Anderson (de)localization of Dirac fermions in graphene with resonant scatterers

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PRL **104**, 076802 (2010) arXiv:1006:3299

Landau Days, 21 June 2010

Outline

Introduction

- Model
- Experimental motivation
- Transport in clean graphene

2 Single strong impurity

- General formalism
- S-wave approximation
- S- & p-wave scattering

3 Many resonant scatterers

- General formalism
- Resonant scalar impurities
- Vacancies

Model Experimental motivation Transport in clean graphene

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Introduction

Model

Single strong impurity Many resonant scatterers

Clean graphene model



Tight-binding approximation

- two sublattices: A. B
- two valleys: K, K'
- linear dispersion: $\varepsilon = v_0 |\mathbf{p}|$
- massless Dirac Hamiltonian:

$$H = v_0 \boldsymbol{\sigma} \mathbf{p} \qquad \boldsymbol{\sigma} = \{\sigma_x, \sigma_y\}$$

- velocity: $v_0 \approx 10^8 \text{ cm/s}$
- band width: $\Delta \sim 1 \text{ eV}$

Model Experimental motivation Transport in clean graphene

Ballistic setup



- rectangular sample with dimensions $L \times W$
- large aspect ratio: $W \gg L$
 - \implies boundary conditions (edge modes) irrelevant
- zero energy (Dirac point)
- ideal contacts
- perfect metallic leads (highly doped regions of graphene)

Model Experimental motivation Transport in clean graphene

Ballistic transport experiment

Danneau et al. '07

Setup

- Rectangular sample
- Temperature 4.2 ÷ 30 K
- Large aspect ratio W/L = 24
- Ballistic limit $L \sim 200 \text{ nm}$

At the Dirac point

• Conductance $G(\epsilon = 0) \approx \frac{4e^2}{\pi h} \frac{W}{L}$ • Fano factor $F(\epsilon = 0) \approx 1/3$



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Electron transport in the clean sample



ransport properties
ullet vertical momentum p is conserved
• transmission probability $T = t ^2 = \frac{1}{\cosh^2 pL}$
• conductance $G = \frac{4e^2 W}{h} \int \frac{dp}{2\pi} T = \frac{4e^2}{\pi h} \frac{W}{L}$
• Fano factor $F = 1 - \frac{\int dp T^2}{\int dp T} = \frac{1}{3}$
• Distribution of transmission probabilities $P(T) = \frac{W}{\pi} \left \frac{dp}{dT} \right = \frac{W}{2\pi L} \frac{1}{T\sqrt{1-T}}$

Model Experimental motivation Transport in clean graphene

Green functions formalism

- Green functions: $G^{R,A} = (\epsilon \pm i0 H)^{-1}$
- Velocity operator: $\mathbf{v} = \partial H / \partial \mathbf{p} = v_0 \boldsymbol{\sigma}$
- Transmission moments (generalized Kubo formula) Tr $T^n = \text{Tr}[v_x G^R(0, L) v_x G^A(L, 0)]^n$



Model Experimental motivation Transport in clean graphene

Generating function

Matrix Green function [Nazarov '94]

$$\check{G} = egin{pmatrix} \epsilon + i0 - H & -\delta(x)v_x\sinrac{\phi}{2} \ -\delta(x-L)v_x\sinrac{\phi}{2} & \epsilon - i0 - H \end{pmatrix}^{-1}$$

Generating function (free energy)

$$\mathcal{F}(\phi) = \mathbf{Tr} \log \check{G}^{-1}(\phi)$$
Conductance: $G = -\frac{2e^2}{h} \left. \frac{\partial^2 \mathcal{F}}{\partial \phi^2} \right|_{\phi=0}$
Fano factor: $F = \frac{1}{3} - \frac{2}{3} \left. \frac{\partial^4 \mathcal{F}/\partial \phi^4}{\partial^2 \mathcal{F}/\partial \phi^2} \right|_{\phi=0}$

Clean graphene

$$\mathcal{F}_0(\phi)=-rac{W\phi^2}{\pi L}, \qquad G=rac{4e^2}{\pi h}rac{W}{L}, \qquad F=rac{1}{3}$$

Anderson (de)localization in graphene with resonant scatterers

General formalism -wave approximation - & p-wave scattering

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General formalism S-wave approximation S- & p-wave scattering

Single strong impurity: numerics Bardarson, Titov, Brouwer '09



General formalism

Generating function

$$\mathcal{F}(\phi) = \mathbf{Tr}\log(\check{G}_0^{-1} - V) = \mathcal{F}_0 + \mathbf{Tr}\log(1 - \check{G}_0 V)$$

Small impurity \Rightarrow G_0 at coincident points \Rightarrow diverge!

How to resolve? Introduce T-matrix!

$$T = V(1 - gV)^{-1} \text{ with } g(\mathbf{r}) = -\frac{i\sigma\mathbf{r}}{2\pi r^2} \leftarrow \text{ Green function of infinite graphene}$$

$$\delta \mathcal{F} = \mathbf{Tr} \log[1 - gV - (\check{G}_0 - g)V] = \mathbf{Tr} \log[1 - (\check{G}_0 - g)T] + \mathbf{Tr} \log[1 - gV]$$

With regularized Green function $\check{G}_{reg}(\mathbf{r}) = \lim_{\mathbf{r}' \to \mathbf{r}} \left[\check{G}_0(\mathbf{r}, \mathbf{r}') - g(\mathbf{r} - \mathbf{r}')\right]$ $\delta \mathcal{F} = \log \det[1 - \check{G}_{reg}(\mathbf{r}) T] \leftarrow \text{just } 2 \times 2 \text{ determinant!}$

General formalism S-wave approximation S- & p-wave scattering

Scattering of Dirac fermions



Scattering state

$$egin{aligned} \psi &= e^{ikx} inom{1}{1} + rac{f(\phi)}{\sqrt{-ir}} e^{ikr} inom{1}{e^{i\phi}} \ f(\phi) &= -\sqrt{rac{k}{2\pi}} \langle \mathbf{k}' | T | \mathbf{k}
angle \end{aligned}$$

s-wave scattering $T = \ell \leftarrow \text{ scattering length}$ $T = -\lim_{k \to 0} \sqrt{\frac{2}{\pi k}} \int_{-\pi}^{\pi} d\phi f(\phi) \begin{pmatrix} 1 & 0\\ 0 & e^{i\phi} \end{pmatrix}$ Cross section: $\Lambda = k\ell^2/2$

Sharp impurity [cf. Novikov '07]

$$U(r) = \begin{cases} V, & r < R\\ 0, & r > R \end{cases}$$

$$\ell = 2\pi R \frac{J_1(VR)}{J_0(VR)} \simeq 2\pi R \tan(VR - \pi/4)$$

General formalism S-wave approximation S- & p-wave scattering

Single strong impurity: s-wave approximation



Correction to conductance

$$\delta G = rac{32 e^2}{\pi^2 h} \left[rac{16 L^2}{\ell^2} + rac{1}{\sin^2(\pi x/L)}
ight]^{-1}$$

General formalism S-wave approximation S- & p-wave scattering

Single strong impurity: s-wave + p-wave



Include two channels in the T-matrix $T = \begin{pmatrix} \ell & 0 \\ 0 & \ell_1 \end{pmatrix} \quad \text{with} \quad \ell = 2\pi R \frac{J_1(VR)}{J_0(VR)} \quad \ell_1 = 2\pi R^3 \frac{J_2(VR)}{J_1(VR)}$

General formalism Resonant scalar impurities /acancies

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General formalism

Generating function

 $\mathcal{F}(\phi) = \mathcal{F}_0 + \mathbf{Tr} \log(1 - \check{G}_0 V) \quad ext{ with } \quad V = \sum_n \, V_n(\mathbf{r})$

Unfolding

$$\mathcal{F}(\phi) = \mathcal{F}_0 + \mathbf{Tr}\log(1-\hat{G}_0\,\hat{V}) = \mathcal{F}_0 + \mathbf{Tr}\log[1-(\hat{G}_0-g)\,\hat{T}]$$

 $\hat{G}_0 \implies N \times N$ matrix with all elements equal to \check{G}_0 $\hat{V} = \text{diag}\{V_1, V_2, \dots, V_N\}$ $\hat{T} = \text{diag}\{T_1, T_2, \dots, T_N\}$

Small impurities (s-wave scattering)

$$\begin{array}{ll} \mathsf{Regularized} \ \mathsf{Green} \ \mathsf{function} \ \ \hat{G}_{\mathsf{reg}} = \begin{cases} \check{G}_{\mathsf{reg}}(\mathbf{r_n}), & n = m, \\ \check{G}_0(\mathbf{r_n}, \mathbf{r_m}), & n \neq m \end{cases} \end{array}$$

 $\delta \mathcal{F} = \log \det(1 - \hat{G}_{\mathsf{reg}} \hat{T}) \leftarrow 2N \times 2N$ determinant!

General formalism Resonant scalar impurities Vacancies

Resonant scalar impurities

At resonance

 $T = \ell \to \infty \quad \Rightarrow \quad \delta \mathcal{F} = \log \det G_{reg}$

Conductance

$$G = \frac{4e^2}{\pi h} \left[\frac{W}{L} + \frac{2}{\pi} \operatorname{Tr} M^{-1} M^{-T} \right] \qquad M = \begin{pmatrix} A & B \\ B^{\dagger} & -A^T \end{pmatrix}$$
$$A_{mn} = \frac{1}{\sin \frac{\pi}{2L} [x_m + x_n + i(y_m - y_n)]} \qquad A = A^{\dagger}$$
$$B_{mn} = \frac{1 - \delta_{mn}}{\sin \frac{\pi}{2L} [x_m - x_n + i(y_m - y_n)]} \qquad B = -B^T$$

Symmetry class DIII

General formalism Resonant scalar impurities Vacancies

Resonant scalar impurities: numerics



Weak antilocalization in class DIII $\frac{d\bar{\sigma}}{d\log L} = 2 - \frac{2}{\bar{\sigma}} + O(\bar{\sigma}^{-2}) \qquad G = \frac{\sigma W}{L} \qquad \sigma = \frac{4e^2}{\pi h}\bar{\sigma}$ $\sigma = \frac{4e^2}{\pi h}(\log nL^2 - \log\log nL^2)$

General formalism Resonant scalar impurities Vacancies

Vacancies



Strong on-site potential \Leftrightarrow vacancy

$$T_A = rac{\ell}{2} egin{pmatrix} 1 & 0 & 0 & -e^{i heta} \ 0 & 0 & 0 & 0 \ -e^{-i heta} & 0 & 0 & 1 \ \end{pmatrix} \qquad T_B = rac{\ell}{2} egin{pmatrix} 0 & 0 & 0 & 0 \ 0 & 1 & e^{i heta} & 0 \ 0 & e^{-i heta} & 1 & 0 \ 0 & 0 & 0 & 0 \ \end{pmatrix}$$

T matrix projects on sublattice (A or B) and on direction θ in valleys

Resonance: $\ell \to \infty$

General formalism Resonant scalar impurities Vacancies

Conductance with vacancies

$$G = \frac{4e^2}{\pi h} \left\{ \frac{W}{L} + \pi \operatorname{Tr}[K, Y](K + K^T)^{-1}[K^T, Y](K + K^T)^{-1} \right\}$$

$$K_{mn} = \frac{e^{\frac{i\pi}{4}(\zeta_m - \zeta_n) + \frac{i}{2}(\theta_m - \theta_n)}}{\sin\frac{\pi}{2L}[\zeta_m x_m + \zeta_n x_n + i(y_m - y_n)]} \qquad K = K^{\dagger}$$
$$Y = L^{-1} \operatorname{diag}\{y_1, y_2, \dots, y_N\}$$
$$\zeta_i = \pm 1 \text{ and } \theta_i \text{ are sublattice and color of } ith vacancy}$$

Symmetry class BDI [Gade & Wegner '91] $\frac{d\bar{\sigma}}{d\log L} = 0 \qquad \text{perturbatively in ALL loop orders!}$

General formalism Resonant scalar impurities Vacancies

Vacancies: preliminary numerics (only one color)



- Unstable fixed point for $n_B = n_A$ (probably conductivity saturates)
- Stable fixed point for $n_B \neq n_A$ with $\sigma \approx \frac{4e^2}{\pi h}$



- Novel efficient approach to studying transport in strongly disordered systems is developed
- In the ory is applied to graphene with resonant scatterers
- Resonant scalar impurities lead to antilocalization
- Vacancies establish various critical regimes
- Results agree with the symmetry analysis based on the nonlinear sigma model but extend beyond its applicability

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