Zero-energy vortices in gated graphene

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Quantum transport in 2D systems
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Graphene dispersion


Unconventional QHE; huge mobility (suppression of backscattering), universal optical absorption...

Theory: use of 2D relativistic QM, optical analogies, Klein paradox, valleytronics...

Dispersion Relation

\[ E = \pm \gamma_0 \sqrt{|f(k)|} \]

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

\[ E = \pm \hbar \nu_F |q| \quad \text{with} \quad c/\nu_F \approx 300 \]

“Dirac Points”

Expanding around the K points in terms of small q

\[
\hat{H} = \hbar v_F \begin{pmatrix}
0 & \hat{q}_x - i\hat{q}_y \\
\hat{q}_x + i\hat{q}_y & 0
\end{pmatrix}
\]
Light-like Dispersion:  \[ E = \pm \hbar v_F |q| \]

Graphene’s charge carriers behave in an ultra-relativistic manner.

Optical Analogies
- Veselago lens
- Goos–Hänchen effect
- Fabry-Pérot etalons
- Waveguides
- Whispering-gallery modes
Fully-confined states in quantum dots and rings

Circularly-symmetric potential $V(r)$

$$\psi(r, \varphi) = \begin{pmatrix} e^{im\varphi} \chi_A(r) \\ e^{i(m+1)\varphi} \chi_B(r) \end{pmatrix}$$

$$\left( -i \frac{\partial}{\partial r} + \frac{im}{r} - i \frac{\partial}{\partial r} \frac{i(m+1)}{r} V(r) \right) [\chi] = E [\chi]$$

$E \neq 0$ -- confinement is not possible for any fast-decaying potential…
"Theorem" - no bound states

\[ \hat{H} = v_F \sigma \cdot \hat{p} + V(r) \]

Inside well

\[ J_n(|E| + v_0|)r \]

Outside well

\[ J_n(|E|r) \quad \text{and} \quad N_n(|E|r) \]

With asymptotics

\[ J_\alpha(z) = \sqrt{\frac{2}{\pi z}} \left( \cos \left( z - \frac{\alpha \pi}{2} - \frac{\pi}{4} \right) + e^{\text{Im}(z)} |O(|z|^{-1}) \right) \]

\[ Y_\alpha(z) = \sqrt{\frac{2}{\pi z}} \left( \sin \left( z - \frac{\alpha \pi}{2} - \frac{\pi}{4} \right) + e^{\text{Im}(z)} |O(|z|^{-1}) \right) \]

Equation (20) involves only the square of energy. Therefore, its solutions do not depend on the sign of \( E \). These solutions are equivalent to the scattering states for the ordinary radial Schrödinger equation with \( E > 0 \). Hence, it follows that, in such a potential well, bound states are absent. We stress that this conclusion does not depend on the depth and width of the well; i.e., a two-dimensional localization of quasiparticles in graphene (quantum dot) is fundamentally impossible (evidently,

Tudorovskiy and Chaplik, JETP Lett. 84, 619 (2006)
Fully-confined states for $E = 0$

$\Rightarrow \text{DoS}(0) \neq 0$

Square integrable solutions require $m > 0$ or $m < -1$

$\Rightarrow$ vortices!
Exactly-solvable potential for $E = 0$

$$V(r) = \frac{V_0}{1 + (r/d)^2}$$

Condition for zero-energy states:

$$V_0 d = \begin{cases} 2(n + m + 1) & m > 0 \\ 2(n - m) & m < -1 \end{cases}$$

C.A. Downing, D.A. Stone & MEP, PRB 84, 155437 (2011)
Wavefunction components and probability densities for the first two confined $m=1$ states in the Lorentzian potential

C.A. Downing, D.A. Stone & MEP, PRB 84, 155437 (2011)
Relevance of the Lorentzian potential

STM tip above the graphene surface
STM tip above the graphene surface

\[ U_{\text{STM}}(r) \approx \frac{e Q_{\text{tip}}}{4\pi \kappa} \left( \frac{1}{\sqrt{r^2 + (h_1 - h_2)^2}} - \frac{1}{\sqrt{r^2 + (h_1 + h_2)^2}} \right) \]

\[ V_0 = \frac{e Q_{\text{tip}}}{4\pi \kappa \hbar v_F} \frac{2h_1}{h_2^2 - h_1^2} \]

\[ d = \frac{h_2^2 - h_1^2}{\pi h_1} \ln \left( \frac{h_2 + h_1}{h_2 - h_1} \right) \]

Coulomb impurity + image charge in a back-gated structure
Exactly-solvable smooth quantum rings

\[ V(r) = \frac{V_0 (r/d)^k}{1 + (r/d)^{2(k+1)}} \]

\[ \eta(r) = c_1 \, _2F_1\left( p_1, -p_1; q_1; \frac{1}{1 + \xi^{-1}} \right) + c_2 \, _2F_1\left( p_2, -p_2; q_2; \frac{1}{1 + \xi} \right), \]

\[ q_1 = \frac{k + 2m + 2}{2k + 2}, \quad q_2 = \frac{k - 2m}{2k + 2}, \quad \xi = \left( \frac{r}{d} \right)^{2k+2}. \]

\[ p_{1,2} = \frac{V_0 d}{2k + 2} = N + q_{1,2} \quad - \text{should be integer.} \]
Exactly-solvable smooth quantum rings
Numerical experiment: $300 \times 200$ atoms graphene flake, Lorentzian potential is decaying from the flake center (on-site energy is changing in space)

Potential is centred at an “A” atom.

Potential is centred at a “B” atom.
Numerical experiment: $300 \times 200$ atoms graphene flake, Lorentzian potential is decaying from the flake center (on-site energy is changing in space)

Potential is centred at the hexagon centre.  
Potential is centred in the centre of a bond.
Numerical experiment: $300 \times 200$ atoms graphene flake, Lorentzian potential is decaying from the flake center (on-site energy is changing in space)

Variable-phase method + Levinson’s theorem can be used to find “optimal strength” for any short-range potential

\[ \frac{d}{dr} \delta_m(r) = \frac{\pi r}{2} p(r) \left[ \frac{1}{k - V(r)} \frac{dV(r)}{dr} \left( q(r) - \frac{m}{r} p(r) \right) + \left( V(r)^2 - 2kV(r) \right) p(r) \right], \]

\[ p(r) = J_m(kr) \cos(\delta_m(r)) - N_m(kr) \sin(\delta_m(r)), \quad \delta_m(0) = 0 \]

\[ q(r) = J'_m(kr) \cos(\delta_m(r)) - N'_m(kr) \sin(\delta_m(r)), \quad \delta_m = \lim_{r \to \infty} \delta_m(r) \]

Zero-energy states \((k \to 0)\): \( \delta_m = n\pi, \quad n = 1, 2, 3... \)

\[ V(r) = -V_0/[1 + (r/d)^2] \quad V(r) = -V_0/[1 + (r/d)^3] \]

Experimental manifestations

PRB 82, 165445 (2010)
Klaus Ensslin & Co
Experimental manifestations
Creating and probing electron whispering-gallery modes in graphene

Yue Zhao, Jonathan Wyrick, Fabian D. Natterer, Joaquin F. Rodriguez-Nieva, Cyprian Lewandowski, Kenji Watanabe, Takashi Taniguchi, Leonid S. Levitov, Nikolai B. Zhitelev, Joseph A. Stroscio

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?? \( \rho(r) \propto 1/(d + r^2/2R) \)

\( \varepsilon u(r) = \left( -i\sigma_x \partial_r + \frac{m+1/2}{r} \sigma_y + kr^2 \right) u(r) \)
Crommie experiments

– Ca dimers on graphene have two states, charged and uncharged
– They can be moved around by STM tip, and the charge states can be manipulated
– Thus, one can make artificial atoms and study them via tunneling spectroscopy

Features not explained by the atomic collapse theory

- The resonance is sensitive to doping.
- Sometimes, it occurs on the wrong side with respect to the Dirac point.
- Distance dependence of peak intensity.
How to combat precise tailoring of potential?

-- What happens to massless Dirac fermions when you add a magnetic flux?

-- Can we get better control of zero-energy bound states?

-- Any interesting physical or mathematical effects?
Adding a magnetic flux

2D-DE

\[ \hat{H} = v_F \sigma \cdot \hat{p} + V(r) \]

Introduce vector potential via modification of momentum

\[ \hat{p} \rightarrow \hat{p} + eA \]

Choose flux

\[ A_\theta(r) = \frac{\hbar f}{e r}, \quad f = \frac{\Phi}{\Phi_0} \]

\[ (\Phi_0 = \hbar/e) \]

Resulting in a relabeling of quantum number

\[ m \rightarrow \tilde{m} = m + f \]
Quantum dots with a magnetic flux

\[ U(r) = \frac{-U_0}{1 + r^2/d^2} \]

Solutions with short-range asymptotics

\[ \chi_A \sim r|\tilde{m}| \]

\[ U_0d = 2n + p, \quad n = 0, 1, 2... \quad p = 1 + |\tilde{m}| + |1 + \tilde{m}|. \]

FIG. 3: Plot of density $|\Psi|^2 d^2$ as a function of distance measured in units of $d$, for a dot with $U_0d = 8$ and (left-to-right) parameters $(\tilde{m}, n) = (1, 2), (2, 1)$ and $(3, 0)$.

Zero-energy states – So what?

- Non-linear screening favors zero-energy states. Could they be a source of minimal conductivity in graphene for a certain type of disorder?
- Could the BEC of zero-energy bi-electron vortices provide an explanation for the Fermi velocity renormalization in gated graphene?
- Where do electrons come from in low-density QHE experiments?

Novoselov et al., PNAS 102, 10451 (2005)  
Elias, …, Geim, Nature Physics 7, 201 (2011)
QHE experiments

Nicholas group, PRL 111, 096601 (2013)

Also seen by many other groups:
Janssen et. al, PRB 83, 233402 (2011)
Benoit Jouault (2011-2015)
A. Lebedev etc…

Apparent difference in carrier densities without B and in a strong magnetic field.
Reservoir of “silent” carriers?
The puzzle of the mass of an exciton in graphene

Excitonic gap & gost insulator (selected papers):

D. V. Khveshchenko, PRL. 87, 246802 (2001).
and many-many others (Guinea, Lozovik, Berman etc…)

Warping => angular mass: Entin (e-h, K≠0), Shytov (e-e, K=0)

Massless particles do not bind!
Or do they?
Excitonic gap has never been observed!

Experiment: Fermi velocity renormalization...

\[ m_c = \frac{\hbar}{2\sqrt{\pi n}} / v_F^* \]

?? \[ v_F(n) = v_F(n_0) \left[ 1 + \frac{\alpha}{8\varepsilon_G} \ln(n_0/n) \right] \]

Elias, …, Geim, Nature Physics 7, 201 (2011)
Mayorov et al., Nano Lett. 12, 4629 (2012)
Two-body problem – construction

Construct wavefunction

$$
\begin{pmatrix}
\psi_{A,A}(\mathbf{r}_1, \mathbf{r}_2) \\
\psi_{A,B}(\mathbf{r}_1, \mathbf{r}_2) \\
\psi_{B,A}(\mathbf{r}_1, \mathbf{r}_2) \\
\psi_{B,B}(\mathbf{r}_1, \mathbf{r}_2)
\end{pmatrix}
$$

Electron-hole

$$
H_{e-h} = v_F \begin{pmatrix}
V(r) & p_{x_e} - ip_{y_e} & -p_{x_h} + ip_{y_h} & 0 \\
p_{x_e} + ip_{y_e} & V(r) & 0 & -p_{x_h} + ip_{y_h} \\
-p_{x_h} - ip_{y_h} & 0 & V(r) & p_{x_e} - ip_{y_e} \\
0 & -p_{x_h} - ip_{y_h} & p_{x_e} + ip_{y_e} & V(r)
\end{pmatrix}
$$

Electron-electron

$$
H_{e_1-e_2} = v_F \begin{pmatrix}
V(r) & p_{x_{e_1}} - ip_{y_{e_1}} & p_{x_{e_2}} - ip_{y_{e_2}} & 0 \\
p_{x_{e_1}} + ip_{y_{e_1}} & V(r) & 0 & p_{x_{e_2}} - ip_{y_{e_2}} \\
p_{x_{e_2}} + ip_{y_{e_2}} & 0 & V(r) & p_{x_{e_1}} - ip_{y_{e_1}} \\
0 & p_{x_{e_2}} + ip_{y_{e_2}} & p_{x_{e_1}} + ip_{y_{e_1}} & V(r)
\end{pmatrix}
$$
Two body problem – free solutions

Diagonalize

\[
E = \pm v_F \left( p_{x_1}^2 + p_{y_1}^2 \right)^{1/2} \pm v_F \left( p_{x_2}^2 + p_{y_2}^2 \right)^{1/2}
\]

Centre-of-mass (COM) and relative coordinates

\[
X = (x_1 + x_2)/2, \quad Y = (y_1 + y_2)/2
\]

\[
x = x_1 - x_2, \quad y = y_1 - y_2
\]

So equivalently

\[
E/\hbar v_F = \pm \left( (K_X/2 + k_x)^2 + (K_Y/2 + k_y)^2 \right)^{1/2}
\]

\[
\pm \left( (K_X/2 - k_x)^2 + (K_Y/2 - k_y)^2 \right)^{1/2}
\]

COM and relative ansatz

\[
\Psi_i(R, r) = \exp(iK \cdot R)\psi_i(r)
\]

COM momentum K=0, system reduces to 3 by 3 matrix

\[
\begin{bmatrix}
\frac{U(r)-E}{\hbar v_F} & \partial_r + \frac{m}{r} & 0 \\
2 \left( -\partial_r + \frac{m-1}{r} \right) & \frac{U(r)-E}{\hbar v_F} & -2 \left( \partial_r + \frac{m+1}{r} \right) \\
0 & \partial_r - \frac{m}{r} & \frac{U(r)-E}{\hbar v_F}
\end{bmatrix}
\begin{bmatrix}
\phi_1(r) \\
\phi_2(r) \\
\phi_4(r)
\end{bmatrix}
= 0,
\]

(4)
Two body problem – bound states

\[
\begin{bmatrix}
\frac{U(r) - E}{\hbar v_F} & \partial_r + \frac{m}{r} & 0 \\
2 \left(-\partial_r + \frac{m-1}{r} \right) & \frac{U(r) - E}{\hbar v_F} & -2 \left(\partial_r + \frac{m+1}{r} \right) \\
0 & \partial_r - \frac{m}{r} & \frac{U(r) - E}{\hbar v_F}
\end{bmatrix}
\begin{bmatrix}
\phi_1(r) \\
\phi_2(r) \\
\phi_4(r)
\end{bmatrix} = 0,
\]

Only binding at Dirac point energy \( E=0 \), consider interaction potential

\[
U(r) = -\frac{U_0}{1 + \left(\frac{r}{d}\right)^2}
\]

Angular momentum

\[
m = 0, \pm 1, \pm 2, ...
\]

Gauss hypergeometric

\[
f(\xi) = \, _2F_1 \left( -n, -n + \frac{1}{2} \frac{U_0 d}{\hbar v_F}; |m| + 1; \frac{\xi}{1+\xi} \right)
\]

useful to define

\[
\eta = \frac{|m| + 1 + \sqrt{|m|^2 + 1}}{2},
\]
Two-body problem – exactly solvable model

\[ \frac{U_0 d}{\hbar \nu_F} = \frac{300}{137} \frac{1}{\epsilon r_0} = 4(n + \eta), \quad n = 0, 1, 2... \]

\[ \eta = \frac{|m| + 1 + \sqrt{|m|^2 + 1}}{2} \]

1. Length scale \( d \) of the order of 30 nm due to necessity of gate
2. Cut-off energy depends on geometry and differs strongly for monolayer graphene or interlayer exciton in spatially separated graphene layers
3. Results do not depend on the sign of the interaction potential

1. Monolayer vortex
   Cut-off comes from
   Ohno strength of 11.3 eV,
   thus \( r_0 = 0.04 \text{nm} \)

2. Interlayer exciton
   Cut-off comes from interlayer spacing of \( r_0 = 1.4 \text{nm} \)

\( U_0 = \frac{e^2}{4\pi \varepsilon_0 \epsilon r_0^{-1}} \)

\( \epsilon = 3.2 \)

Nb assuming BN with relative permittivity of \( \epsilon = 3.2 \)
Exactly solvable model – two systems

1. Monolayer exciton or e-e pair

\[ U_{0d} = 515.39\ldots \]

\[(m, n) = (128, 0), \text{ size } <r> = 1.006 \text{ d}\]
\[(m, n) = (127, 1), \text{ size } <r> = 1.018 \text{ d}\]
\[(m, n) = (126, 2), \text{ size } <r> = 1.030 \text{ d}\]

2. Interlayer exciton

\[ U_{0d} = 14.66\ldots \]

\[(m, n) = (3, 0), \text{ size } <r> = 1.433 \text{ d}\]
\[(m, n) = (2, 1), \text{ size } <r> = 2.639 \text{ d}\]
\[(m, n) = (1, 2), \text{ size } <r> = 4.415 \text{ d}\]
Two-body problem – exactly solvable model

Results for $d = 100$ nm, monolayer graphene, repulsive interaction

**FIG. 1:** Radial probability densities for the pair states with quantum numbers $(n, m) = (0, 429), (1.428)$ left-to-right.

**FIG. 2:** A plot of the average size of the pair state as a function of quantum number $m$. 

Numerics – expansion in Fourier-Bessel series

When $K=0$, $E=0$, one can reduce the problem to a single differential equation in one of the four wavefunction components, which can be solved by expanding in a Fourier-Bessel series

$$
\phi_2(r) = \frac{\sqrt{2}}{L} \sum_{n=1}^{\infty} \frac{a_n}{J_{m+1}(\alpha_n)} J_m(\alpha_n \frac{r}{L}),
$$

where $\alpha_n$ are roots of the first Bessel function and $L$ is a large distance over which we satisfy orthonormality.

To find the parameters of the potential required for the existence of zero-energy states, one needs to solve the resulting secular equation.
Electron-hole puddles in disordered graphene or droplets of two-particle vortices?

Is it a step in the on-going search for Majorana fermions in condensed matter systems?

“Majorana had greater gifts than anyone else in the world. Unfortunately he lacked one quality which other men generally have: plain common sense.” (E. Fermi)

Ettore Majorana
1906 - ?
Practical applications?

Graphene—A rather ordinary nonlinear optical material

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Essentially, all the electrons residing further away from the Dirac point hardly contribute to nonlinearity at all, but they are needed to keep the Fermi level high enough to mitigate the loss due to band-to-band absorption. Clearly, absence of a real bandgap (rather than one induced by blocking the absorption) is a handicap that seems to have no remedy.

Remedy – a reservoir of charged vortices at the Dirac point.
Highlights
Highlights

Contrary to the widespread belief electrostatic confinement in graphene and other 2D Weyl semimetals is indeed possible!

Several smooth fast-decaying potential have been solved exactly for the 2D Dirac-Weyl Hamiltonian.

Precisely tailored potentials support zero-energy states with non-zero values of angular momentum (vortices). The threshold in the effective potential strength is needed for the vortex formation.

An electron and hole or two electrons (holes) can also bind into a zero-energy vortex reducing the total energy of the system.

The existence of zero-energy vortices explains several puzzling experimental results in gated graphene.

Confined modes might also play a part in minimum conductivity (puddles)?
Variable-phase method: Scattering cross-sections

\[
\zeta = \frac{4}{k} \sum_{m=-\infty}^{\infty} \sin^2(\delta_m), \quad \zeta_T = \frac{2}{k} \sum_{m=-\infty}^{\infty} \sin^2(\delta_{m+1} - \delta_m)
\]

\[
k\zeta_m = \sin^2(\delta_m)
\]

for \( V(r) = \frac{-V_0}{1 + (r/d)^3} \)

(a) \(V_0d = 1.00\) and critical \(V_0d = 2.27\). We show results for \(m = 0,1,2\), corresponding to the solid line (red), dashed line (blue) and dotted line (green) respectively.