Chirality & Correlations in Graphene

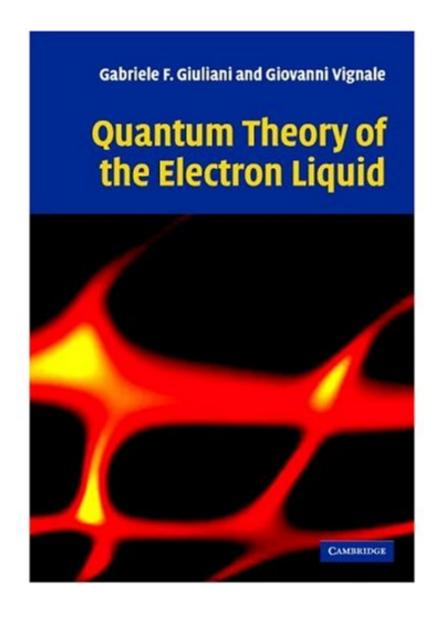
KITP Workshop - 01.07



University of Texas at Austin

Yafis Barlas Tami Pereg-Barnea Marco Polini Reza Asgari

Electron Gas Theory



The MDF model for Graphene

$$v = 2 \pi e^2/q$$

$$\hat{\mathcal{H}} = v \sum_{\mathbf{k}} \hat{\psi}_{\mathbf{k}}^{\dagger} \left(\sigma_1 k_1 + \sigma_2 k_2 \right) \hat{\psi}_{\mathbf{k}} + \frac{1}{2S} \sum_{\mathbf{q} \neq 0} v_{\mathbf{q}} (\hat{n}_{\mathbf{q}} \hat{n}_{-\mathbf{q}} - \hat{N})$$

Wikipedia on Helicity vs. Chirality

Helicity (particle physics)

From Wikipedia, the free encyclopedia

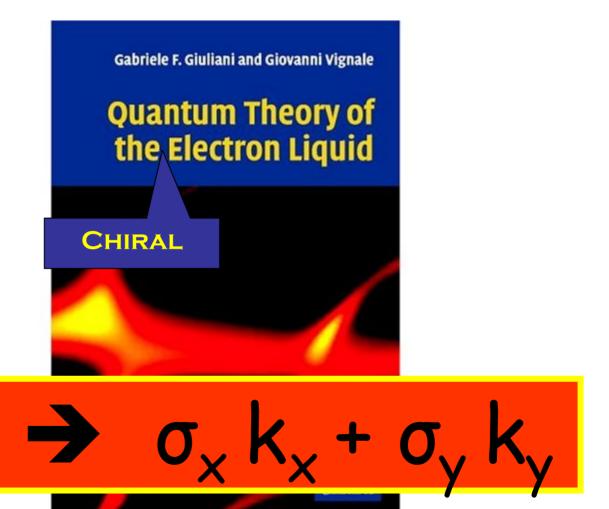
In <u>particle physics</u>, **helicity** is the projection of the <u>angular momentum</u> to the direction of motion:

Because the angular momentum with respect to an axis has discrete values, helicity is discrete, too. For spin-1/2 particles such as the <u>electron</u>, the helicity can either be positive - the particle is then "right-handed" - or negative - the particle is then "left-handed".

For massless (or extremely light) spin-1/2 particles, helicity is equivalent to the operator of chirality multiplied by h/2

.

Electron Gas Theory



The MDF model for Graphene

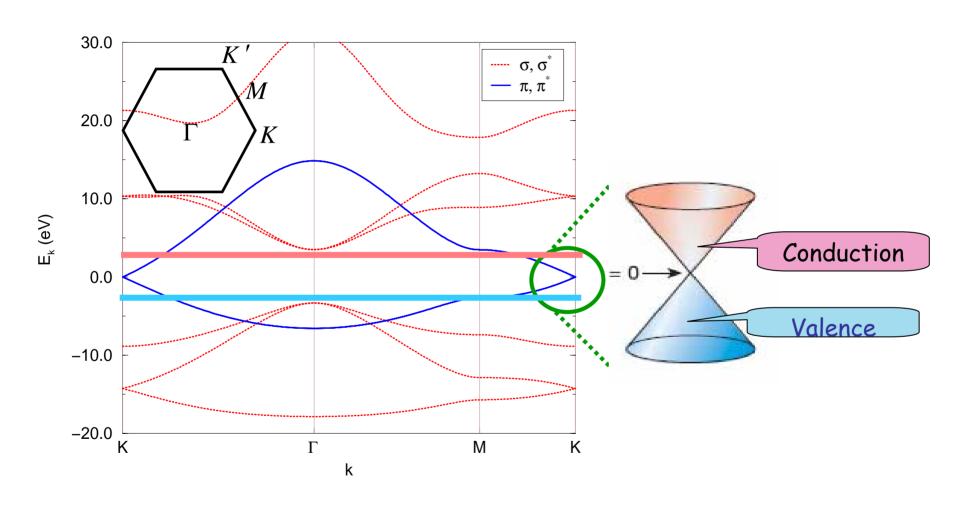
$$v = 2 \pi e^2/q$$

$$\hat{\mathcal{H}} = v \sum_{\mathbf{k}} \hat{\psi}_{\mathbf{k}}^{\dagger} \left(\sigma_1 k_1 + \sigma_2 k_2 \right) \hat{\psi}_{\mathbf{k}} + \frac{1}{2S} \sum_{\mathbf{q} \neq 0} v_{\mathbf{q}} (\hat{n}_{\mathbf{q}} \hat{n}_{-\mathbf{q}} - \hat{N})$$



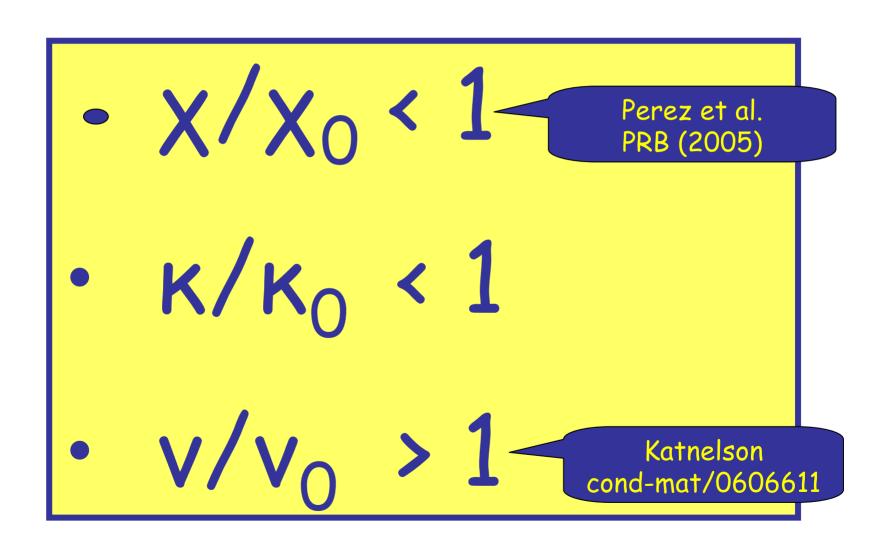
... plus uv cutoff

Graphene Bands



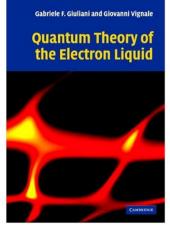
$$K_c \sim 0.5 (\Gamma - M) = \pi/3a \sim 1/a$$

Chiral Electron Gas Properties



Coupling Constant Integration

$$E_{\text{int}} = \frac{N}{2} \int_0^1 d\lambda \int \frac{d^2 \mathbf{q}}{(2\pi)^2} v_q \left[S^{(\lambda)}(q) - 1 \right]$$



Static Structure Factor

Fluctuation-Dissipation Theorem

$$S^{(\lambda)}(q) = -\frac{1}{\pi n} \int_{0}^{+\infty} d\Omega \ \chi_{\rho\rho}^{(\lambda)}(\mathbf{q}, i\Omega)$$

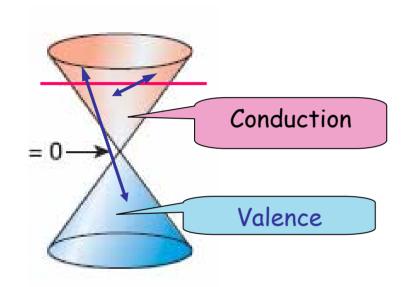
RPA Theory

$$\chi_{\rho\rho}^{(\lambda)}(\mathbf{q},i\Omega) = \frac{\chi^{(0)}(\mathbf{q},i\Omega)}{1 - \lambda v_q \chi^{(0)}(\mathbf{q},i\Omega)}$$



Why RPA?

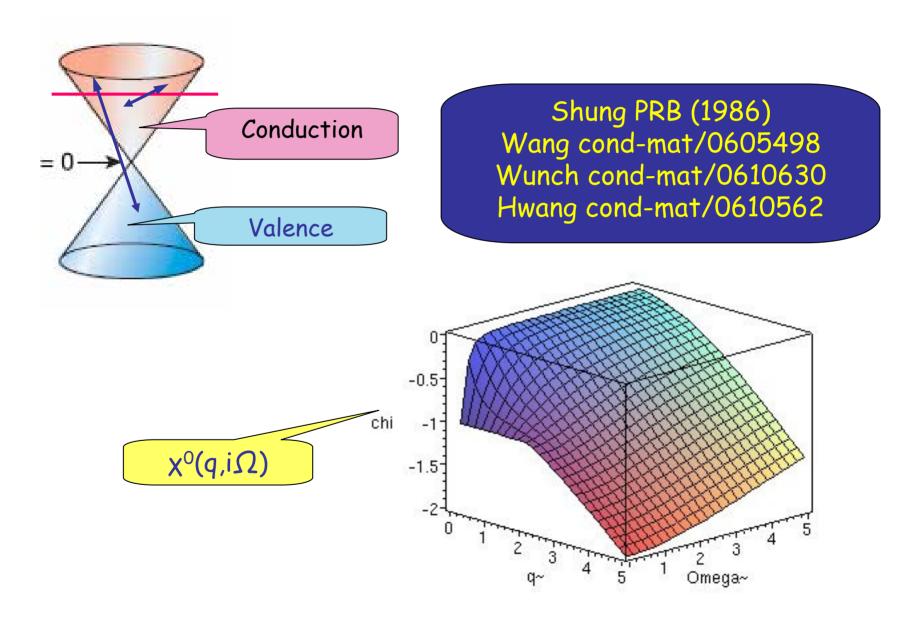
Chiral `Lindhard' Function



Shung PRB (1986)
Wang cond-mat/0605498
Wunch cond-mat/0610630
Hwang cond-mat/0610562

$$\chi^{MDF}(\mathbf{q}, i\Omega) = -\frac{q^2}{16\sqrt{\Omega^2 + v^2q^2}} - \frac{\varepsilon_{\mathrm{F}}}{2\pi v^2} + \frac{q^2}{8\pi\sqrt{\Omega^2 + v^2q^2}} \Re e \left[\sin^{-1}\left(\frac{2\varepsilon_{\mathrm{F}} + i\Omega}{vq}\right) + \left(\frac{2\varepsilon_{\mathrm{F}} + i\Omega}{vq}\right) \sqrt{1 - \left(\frac{2\varepsilon_{\mathrm{F}} + i\Omega}{vq}\right)^2} \right]$$

Chiral 'Lindhard' Function



Regularization

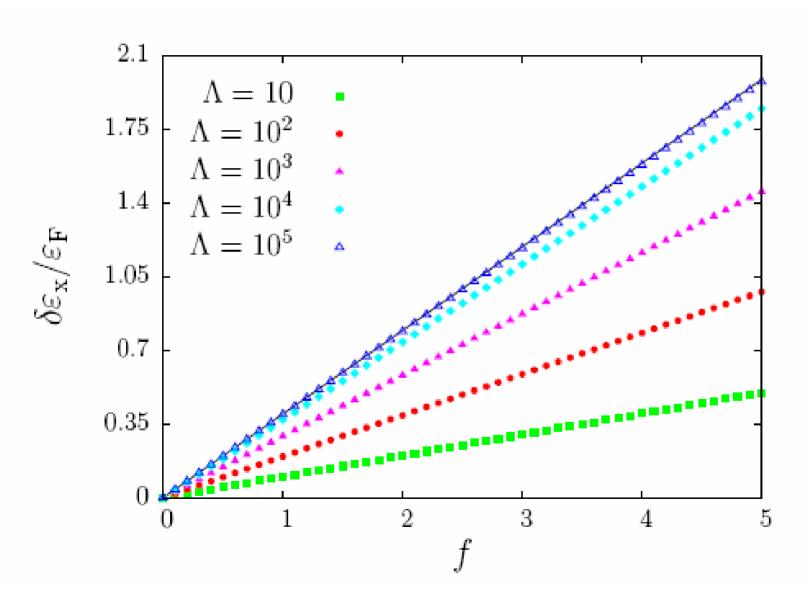
$$E=E-E(\varepsilon_F=0)$$

$$\delta \varepsilon_{\rm x} = -\frac{1}{2\pi n} \int \frac{d^2 {\bf q}}{(2\pi)^2} \; v_q \int_0^{+\infty} d\Omega \; \left[\chi^{(0)}({\bf q}, i\Omega, \varepsilon_{\rm F}) - \chi^{(0)}({\bf q}, i\Omega, \varepsilon_{\rm F} = 0) \right] \label{eq:epsilon}$$
 Exchange

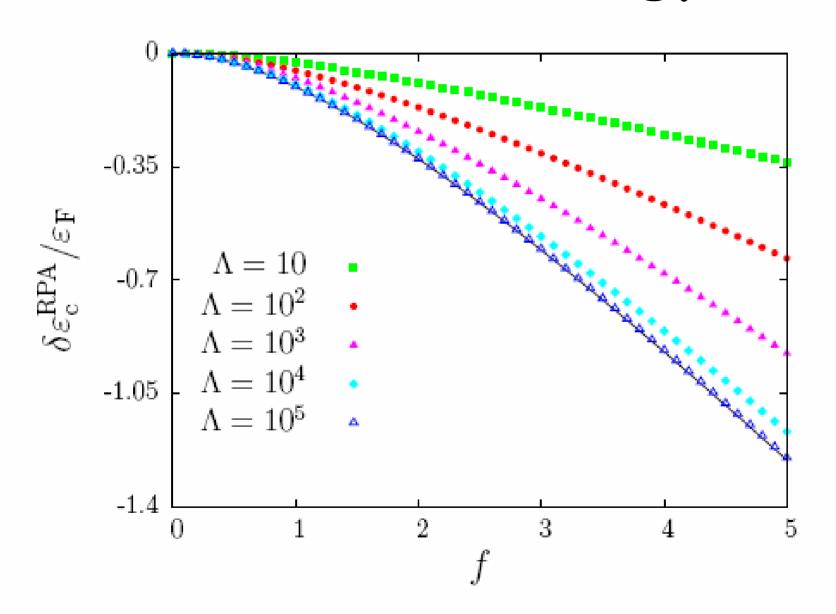
Correlation

$$\delta \varepsilon_{\rm c}^{\rm RPA} = \frac{1}{2\pi n} \int \frac{d^2\mathbf{q}}{(2\pi)^2} \int_0^{+\infty} d\Omega \left\{ v_q \delta \chi^{(0)}(\mathbf{q}, i\Omega) + \ln \left[\frac{1 - v_q \chi^{(0)}(\mathbf{q}, i\Omega, \varepsilon_{\rm F})}{1 - v_q \chi^{(0)}(\mathbf{q}, i\Omega, \varepsilon_{\rm F} = 0)} \right] \right\}$$

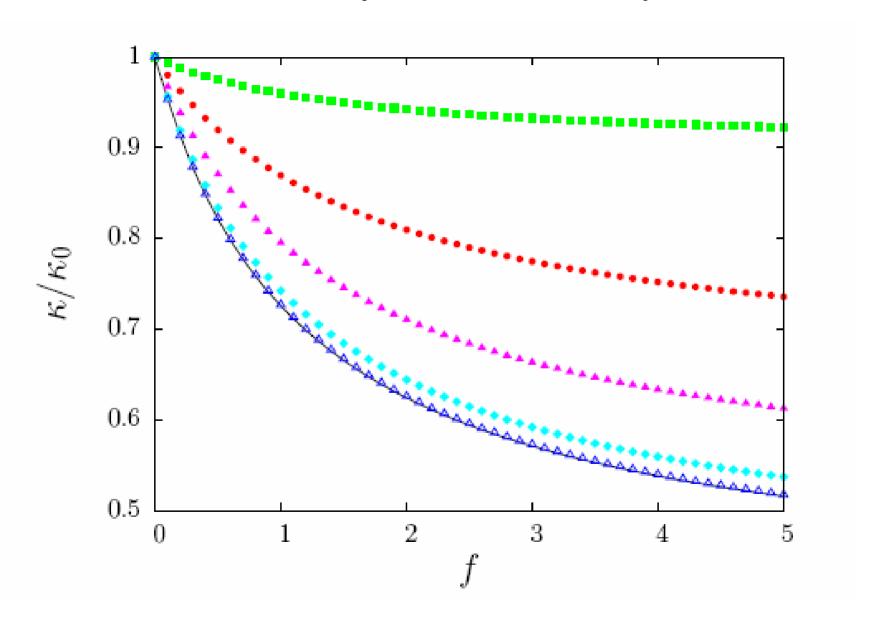
Exchange Energy



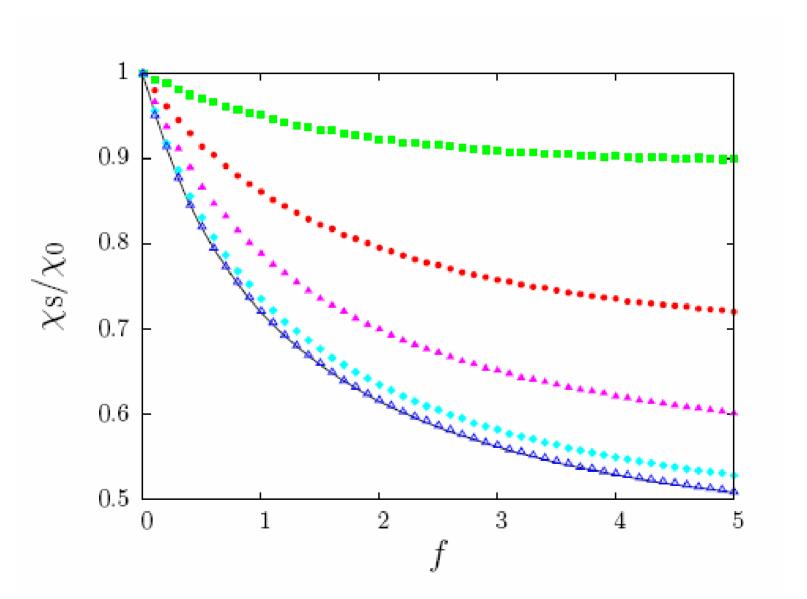
Correlation Energy



Compressibility



Spin-susceptibility



Alternate Form for X-energy

$$\delta \varepsilon_{\mathbf{x}} \ = \ -\frac{1}{2nS^2} \sum_{s,s'} \sum_{\mathbf{k},\mathbf{k}'} V_{s,s'}(\mathbf{k},\mathbf{k}') \, \delta n_{\mathbf{k}s} \delta n_{\mathbf{k}'s'}$$

$$+ \ \frac{1}{nS} \sum_{\mathbf{k},s} \Sigma_{\mathbf{k},s}^{(0)} \delta n_{\mathbf{k}s} \qquad \text{Extra-ordinary}$$

Renormalized Velocity

$$\Sigma_{\mathbf{k},s}^{(0)} = -\frac{1}{S} \sum_{\mathbf{k}',s'} V_{ss'}(\mathbf{k},\mathbf{k}') n_{s'}^{(0)}(\mathbf{k}')$$

$$V_{s,s'}(\mathbf{k}, \mathbf{k}') = \frac{2\pi e^2}{|\mathbf{k} - \mathbf{k}'|} \left[\frac{1 + ss' \cos(\theta_{\mathbf{k}, \mathbf{k}'})}{2} \right]$$

Contribution to Band Energy

$$\Rightarrow v \to v \left[1 + \frac{f}{4g}\ln(\Lambda)\right]$$

Katnelson cond-mat/0606611

Mischenko cond-mat/0612651

$$\frac{v_p}{v_0} = 1 + \left[\frac{g}{4} - g^2 \left(\frac{5}{6} - \ln 2 \right) + O(g^3) \right] \ln(\mathcal{K}/p).$$

Chiral Electron Gas Theory



The Cast



Chiral Electron Gas Properties

