\hat{A}, \hat{B}] \rangle + \frac{i}{\omega} \langle \langle \partial_t \hat{A}; \hat{B} \rangle \rangle_{\omega}$$

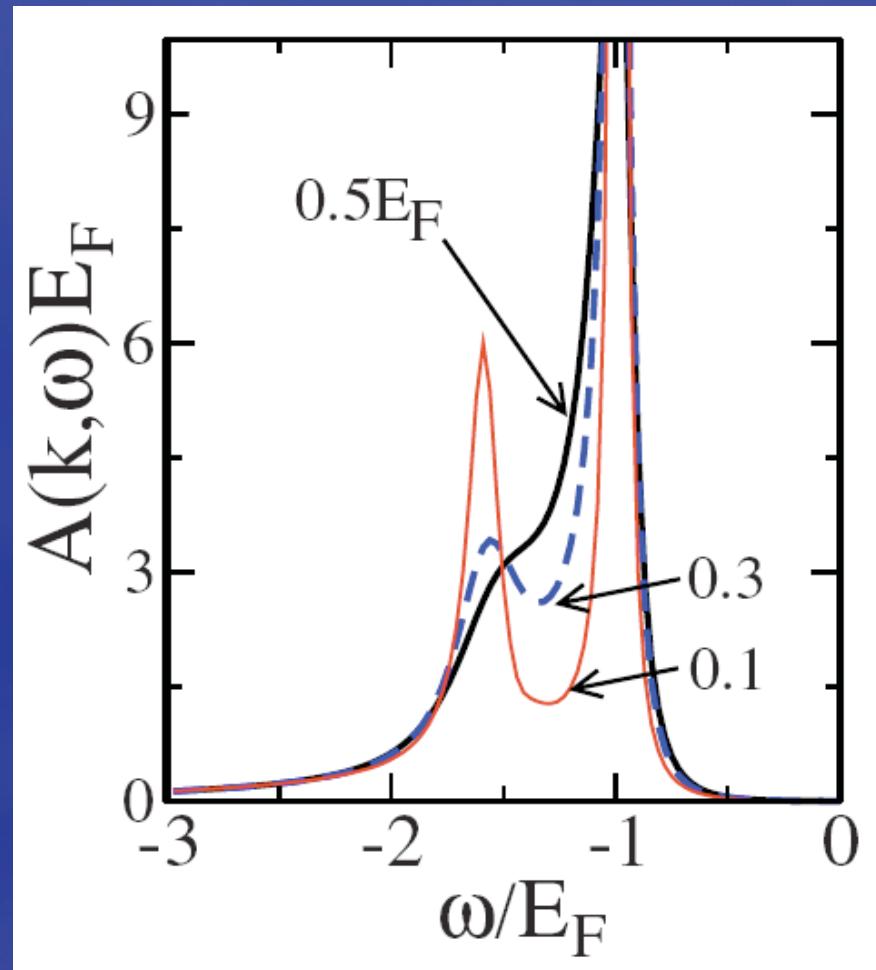
R. Nifosi, S. Conti, and M.P. Tosi, PRB **58**, 12758 (1998)

S.H. Abedinpour, MP, A.H. MacDonald, B. Tanatar, M.P. Tosi, and G. Vignale, Phys. Rev. Lett. **99**, 206802 (2007)

Satellite band not seen in experiments: why?

Maybe disorder ?
(on which it has been
commented at great length
yesterday by Rotenberg)

Maybe interactions
with the buffer layer ?



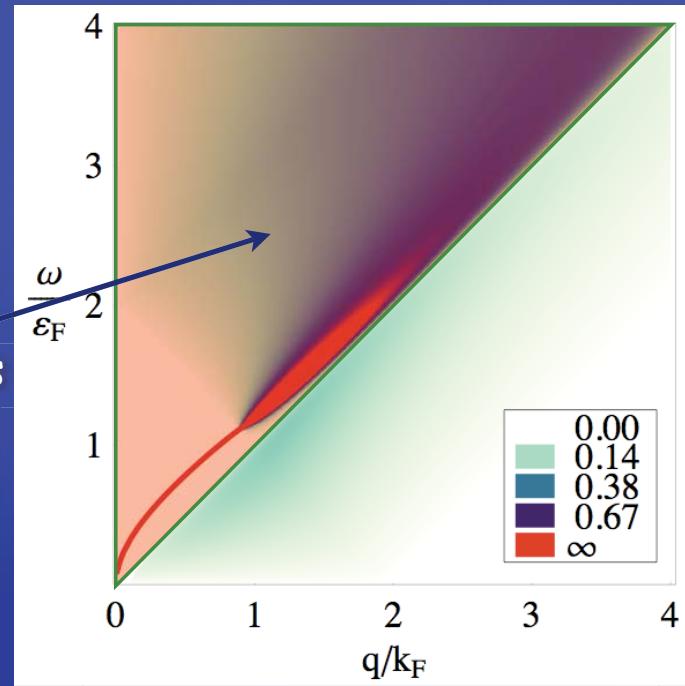
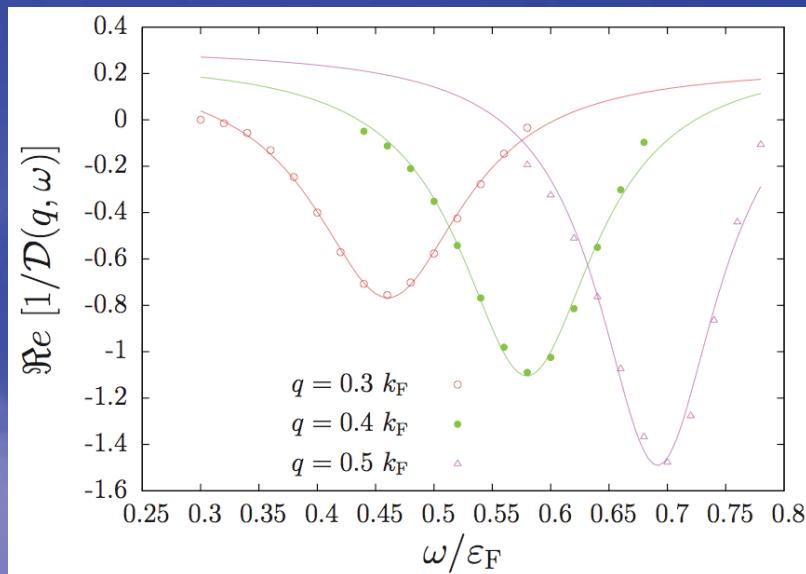
Plasmon damping in the presence of nearby layers

Coulomb coupled nearby layers ?

— doped

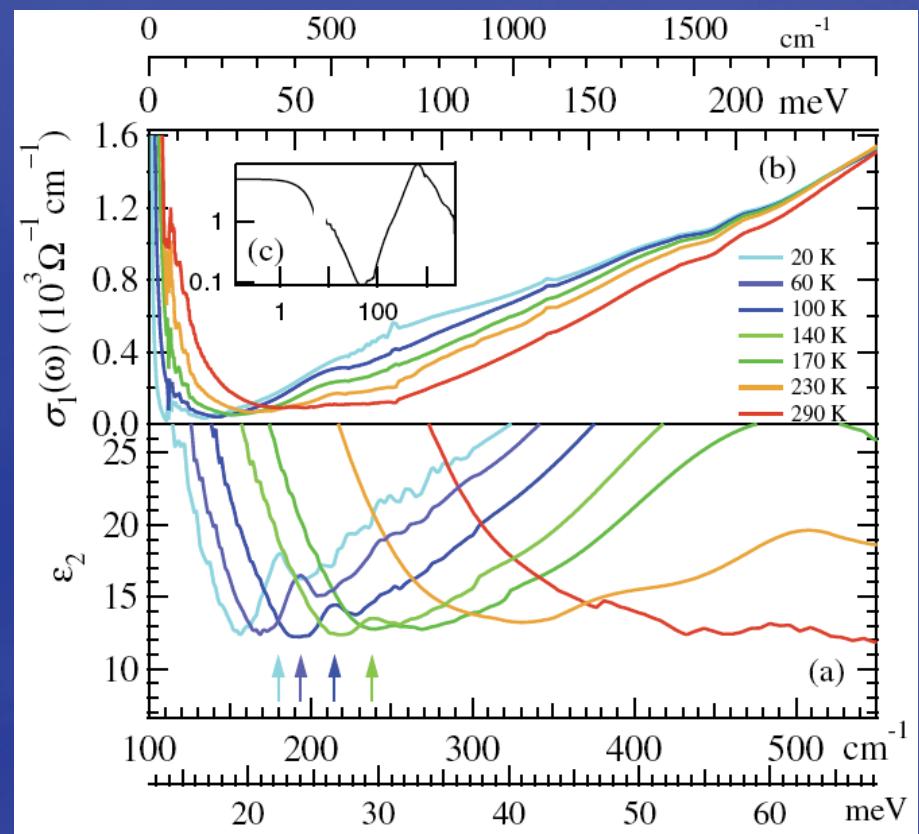
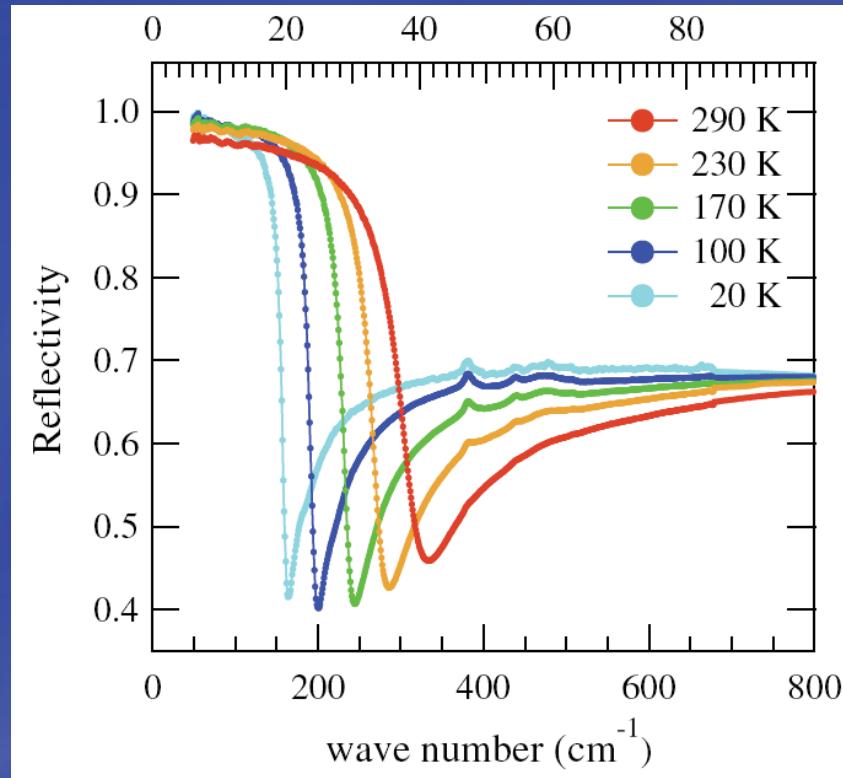
— undoped

Inter-band
particle-hole excitations
of the undoped layer



Plasmon damping
 $\gamma(q)/\varepsilon_F \sim 10\% - 20\%$

Plasmarons in Bismuth (optics)



R. Tediosi, N.P. Armitage, E. Giannini, and D. van der Marel, Phys. Rev. Lett. **99**, 016406 (2007)

Conclusions

Doped graphene is a 2D chiral electron gas with interesting new features because of

- i) interband electron-hole excitations and interband exchange interactions
- ii) (sublattice pseudospin) chirality of eigenstates

Most important consequences:

- i) Quasiparticle velocity is enhanced rather than suppressed
- ii) Charge and spin susceptibilities are suppressed rather than enhanced
- iii) Stronger plasmon features that might emerge in ARPES spectra on better samples in the near future

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Financial support

CNR-INFM ``Seed'' Project
for young researchers

