Electron interaction effects in graphene

Daniel E. Sheehy

LOUISIANA STATE UNIVERSITY

SESAPS: Nov. 15, 2012

sheehy@lsu.edu

Work in collaboration with: J. Schmalian

Outline

- Graphene: One-atom thick sheet of graphite

- Low-energy theory: Coulomb-interacting Dirac fermions

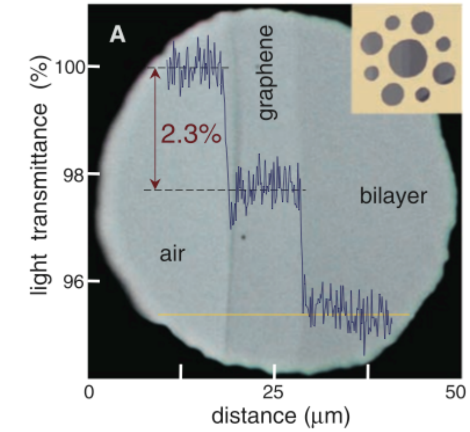
- Theoretical research: Neglects effect of Coulomb interactions

- Compute interaction corrections for several quantities

  Renormalization Group Hertz PRB 76, Millis PRB 1993

  Graphene: at a quantum critical point

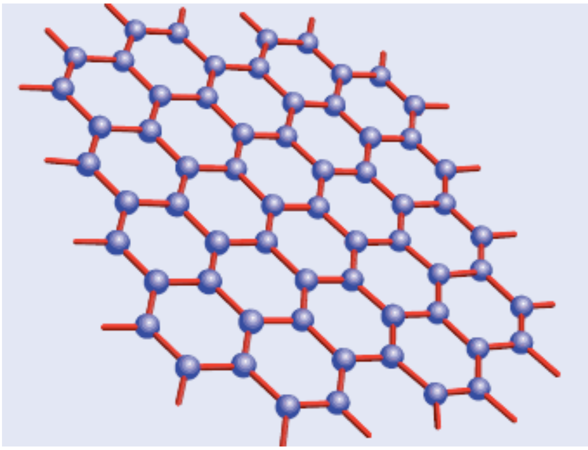
- Interaction effects in optical transparency?



Nair et al Science 2008

Graphene

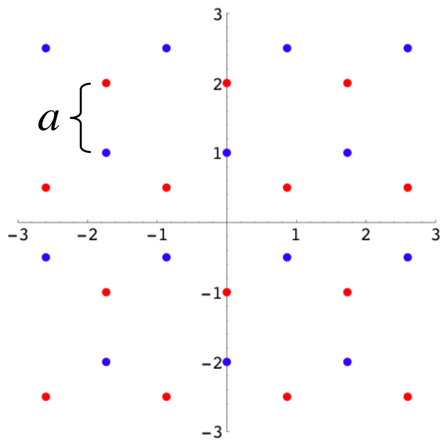
- Single-atom thick layer of graphite
  - –Theory: Wallace 47, Semenoff 84
  - – Exp't: Novoselov et al 2004
    Zhang et al 2005



- Model:
  - – Coulomb-interacting fermions on honeycomb lattice
  - – Half-filled: One fermion/site

- Kinetic energy $$H_0 = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma}$$

Nearest-neighbor hopping ⇒ Connects two sublattices



$$H_0 = -t \sum_{\mathbf{k},\sigma} \left(a^\dagger_{\mathbf{k}\sigma} \;\; b^\dagger_{\mathbf{k}\sigma} \right) \begin{pmatrix} 0 & f(\mathbf{k}) \\ f^*(\mathbf{k}) & 0 \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}\sigma} \\ b_{\mathbf{k}\sigma} \end{pmatrix}$$

$$f(\mathbf{k}) = \mathrm{e}^{ik_y a} + 2\cos\left[\frac{\sqrt{3}}{2} k_x a\right] \mathrm{e}^{-\frac{i}{2} k_y a}$$

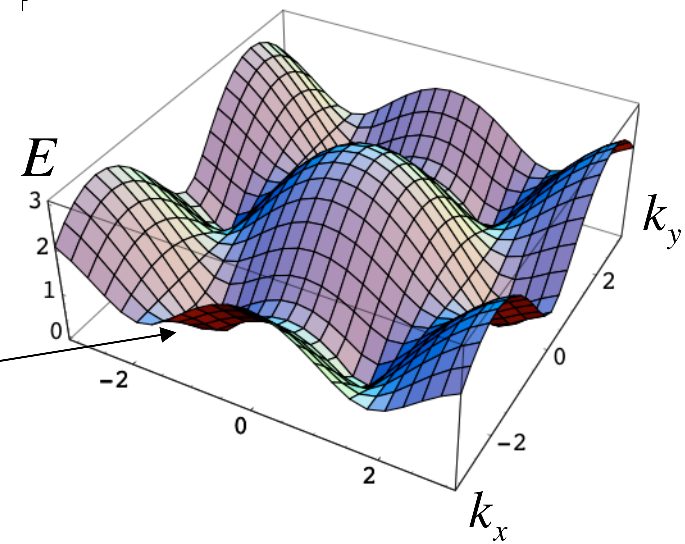
$a_{\mathbf{k}\sigma}, b_{\mathbf{k}\sigma}$ fermions on two sublattices

Next: Low energy

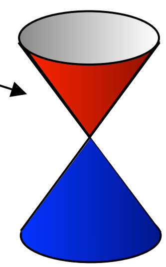
Low-energy theory of graphene

- Eigenvalues → Energy bands

$$E(\mathbf{k}) = \pm t\sqrt{1 + 4\cos^2\left[\frac{\sqrt{3}}{2}k_x a\right] + 4\cos\left[\frac{\sqrt{3}}{2}k_x a\right]\cos\left[\frac{3}{2}k_y a\right]}.$$



  - "Conduction band": two inequivalent nodes in Brillouin zone
  - "Valence band": Minus this



- Cone-like dispersion near nodes:

$$E(\mathbf{k}) \cong \pm v\,|\mathbf{k}| \quad \text{Velocity} \quad v = 3ta/2$$

- Effective Hamiltonian near nodes:

$$H_0 \simeq -v\sum_{\mathbf{k},i}\psi_i^\dagger(\mathbf{k})\begin{pmatrix} 0 & -k_x + ik_y \\ -k_x - ik_y & 0 \end{pmatrix}\psi_i(\mathbf{k})$$

$i = 1,\ldots 4$

Spin, node

- Applies at low momenta! ⇨ Cones don't go to infinity! $k << \Lambda \cong a^{-1}$

Free fermions on the honeycomb lattice

- "Relativistic" low-energy Hamiltonian

$$H = \sum_{\mathbf{p},i} \psi_i^{\dagger}(\mathbf{p})[v\mathbf{p}\cdot\sigma]\psi_i(\mathbf{p})$$

Pauli matrices.

Two-component spinor

- Condensed-matter phenomena: Observe $v \approx c/300$ Novoselov Nature 2005

Photoemission, Infrared spectroscopy

Bostwick Nat. Phys 2007; Li Nat. Phys. 2008

Novel Quantum Hall effect $\longrightarrow$ Dirac fermions in B-field

Zhang et al Nature 2005

- "Relativistic" quantum field theory phenomena

Zitterbewegung Katsnelson 2006

"jittery motion" of Dirac fermions

- What about Coulomb interaction?

Unscreened (No Fermi surface)

Next: Full Hamiltonian

Full Hamiltonian: Coulomb

$$H = \sum_{\mathbf{p},i} \Psi_i^\dagger(\mathbf{p})[v\mathbf{p}\cdot \sigma]\Psi_i(\mathbf{p}) + \frac{1}{2}\int d^2\mathrm{r}d^2\mathrm{r}' n(\mathbf{r})n(\mathbf{r}')\frac{e^2}{\varepsilon|\mathbf{r}-\mathbf{r}'|}$$

Kinetic energy

Coulomb interaction

$$n(\mathbf{r}) = \sum_{i=1}^{N}\Psi_i^\dagger(\mathbf{r})\Psi_i(\mathbf{r})$$

- Is the Coulomb interaction important?

Quantum Electrodynamics: Fine structure constant $\alpha_{QED} = \dfrac{e^2}{c\hbar} = \dfrac{1}{137}$

- Graphene: Dimensionless interaction strength $\alpha = \dfrac{e^2}{v\hbar}$ ← Note: $v \approx c/300$!

$$\alpha = 300\alpha_{QED} \approx 2.2$$

- Graphene's fine-structure constant can be quite large…

Dielectric screening: $\alpha = \dfrac{e^2}{\varepsilon v\hbar}$

Substrate-dependent ⇒ $\varepsilon = 1$ in vacuum

Next: Scaling…

Scaling analysis

- Relative importance of kinetic energy & potential energy?
  - ➢ Usual 2D Fermi gas: $\varepsilon_p = \dfrac{p^2}{2m}$
  - ➢ Kinetic energy per particle: $E_{\mathrm{KE}} \propto \varepsilon_F n \propto n^2$

    in 2D… $\varepsilon_F \propto n$
  - ➢ Potential energy per particle: $V(r) = \dfrac{e^2}{r}$ ⇒ Typical length scale is interparticle spacing… $r \approx \dfrac{1}{\sqrt{n}}$

$$E_{\mathrm{Coulomb}} \propto n\sqrt{n} \propto n^{3/2}$$

Density of other electrons to interact with

Interparticle spacing

  - ➢ High density: $E_{\mathrm{Coulomb}} << E_{\mathrm{Kinetic}}$ ⇒ Strong screening regime
  - ➢ Low density: $E_{\mathrm{Coulomb}} >> E_{\mathrm{Kinetic}}$ ⇒ Wigner crystal

- Relative importance depends on density!

Next: What about graphene?

Scaling analysis: Graphene

- Now, the kinetic energy has the Dirac form!

  - Graphene $\varepsilon_p = vp$

  - Kinetic energy per particle: $E_{\mathrm{KE}} \propto p_F n \propto n^{3/2}$

  - Potential energy per particle: $E_{\mathrm{Coulomb}} \propto n\sqrt{n} \propto n^{3/2}$ (Same as previous)

Relative importance of Kinetic & Coulomb independent of n! $\Rightarrow$ No characteristic length scale

- Scale invariance: Like at a quantum critical point

  - External perturbations: Introduce length scales

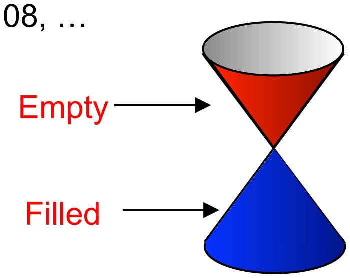
    – Applied Magnetic field: $\ell_B = \sqrt{\frac{\hbar c}{2e}}\frac{1}{\sqrt{B}}$ Magnetic length

    – Finite temperature: $\lambda_T = \frac{2\pi\hbar v}{k_B T}$ de Broglie wavelength (different for Dirac!)

Next: RG

Wilsonian renormalization group

Gonzalez Nucl. Phys. B 94, Khveshchenko PRB 06,
Son PRB 07, DES & J. Schmalian PRL 07, Herbut et al PRL 08, …



- Graphene Hamiltonian:
  - Quasiparticle velocity $v \approx c/300$
  - Coulomb interaction parameter $\alpha = \dfrac{e^2}{\hbar v} \approx 2.2$
  - Ultraviolet (large momentum) cutoff $\Lambda \approx \dfrac{\hbar}{a}$

Theory in BZ
Became Dirac theory

- Partition function: $Z = Tr \exp\left[-\beta H[\Psi^\dagger(\mathbf{p}), \Psi(\mathbf{p})]\right]$

$\beta = 1/(k_B T)$

  - Trace over states with $p < \Lambda$

How does the theory change if we change the cutoff?

- Idea behind renormalization group (RG):
  - Partial trace over high momentum states $\Lambda / b < p < \Lambda$
  - New theory: Lower cutoff, smaller coupling $\alpha(b) = \dfrac{\alpha}{1 + \frac{1}{4}\alpha \ln b}$

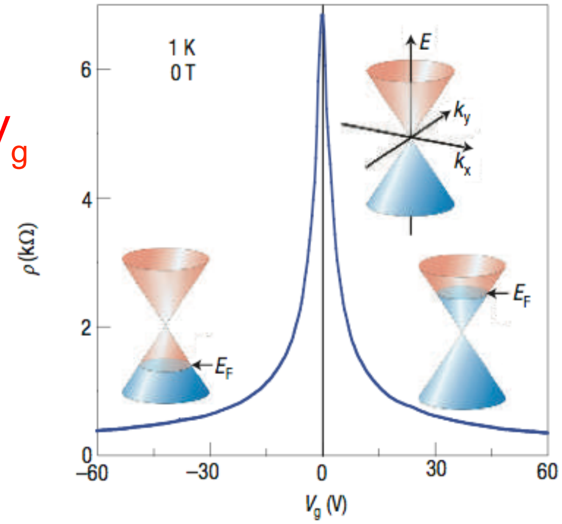
Since coupling is smaller, the theory is easy to solve!

Next: Other parameters?

Electron density

- Fermion density: adjustable via doping or external gate V_g
  - Impose chemical potential $\mu \leftrightarrow V_g$

Intrinsic: $\mu = 0, n = 0$ (No Fermi surface)
Electron doped: $\mu > 0, n > 0$ (e Fermi surface)
Hole doped: $\mu < 0, n < 0$ (h Fermi surface)



Geim & Novoselov Nat. Mat. 2007

- How do chemical potential & temperature evolve under RG?

Chemical potential & temperature increase:

$$\mu(b) = \frac{\mu b}{1 + \frac{1}{4}\alpha \ln b} \qquad T(b) = \frac{Tb}{1 + \frac{1}{4}\alpha \ln b}$$

- Density scaling relation:

$$n(\mu, T, \alpha) = b^{-2} n(\mu(b), T(b), \alpha(b))$$

What we want

In renormalized system $\begin{cases} \alpha(b) & \text{small} \\ T(b) & \text{large} \end{cases}$

- Need: Choice for *b* ➡ renormalization condition

Next: RG condition

Renormalization condition

- Graphene: critical point at $T = \mu = B = n = 0$

Magnetic field

- Relevant perturbations: Grow under RG, leave vicinity of critical point

  - E.g., if original system is at nonzero *T*, renormalized system has larger *T*

Nodal "Dirac" approximation breaks down!

  - Terminate RG flow when perturbation reaches UV scale (bandwidth)

$$k_B T(b) = \hbar v \Lambda$$

- Graphene at fixed density *n* but low *T*: $n(b) = b^2 n$

  - Terminate RG flow when $n(b)$ gets too large!

$$n(b) = a^{-2}$$

Renormalized density *lattice scale*

- Question: What does this get us?

Interaction corrections to equations for graphene obesrvables

Compressibility at low T

- Scanning Single electron transistor: Measure $\kappa^{-1} = \dfrac{\partial \mu}{\partial n}$

Inverse compressibility

J. Martin, N. Akerman, G. Ulbricht, T. Lohmann, J. H. Smet, K. von Klitzing, A. Yacoby, Nat. Phys. (2007)

- RG equation for inverse compressibility

$$\kappa^{-1}[n,\alpha] = b\left(1 + \frac{1}{4}\alpha \ln b\right)\kappa^{-1}[n(b),\alpha(b)]$$

What we want

In renormalized system, approximate $\alpha(b) \approx 0$

- Inverse compressibility of ***interacting*** graphene

$$\kappa^{-1} \cong \underbrace{\sqrt{\frac{\pi}{4|n|}}}_{\text{Free Dirac Fermions}}\, v \underbrace{\left(1 + \frac{\alpha}{4}\ln\sqrt{\frac{n_0}{|n|}}\right)}_{\text{Log correction depends on density}}$$

See Also: Hwang et al PRL 07

$$n_0 \approx 4\times10^{15}\,cm^{-2}$$

- Looks like: Density-dependent velocity!

Need: Many decades of data to observe…

$$v(n) = v\left(1 + \frac{\alpha}{4}\ln\sqrt{\frac{n_0}{|n|}}\right)$$

Recent compressibility data

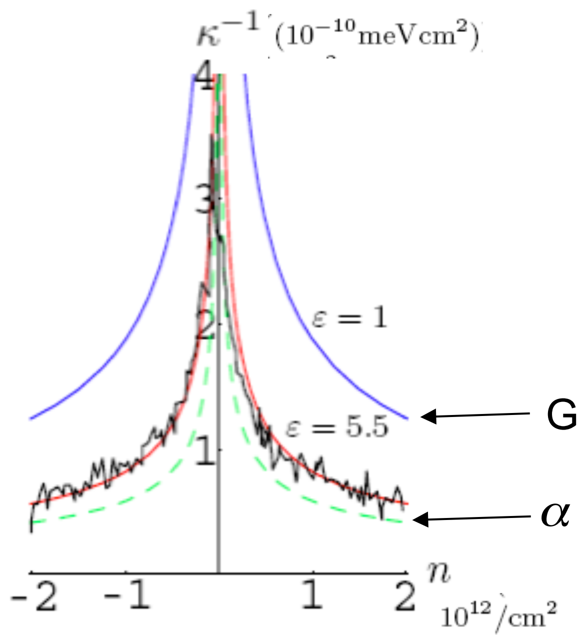
J. Martin, N. Akerman, G. Ulbricht, T. Lohmann, J. H. Smet, K. von Klitzing, A. Yacoby, Nat. Phys. (2007)

- We attempted to fit the data: $$\kappa^{-1} \cong v\sqrt{\frac{\pi}{4|n|}}\left(1+\frac{\alpha}{4}\ln\sqrt{\frac{n_0}{|n|}}\right)$$

DES & J. Schmalian PRL 2007

Substrate: Alters dielectric const.

$$\alpha = \frac{e^2}{\varepsilon v \hbar}$$



Graphene in vacuum

$\alpha = 0$ Doesn't fit….

- Interactions necessary to understand data
  - Best fit $\varepsilon = 5.5$
- Difficult to observe ln(n) dependence
  - Uncertainty in velocity

Next: Other experiments?

Shubnikov-de Haas oscillations

"Dirac cones reshaped by interaction effects in suspended graphene"
Elias, et al Nat. Phys. 8, 172 (2012)

- SdH Oscillations: Also measure v at fixed n!
  - Resistivity oscillates with applied B field

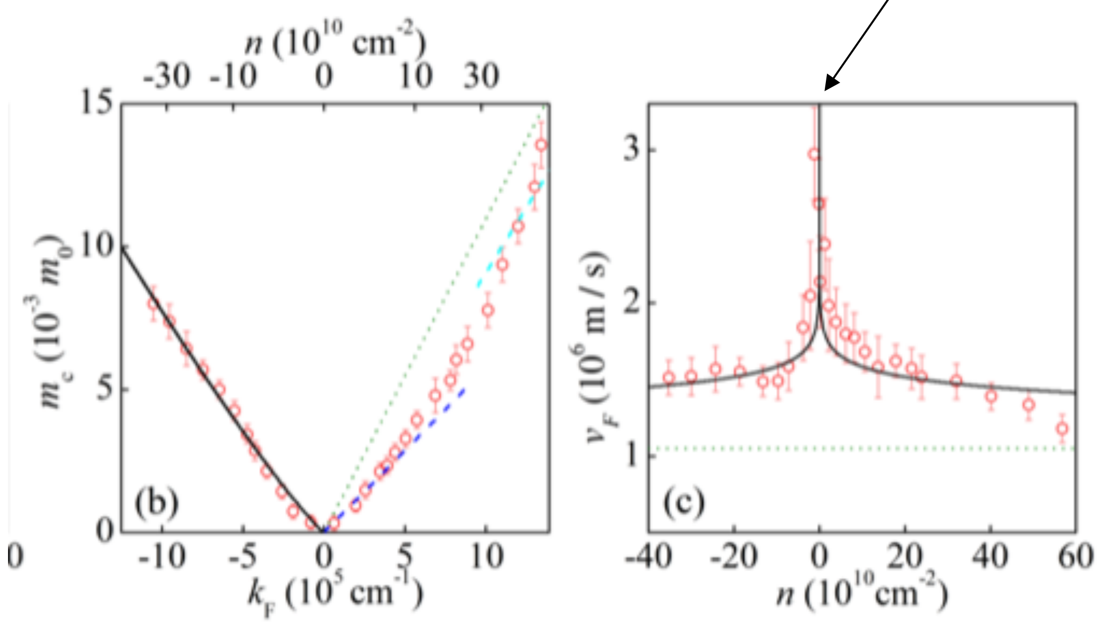
Measure cyclotron mass, and velocity

Effective velocity at fixed density:

$$v(n) = v\left(1 + \frac{\alpha}{4}\ln\sqrt{\frac{n_0}{|n|}}\right)$$

Diverges logarithmically for vanishing carrier density

- Data: Consistent with this picture:

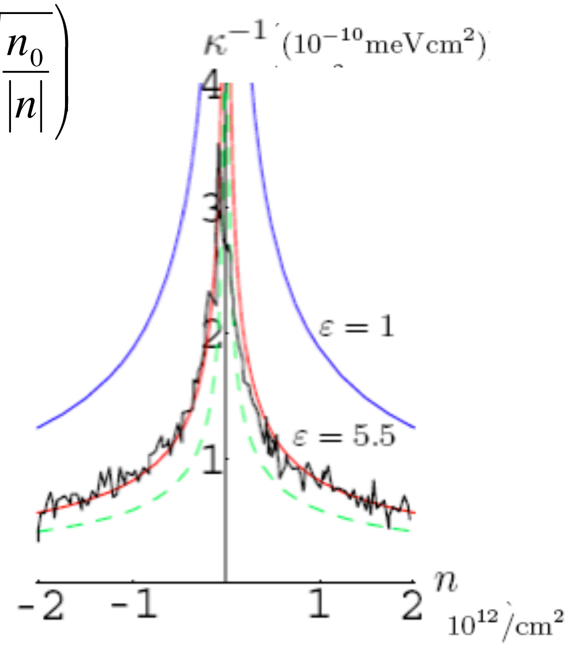


Next: Does the velocity really diverge?

Back to inverse compressibility…

- Low-T inverse compressibility vs. carrier concentration:

$$\kappa^{-1} \cong v\sqrt{\frac{\pi}{4|n|}}\left(1+\frac{\alpha}{4}\ln\sqrt{\frac{n_0}{|n|}}\right)$$



- ➢ We assumed: density is the dominant perturbation
- ➢ All experiments at finite T

Temperature dependence of Inverse compressibility of intrinsic graphene!

- RG analysis of finite-T inverse compressibility at n=0:

Result:

$$\kappa^{-1} \cong \frac{\pi v^2}{\underbrace{4T\ln 2}_{\text{Free Dirac Fermions}}}\left(1+\frac{1}{4}\alpha\ln\frac{T_0}{T}\right)^2$$

$T_0 \approx 8\times 10^4 K$ *Characteristic temp.*

Log-T enhancement
Depends on temperature!

Next: Heat Capacity

Specific heat capacity

- Two regimes: Is temperature or density (chemical potential) dominant?
  - High temperature $|\mu| << T$ ⇒ Interacting Dirac fermions

$$C \cong \frac{9N\varsigma(3)}{2\pi v^2}\frac{T^2}{\left[1+\frac{1}{4}\alpha\ln(v\Lambda/T)\right]^2} \Rightarrow C \propto \frac{T^2}{\left[\ln(v\Lambda/T)\right]^2}$$

Vafek PRL 07

Low-T behavior

  - High density ($|\mu| >> T$) ⇒ Fermi liquid! (electron or hole)

Metallic ⇒ $C \cong \gamma T$

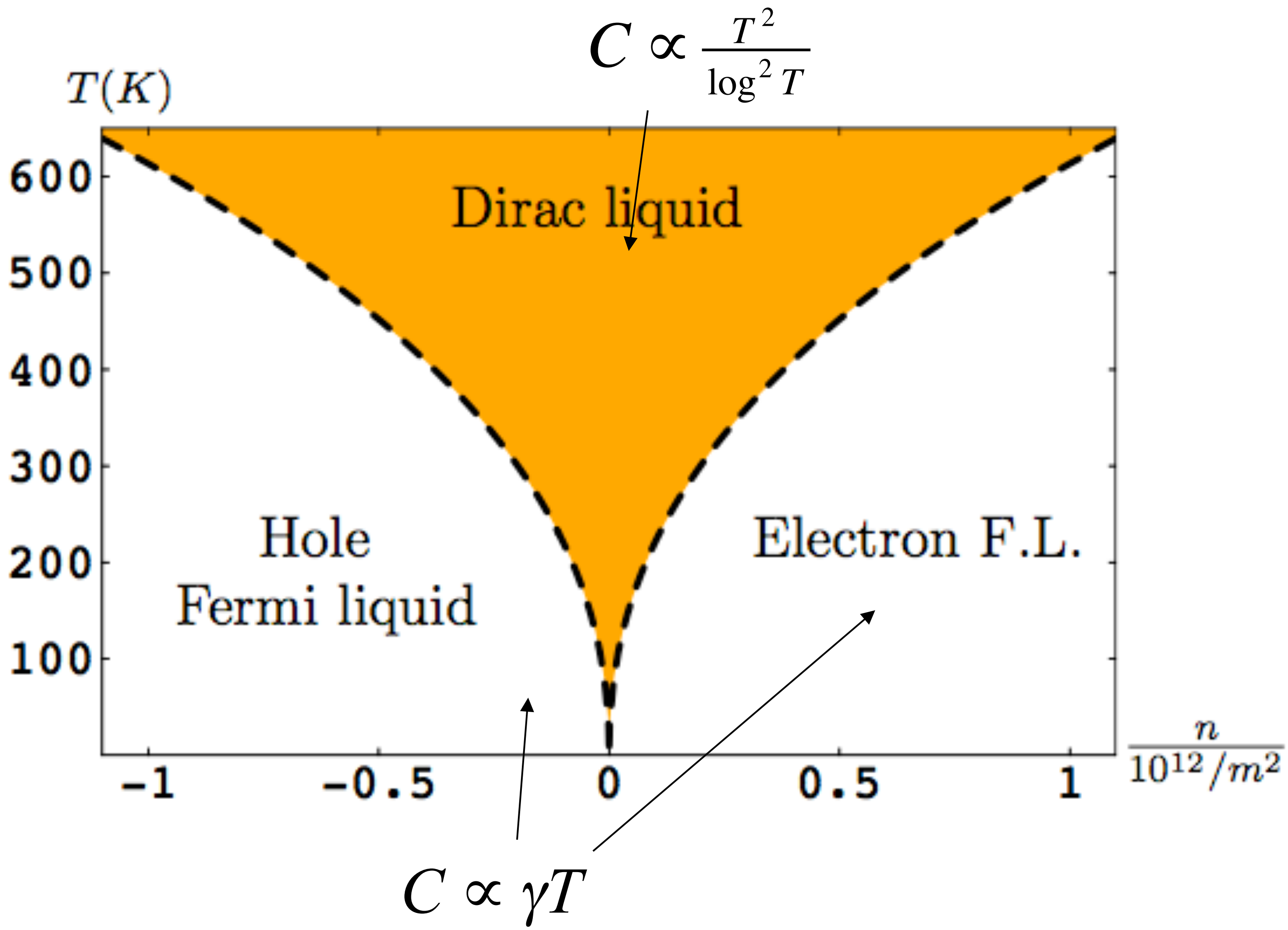
$$\gamma \propto \frac{\sqrt{n}}{v\left(1+\frac{\alpha}{4}\ln\sqrt{\frac{n_0}{n}}\right)}$$

- Heat capacity coefficient also measures density-dependent velocity

- RG: Tells us how to sum perturbative corrections

Next: Phase Diagram

Phase diagram: Crossover behavior



- Dashed line: Crossover between two regimes

Next: Transparency

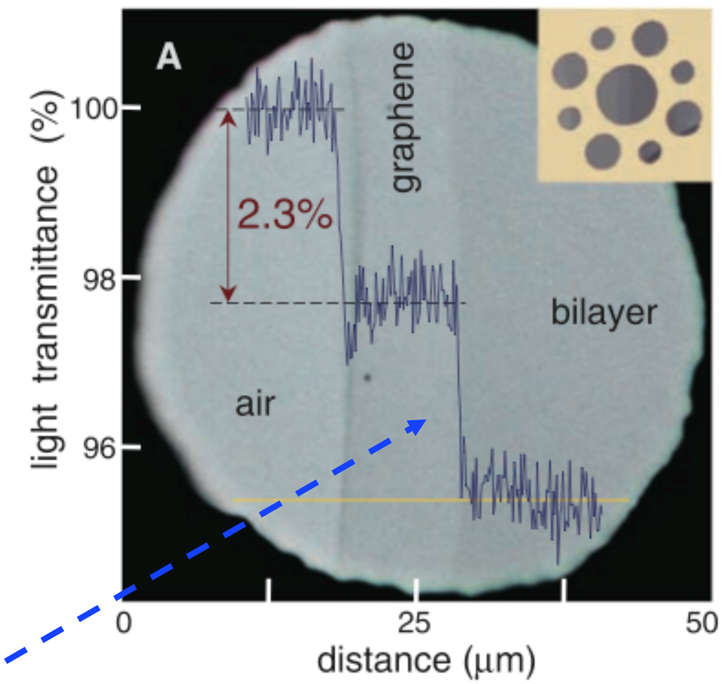
Optical transparency of graphene

- Graphene nearly transparent ➔ What determines the deviation from perfect transparency?

Nair et al, Science 2008: “Fine structure constant defines visual transparency of graphene”

See also Kuzmenko et al PRL 2008 -- graphite

Aperture partially covered by graphene



Transmittance: $t = 97.7\%$

- Theory*: $$t(\omega) = \frac{1}{(1 + 2\pi\sigma(\omega)/c)^2}$$

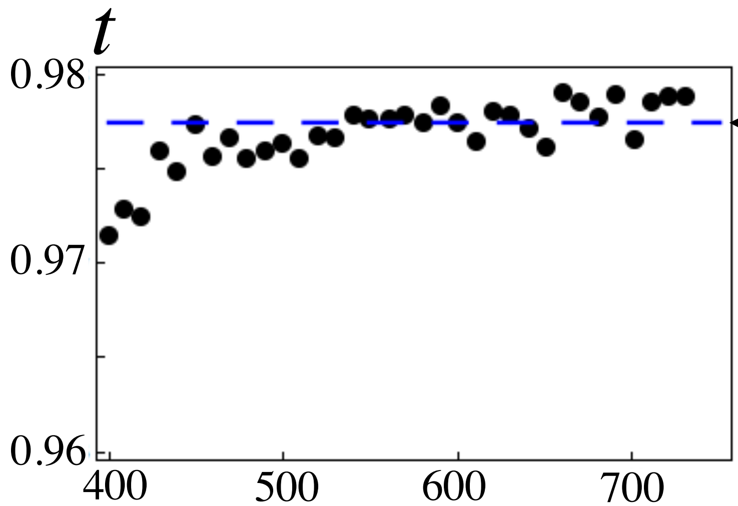
Measures conductivity in optical regime!

*Stauber et al PRB 2008

Next: Are interactions important?

Optical transparency of graphene

• Apparently not: Nair et al results consistent with noninteracting graphene



$$\sigma_0 = \frac{e^2}{4\hbar}$$

"Universal"
Ludwig et al PRB 94

• Transmission $t(\omega) = \dfrac{1}{(1 + \pi\alpha_{QED}/2)^2}$

Fine structure constant!

• Question: Why can we neglect Coulomb interaction?

– No log prefactors in $\sigma(\omega)$

– Small perturbative correction

Next: Are interactions important?

Conductivity of clean graphene

- Scaling: $\sigma(\omega,T,\alpha)=\sigma(\omega(b),T(b),\alpha(b))$

Previously: $\alpha(b)\approx 0$ in renormalized theory

Now we do perturbation theory!

- Perturbation theory in renormalized:

$$\sigma(\omega,T,\alpha)\cong\sigma_0(\omega,T)+\underbrace{\alpha(b)\sigma_1(\omega,T)}_{\text{keep...}}+\alpha(b)^2\sigma_2(\omega,T)+\ldots$$

- Low-T regime: $\omega(b^*)=v\Lambda$

$$\alpha(b^*)\cong\frac{\alpha}{1+\frac{\alpha}{4}\ln(v\Lambda/\omega)}$$

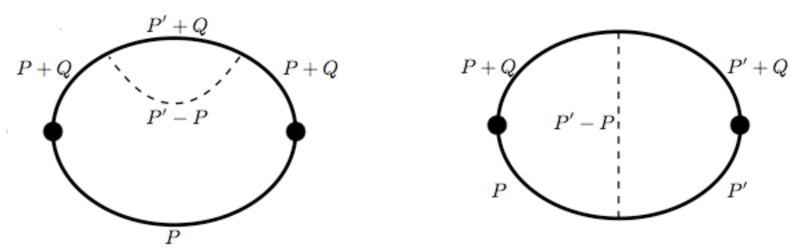
$$\sigma=\frac{e^2}{4\hbar}\left(1+\frac{C\alpha}{\underbrace{1+\frac{1}{4}\alpha\ln(v\Lambda/\omega)}}\right)$$

Herbut, Juricic, Vafek, PRL 08
Mishchenko Europhys. Lett. 08
DES & J Schmalian PRB 09
Juricic et al PRB 10

tiny correction for $\omega\rightarrow 0$; NOT small in optical range!

- What is the coefficient C ?

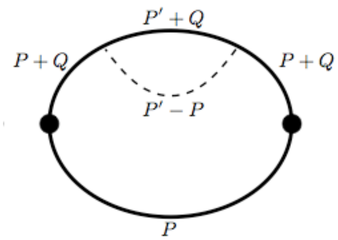
Calculate some diagrams…

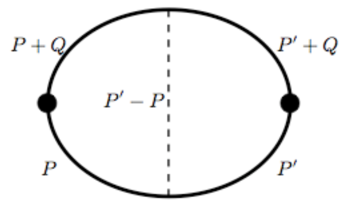


Next: Three different results in literature!

Calculation of the optical transparency of graphene

- Our motivation: Initially two results in the literature for C





$$\sigma = \frac{e^2}{4\hbar}\left(1+\frac{C\alpha}{1+\frac{1}{4}\alpha\ln\left(v\Lambda/\omega\right)}\right)$$

- ➢ Herbut, Juricic, Vafek, PRL 08: $C=\dfrac{25-6\pi}{12}\cong 0.512$ Would give a large correction!
- ➢ Mishchenko EPL 08: $C=\dfrac{19-6\pi}{12}\cong 0.012$ Would give a small correction

- Our insight: Herbut et al used Kubo formula   Phys. Rev. B 80, 193411 (2009)
  - ➢ Diagrams are *separately* divergent, can be combined to give different answer

    How to get the right answer?
  - ➢ Diagrams must satisfy current conservation!

$$\nabla\cdot\mathbf{j}+\frac{\partial\rho}{\partial t}=0 \quad\Rightarrow\quad Q_\mu\left\langle j_\mu(Q)\,j_\nu(-Q)\right\rangle=0$$

- Imposing this: Tells us how to combine divergent diagrams
  - ➢ Obtain result due to Mishchenko…

Next: But wait!

Recent work:

- Juricic et al PRB 2010: Regularize graphene in a different way

  “epsilon expansion”

  - Analytically continue *spatial dimension* $d = 2 - \varepsilon$
  - Their claim: cannot use a UV cutoff for graphene
  - Obtain a third result: $C = \dfrac{11 - 3\pi}{6}$

- What is the resolution?
  - Possibility 1: Latest Juricic et al result is correct:
    - One cannot study graphene in spatial dimension 2 and regularize integrals
    - Note: Original Mishchenko calculation had no cancelling divergences
  - Possibility 2: Latest Juricic et al result is incorrect:
    - “epsilon expansion” is not really probing the AC conductivity
    - We can obtain Mishchenko result by implementing epsilon expansion differently and using different regularization schemes
    - See also Abedinpour et al PRB 2011 – also obtain Mishchenko result

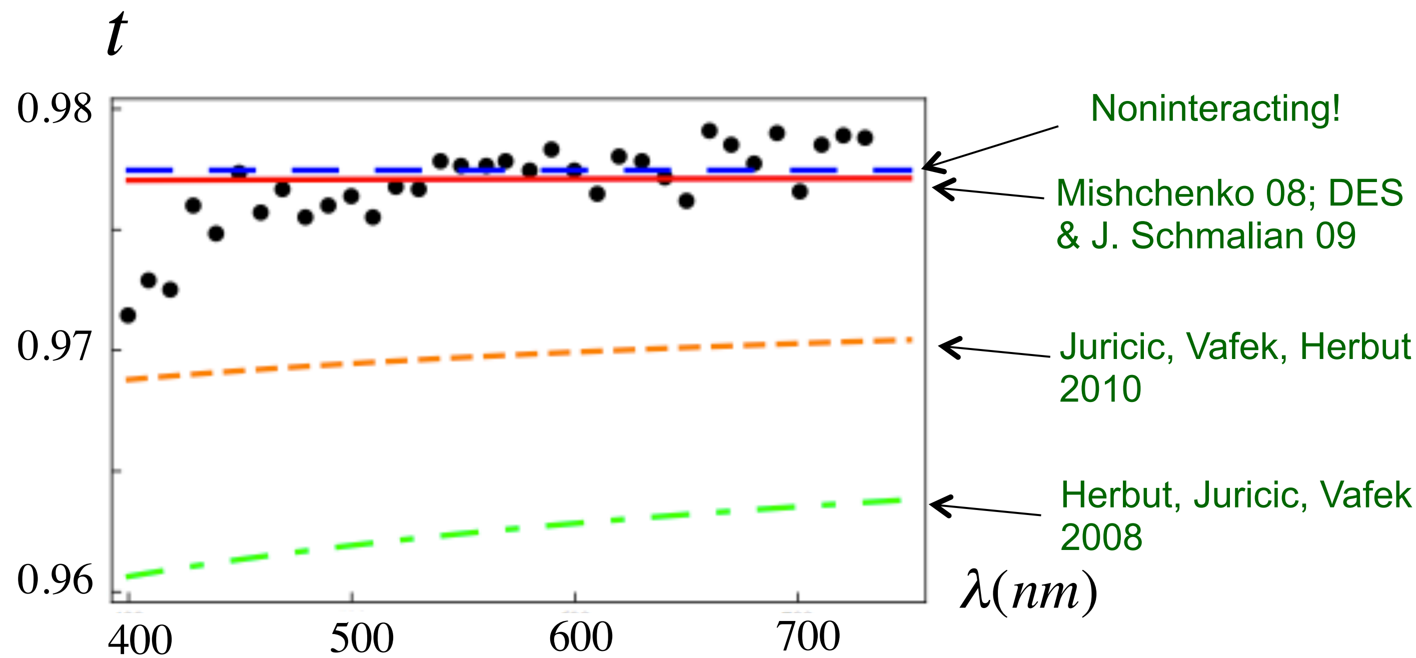
- All these difficulties arise because of the nodal approximation! Why not use the original lattice theory?

Next: What do experiments say?

Conductivity of clean graphene

Transparency:

$$t(\omega) = \frac{1}{(1+2\pi\sigma(\omega)/c)^2} \qquad \sigma(\omega) = \frac{e^2}{4\hbar}\left(1+\frac{C\alpha}{1+\frac{1}{4}\alpha\ln(v\Lambda/\omega)}\right)$$



- Only a very small value of C is consistent with experiments!

Concluding remarks

- Graphene: Dirac fermions with Coulomb interaction (Marginal)
    - Interaction effects: Log corrections to free case (Dirac fermions)
- Renormalization group: Scaling equations for various quantities
    - Specific heat, compressibility, diamagnetic susceptibility, dielectric
    - function, …
    - Interactions only renormalize velocity: $v \to v\left(1+\frac{\alpha}{4}\ln\left[v\Lambda/T\right]\right)$

      (Leading order)
- Optical transparency probes conductivity

$$\sigma = \frac{e^2}{4\hbar}\left(1+\frac{C\alpha}{1+\frac{1}{4}\alpha\ln\left(v\Lambda/\omega\right)}\right)$$

α large! But $C = \frac{19-6\pi}{12} \cong 0.012$

Small correction!

Mishchenko Europhys. Lett. 2008

- We resolved discrepancy with earlier Kubo formula calculation
    - Regularization method must preserve conservation laws