Nonlinear screening in graphene nanostructures

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Acknowledgements

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- Matt Zhang (UCSD)

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Quasi-relativistic ("Dirac") fermions

\[ E(p) = \pm \nu |p| \]

\[ \nu \approx c/300 \]

300 times slower than light

\[ E > 0 \text{ "electrons"} \]
\[ E < 0 \text{ "positrons" or "holes"} \]

Fermi surface shrinks to a single point
Graphene: QED in a pencil trace?

**Similarities**
- Linear spectrum
- Spin-like degree of freedom
- Chirality

**Differences**
- 2+1D instead of 3+1D
- No mass
- Interactions are strong
- No retardation ($\nu < c$)
- Doping, disorder, phonons
- ....
Klein paradox (1929)

An example of what “QED in a pencil trace” may test

- Naïve calculation gives transmission > 1 ??
  - Source of mistake: for the negative-energy states
    (group velocity) = - (quasi-particle velocity)

The result of the correct calculation: transmission < 1 and increases with the barrier height

- Not exactly paradoxical in 2007 but still unusual ...
Supercritical charge: atomic collapse and creation of antimatter

Energy

\[ 2mc^2 \]

\[ Z\alpha < C \sim 1 \]

subcritical

Schwinger, 1950’s
Zeldovich, 1970’s

\[ Z\alpha > C \]
Fine-structure constant in graphene

\[ \alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137} \]

\[ \alpha_{\text{Graphene}} = \frac{e^2}{\kappa \hbar \nu} \approx 0.9 \]

\( \kappa = 2.3 \) dielectric constant

SiO₂
High-k dielectric: weak interactions

\[ \alpha = \frac{e^2}{\kappa \hbar \nu}, \quad \kappa = \text{dielectric constant} \]

If \( \kappa \gg 1 \), \( \alpha \ll 1 \)

HfO\(_2\), water, …
Our work – nonlinear screening in graphene

References: arXiv:0707.1023 (PRB 2007), 0708.0892, and 0710.2150
What is screening?
Linear screening

Poor screening $\varepsilon(q) \approx 1$
- External charge $\sim \sin qx$

Good screening $\varepsilon(q) \gg 1$
- $r_s = \frac{1}{\alpha k_F}$ screening length

Guinea et al.
Ando
Das Sarma et al.
Why would screening be nonlinear in graphene?

- Lots of carriers: good screening
- No carriers: no screening!
- Lots of carriers: good screening
Nonlinear screening

Higher electron density, better screening
Lower density, worse screening
# Summary of possible screening regimes

<table>
<thead>
<tr>
<th>Screening</th>
<th>Poor</th>
<th>Poor</th>
<th>Good</th>
</tr>
</thead>
<tbody>
<tr>
<td>Valid approximation</td>
<td>N/A (Dirac eq.)</td>
<td>Thomas-Fermi</td>
<td>Classical electrostatics</td>
</tr>
</tbody>
</table>

\[ r_s = \frac{\lambda_F}{\alpha} \]

If \( \alpha \ll 1 \)
Graphene $p$-$n$ junction

Electrostatic potential of the gates induces a gradually varying charge density profile, which changes sign.

- The back-gate controls the overall carrier density
- The top gate determines the density difference
Recent experiments

- Resistance of a graphene $p$-$n$ junction is only a few kΩ
- Qualitatively explained by the gapless Dirac spectrum
- Quantitative theory needed

Williams et al., Science 317, 638 (2007)
B. Huard et al., PRL 98, 236803 (2007)
B. Ozyilmaz et al., arXiv/cond-mat:0705.3044
Klein paradox (1929)

An example of what “QED in a pencil trace” may test

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Veselago lensing

Cheianov et al. 2007
Electric field in the junction

- Conductance is determined by the field strength at the interface.
- A naïve estimate (Cheianov 06) assumed uniform field:

  In reality, electric field is:
  - *suppressed* away from junction where screening is good
  - *enhanced* near the interface where screening is poor
Nonlinear screening, case \( \alpha \sim 1 \)

- Electron density is highly non-uniform, how to compute the screened potential?
- It is charge density that must be found first!
- Screened potential \( V(x) \) follows from the density of states
- Three-line derivation, next
Nonlinear screening, $\alpha \sim 1$

- **Charge density**
  \[ \rho(x) = \rho' x \]

- **Potential, T-F approx.**
  \[ eV(x) = \mu(x) = \hbar \nu \sqrt{\rho(x)} \propto \sqrt{x} \]

- **Electric field**
  \[ F = -V'(x) \propto 1/\sqrt{x} \]

- **Cut the divergence**
  \[ x_* = \lambda_F(x_*) \]
Numerical results

3 / 16 / 1

2 ) ' ( 0 . 1

\( \rho_\alpha e hR \)

(a)

\( \alpha = 1 \)
\( \alpha = 0.1 \)

\( x/D \)

Density

(b)

\( \alpha = 1 \)
\( \alpha = 0.1 \)

\( x/D \)

Electric field

(c)

\( \alpha = 0.1 \)

\( x/D \)

Density

Junction resistance

\[
R = 1.0 \frac{h}{e^2 \alpha^{-1/6} (\rho')^{-1/3}}
\]
Results

- Previous results for transmission through p-n junction are off by a (parametrically) large factor (~2-10, in practice)
- Our new results bring theory and experiments in a much better agreement
- Including disorder effects the agreement can be made quantitative (next slide)
Disorder in $p$-$n$ junction
Coulomb impurity in graphene
Why the Coulomb impurity problem?

- Uncontrolled charged impurities in the substrate
- Intentional doping / gating
- Intriguing analogy to atomic collapse and vacuum breakdown in QED

\[ \alpha_{\text{Graphene}} \approx 0.9 > \alpha_c ? \]
Supercritical charge: atomic collapse and creation of antimatter

\[ E = 2mc^2 \]

\( Z\alpha < 1 \) subcritical

\( Z\alpha > 1 \)

Schwinger, 1950’s
Zeldovich, 1970’s
Critical charge in graphene

\[ Z_c \alpha \sim \frac{1}{2} \]

\[ \alpha_{\text{Graphene}} \approx 0.9 \therefore Z_c \sim 1? \]

Khalilov (1998)
Novikov
Shytov, Levitov
Castro-Neto

...
Critical charge in graphene: previous work

Subcritical $Z$

Electron density

$$n(r) \sim \alpha \delta(r)$$

$$V(r) \sim \frac{1}{r}$$

Supercritical $Z$

Electron density

$$n(r) \sim \frac{1}{r^2 \ln^2 r}$$

$$V \sim \frac{1}{r \ln r}$$

DiVincenzo, Katsnelson, Shytov, Castro-Neto
Problem with previous work: range of validity

- Short-range cutoff: bandwidth
- Long-range: zero mass
- For $\alpha Z \sim 1$ both cutoffs $\sim$ lattice constant
Our work – “hyper"critical charge

M.F., Novikov, Shklovskii, PRB (2007)

\[ \alpha Z \gg 1 \]
New result for “vacuum polarization” around a large Coulomb charge

- New universal result for the structure of the supercritical core
- For $\alpha = 1$ this core “squeezes out” the regimes discussed in previous literature
- Such regimes return if $\alpha << 1$ (next slide)
Hypercritical impurity, small $\alpha$
How to realize large-Z charge?

STM / AFM tip