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Voltage-driven quantum oscillations in graphene

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Abstract. We predict unusual (for non-relativistic quantum mechanics) electron states in graphene, which are *localized within* a finite-width potential barrier. The density of localized states in the sufficiently high and/or wide graphene barrier exhibits a number of singularities at certain values of the energy. Such singularities provide *quantum oscillations* of both the transport (e.g. conductivity) and thermodynamic properties of graphene—when increasing the barrier height and/or width, similarly to the well-known Shubnikov–de-Haas (SdH) oscillations of conductivity in pure metals. However, here the SdH-like oscillations are driven by an *electric* field instead of the usual magnetically driven SdH-oscillations.

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Contents

1. Introduction

The Shubnikov–de-Haas (SdH) effect, i.e., the oscillations of the magneto-resistance of metals when increasing an external magnetic field, was one of the first macroscopic manifestations of the quantum-mechanical nature of matter. The key to understanding this remarkable phenomenon was pointed out by Landau and Onsager and it is described in many textbooks on solid state physics (see, e.g. [1]). Namely, electrons in the conduction band of a metal in a strong magnetic field behave like simple harmonic oscillators. The resulting energy spectrum is made up of equidistant Landau levels separated by the cyclotron energy. The density of electron states has singularities at the Landau levels. When the magnetic field is changed, the positions of the Landau levels move and pass periodically through the Fermi energy. As a result, the population of electrons at the Fermi surface also oscillates and, in turn, leads to quantum oscillations of the transport and thermodynamic properties of a metal. The quantum oscillations also manifest themselves in the thermoconductivity, magnetization, sound attenuation, magnetostriction and other quantities.

These quantum oscillations are pronounced in conductors with a long mean free path of charge carriers. This can occur in pure metals, semimetals, and narrow band-gap semiconductors at low temperatures, as well as in graphene, a one-atom-thick sheet of carbon. The SdH oscillations of the magneto-resistivity were observed in graphene [2, 3] soon after its discovery [4]. Due to the monolayer honeycomb-lattice structure of graphene, its electrons obey a massless Dirac-like equation (see, e.g. [3, 5, 6]). This is responsible for the unusual properties of graphene. In particular, the Landau levels in graphene are not equidistant and these influence the period of the SdH oscillations [7]. Graphene has another striking property: it has unusual relativistic effects which are counterintuitive for electrons with speeds much slower than the speed of light [8]. For example, it has been recently shown [5] that graphene could be used for experimentally testing the so-called Klein paradox [9]. This quantum-mechanical effect of relativistic particles penetrating through high and wide potential barriers can be illustrated with massless Dirac fermions in graphene with a potential barrier controlled by an applied voltage. A high potential energy barrier in graphene, as was shown in [10], can also act as an unusual electron lens, due to the negative refraction of electron waves at the edge of the barrier, in analogy to the negative refraction of 3D [11] and 2D [12, 13] electromagnetic waves.

Our goal here is to show that, due to the Dirac-like Hamiltonian of graphene with a potential energy barrier, quantum oscillations similar to the SdH effect can be observed *without an applied magnetic field*. Below we prove that the density of electron states in a graphene sheet with a potential barrier should display quantum oscillations if the strength of the barrier (i.e. the product $V_0 D$ of the barrier's height V_0 and width D) exceeds some threshold value. In these

oscillations, the barrier strength $V_0 D$, that can be controlled by a gate voltage, plays the same role as the external magnetic field in the SdH effect.

The quantum oscillations predicted here originate from a new type of electron states in graphene. Contrary to non-relativistic quantum mechanics, where localized states can only exist inside quantum wells, we find that the electron states in graphene can be localized *within the barrier*. The energy $E(q_y)$ of the localized states (versus the wavevector component q_y along the barrier) becomes *non-monotonic* if

$$V_0 D > \pi \hbar v_F,$$

(v_F is the Fermi velocity). We show that this produces singularities of the density of electron states for energies where $dE/dq_y = 0$. When the magnitude and/or width of the barrier changes, the locations of the singularities move and periodically cross the Fermi level, generating quantum oscillations of both thermodynamic and transport properties, e.g. of the conductance in the y-direction (along the barrier).

2. Electron states localized in a barrier

The tunnelling of relativistic particles through a finite-width potential barrier has recently been studied in [5, 14, 15]. Here, we consider another type of electron waves that propagate *strictly along* the barrier and *damp away from it*. Our analysis shows that a step-like barrier (i.e. a single edge of an infinitely wide barrier) does not support such electron waves, which would be an analogue to surface electromagnetic waves (plasmon-polaritons) at the interface between two different media. Therefore, even though the potential barrier in graphene could act as an electron lens [10], it *cannot* provide the perfect lensing (i.e. subwavelength image reconstruction) that is possible for Veselago's lens in optics [16]. However, as we show in this section, the electron waves in graphene can be localized inside *a finite-width* potential barrier.

We consider electron states in graphene with a potential barrier located in a single-layer graphene occupying the x–y-plane (see figure 1). For simplicity, we assume that the barrier $V(x)$ has sharp edges

$$V(x) = \begin{cases} 0, & |x| > D/2, \\ V_0, & |x| < D/2. \end{cases} \tag{1}$$

Electrons in monolayer graphene obey the Dirac-like equation,

$$\hat{H}\psi = i\hbar \frac{\partial \psi}{\partial t}, \quad \hat{H} = -i\hbar\, v_F\, \boldsymbol{\sigma} \cdot \boldsymbol{\nabla} + V(x), \tag{2}$$

where v_F is the Fermi velocity and $\sigma = (\sigma_x, \sigma_y)$ are Pauli matrices.

We seek stationary spinor solutions of the form,

$$\psi = \psi(x) \exp\left(-\frac{i}{\hbar} E t + iqy\right), \tag{3}$$

with energy E and momentum $\hbar q$ along the barrier. We focus on the states with

$$|q| > |\epsilon| \equiv |E|/\hbar v_F. \tag{4}$$

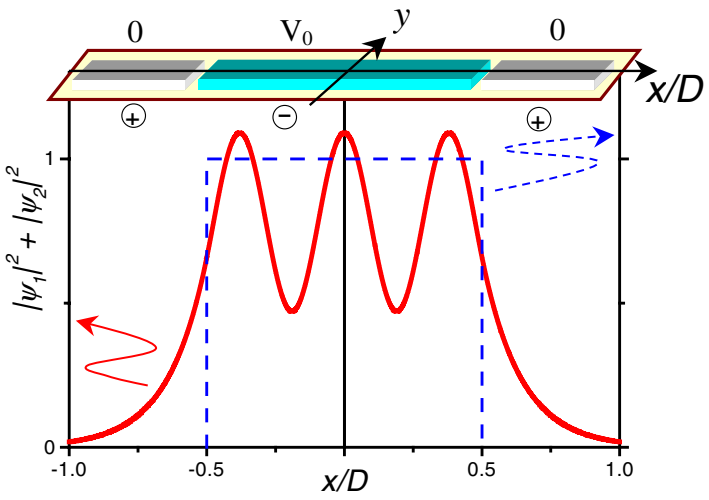

Figure 1. Top: geometry of the problem. A graphene sheet is placed under the voltage gates indicated by block rectangles. Bottom: potential energy barrier $V(x)$ in graphene (dashed blue line) and the probability distribution $W(x) = |\psi_1(x)|^2 + |\psi_2(x)|^2$ for the localized electron state at $qd = 3.5625$, $\epsilon D = 0.003$ and $\mathcal{V} = 9$ (red solid line).

In this case, the electron waves satisfying equation (2) damp away from the barrier, and the components ψ_1 and ψ_2 of the Dirac spinor can be written in the form

$$\psi_1(x) = \begin{cases} a\exp(k_x x), & x < -D/2, \\ b\exp(\mathrm{i}q_x x) + c\exp(-\mathrm{i}q_x x), & |x| < D/2, \\ d\exp(-k_x x), & x > D/2, \end{cases} \tag{5}$$

$$\psi_2(x) = \begin{cases} a\dfrac{\mathrm{i}\epsilon}{(k_x+q)}\exp(k_x x), & x < -D/2, \\ -b\exp(\mathrm{i}q_x x + \mathrm{i}\theta) + c\exp(-\mathrm{i}q_x x - \mathrm{i}\theta), & |x| < D/2, \\ \dfrac{-\mathrm{i}d\epsilon}{(k_x-q)}\exp(-k_x x), & x > D/2, \end{cases} \tag{6}$$

with real

$$k_x = (q^2 - \epsilon^2)^{1/2}$$

and

$$q_x = \left[\left(\epsilon - \frac{\mathcal{V}}{D}\right)^2 - q^2\right]^{1/2}.$$

Here $\mathcal{V} = V_0 D/\hbar v_\mathrm{F}$ is the effective barrier strength and $\tan\theta = q/q_x$.

Matching the functions $\psi_1(x)$ and $\psi_2(x)$ at the points $x = \pm D/2$, we obtain a set of four homogeneous algebraic equations for the constants a, b, c and d. Equating the determinant of this set to zero, we derive a dispersion relation for the localized electron states,

$$\tan(q_x D) = -\frac{k_x q_x}{(\mathcal{V}/D - \epsilon)\epsilon + q^2}. \tag{7}$$

A similar equation was obtained in [17] for non-propagating electron states in ribbons of graphene with armchair boundaries. Figure 1 illustrates the behaviour of the probability distribution $W(x)$ for a localized state. Note that $W(x)$ is an *even* function with *continuous derivative* $W'(x)$, in spite of the fact that each one of the functions $|\psi_1|^2$ and $|\psi_1|^2$ are not even (the chirality of the Dirac spinors) and both have discontinuous derivatives at the points $x = \pm D/2$.

The localized states can also be observed in either a 2D electron gas or graphene (e.g. [18]) when a voltage is applied to produce a potential well. In the 2D electron gas, for electrons with a quadratic dispersion law, this spectrum is

$$\mathcal{E}_n = y_n^2 + 4Q^2 - \mathcal{V},$$

where

$$\mathcal{E} = \frac{mD^2E}{2\hbar^2}, \quad \mathcal{V} = \frac{mD^2V_0}{2\hbar^2}, \quad Q = qD,$$

m is the electron mass. Here y_n is the nth root of the equation

$$y\tan(y) = (\mathcal{V} - y^2)^{1/2}$$

for even states, and

$$y\cot(y) = -(\mathcal{V} - y^2)^{1/2}$$

for odd states.

The spectrum equation (7) of localized states in graphene is shown by the solid black curves in figure 2, for dimensionless variables $Q = qD$ and $\mathcal{E} = \epsilon D$. This spectrum consists of an infinite number of branches $\mathcal{E}_n(Q)$. Each of these branches starts from the lines $\mathcal{E} = \pm|Q|$ (red solid straight lines in figure 1(b)) at

$$\mathcal{E} = \frac{\mathcal{V}}{2} - \frac{\pi^2 n^2}{2\mathcal{V}}$$

and tends asymptotically to the lines $\mathcal{E} = \mathcal{V} \pm Q$ (dashed red lines). Moreover, a particular branch of the spectrum starts at the point ($Q = 0$, $\mathcal{E} = 0$) and also tends to the line $\mathcal{E} = \mathcal{V} - Q$, with increasing Q.

The behaviour of different branches of the spectrum depends on the barrier strength $\mathcal{V}$. If $\mathcal{V} < \pi/2$, all branches satisfy $\mathcal{E} < 0$ (see inset in figure 2). Localized states with positive energies appear only for $\mathcal{V} > \pi/2$. When $\mathcal{V}$ increases, new branches in the spectrum with positive energies appear. When $\mathcal{V}$ is within the interval

$$\left(n + \tfrac{1}{2}\right)\pi < \mathcal{V} < \left(n + \tfrac{3}{2}\right)\pi,$$

the number of branches with $E > 0$ is $(n+1)$, $n = 1, 2, 3, \ldots$. We emphasize that each of the branches with positive energy has a maximum $\mathcal{E}_n^{\max}$ at a certain wavenumber $Q = Q_n^{\max}$. Near these points, the group velocity of localized electron waves tends to zero. This effect is similar to the stop-light phenomenon [19] found in various media, including superconductors [20].

Note that defect-induced localized electron states in graphene and the enhancement of conductivity due to an increase in the electron density of states localized near the graphene edges were recently reported [21]–[23]. Contrary to these examples, the electron states studied here are localized within the barrier and also these *are tunable*, i.e. the energy levels can be shifted by changing the barrier strength (e.g. via tuning a gate voltage).

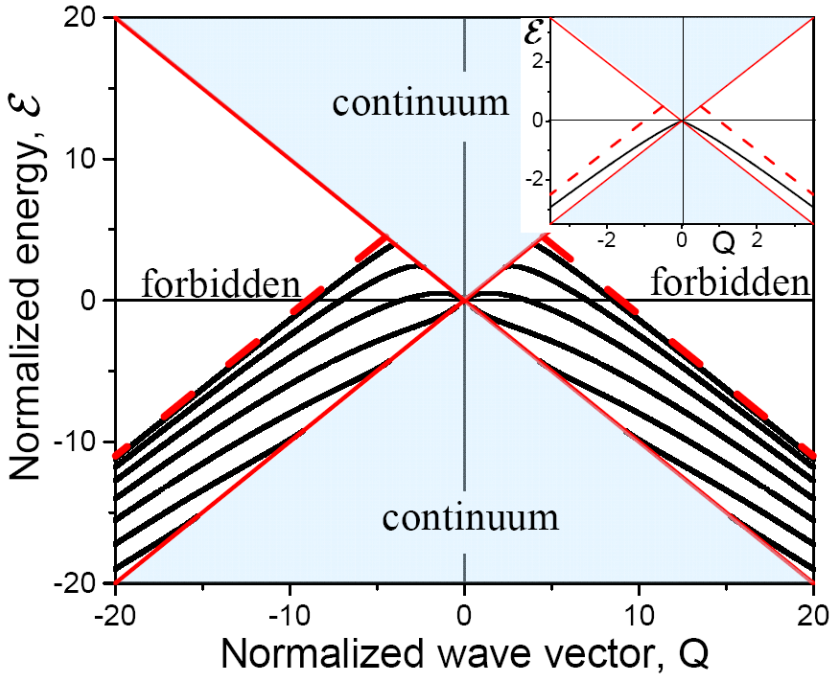

Figure 2. Electron spectrum in graphene obtained for $\mathcal{V} = 1$ (inset) and $\mathcal{V} = 9$ (main panel). The sea of delocalized states (continuum spectrum) is marked by the light-purple regions. The branches of the spectrum for localized states are shown by solid black curves between the straight solid and dashed red lines. There are no states in the forbidden (white) regions.

3. Density of localized electron states

To calculate the density $N(E)$ of electron states, we use the general formula $N(E) = \sum_\alpha \times \delta(E - E_\alpha)$, where α labels the quantum state and $\delta(x)$ is Dirac's delta-function. Using $\sum_\alpha \cdots = 2L_x L_y (2\pi)^{-2} \int_{-\infty}^{\infty} \mathrm{d}k_x\, \mathrm{d}k_y \cdots$ for a continuum spectrum, we derive

$$N_{\mathrm{cont}} = N_0 |\mathcal{E}|, \quad N_0 = \frac{L_x L_y}{\pi \hbar v_{\mathrm{F}} D}, \tag{8}$$

where L_x and L_y are the lengths of the graphene sheet in the x- and y-directions, respectively. For localized states, we obtain

$$N_{\mathrm{loc}}(\mathcal{E}) = 2N_0 \frac{D}{L_x} \sum_n \left| \frac{\mathrm{d}\mathcal{E}_n(Q)}{\mathrm{d}Q} \right|^{-1}_{\mathcal{E}_n(Q)=\mathcal{E}}. \tag{9}$$

Here n runs over the number of positive roots of the equation $\mathcal{E}(Q) = \mathcal{E}$.

The dimensionless density of states $N(\mathcal{E})/N_0$ is shown in figure 3. The localized electron states exhibit two types of peculiarities. First, increasing $\mathcal{E}$, the jumps or steps (each one of magnitude $2D/L_x$) in $N(\mathcal{E})/N_0$ occur at the points

$$\mathcal{E} = \frac{\mathcal{V}}{2} - \frac{\pi^2 n^2}{2\mathcal{V}},$$

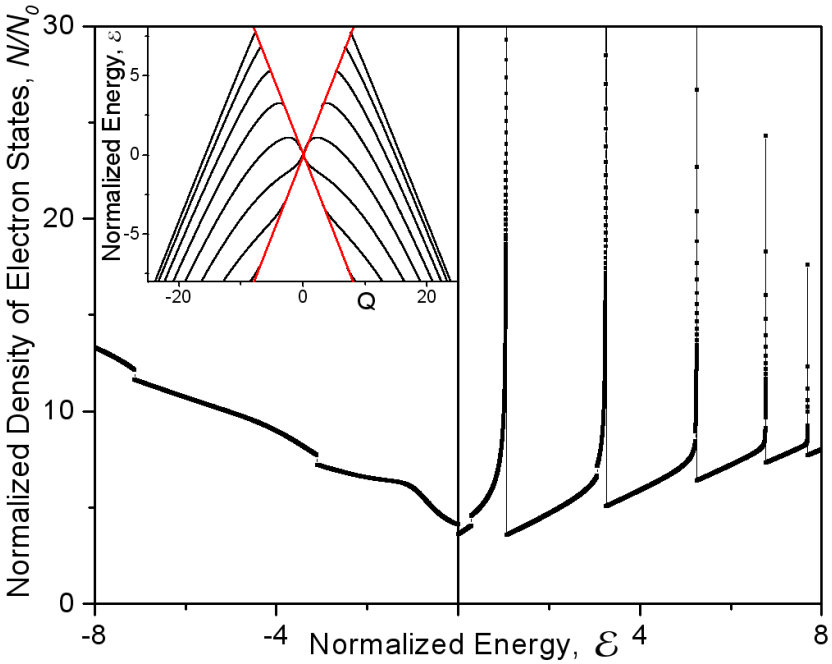

Figure 3. Dimensionless density of electron states $N(\mathcal{E})/N_0$ in graphene with a potential barrier, for $D/L_x = 0.5$ and $\mathcal{V} = 16$.

where new branches of the spectrum arise or disappear. More importantly, singularities are observed when $\mathcal{E} = \mathcal{E}_n^{\max}$, where $|\mathrm{d}\mathcal{E}_n/\mathrm{d}Q|^{-1}$ in equation (9) diverges.

The locations of the singularities shift when changing the barrier strength $\mathcal{V}$. Therefore, they periodically cross the Fermi level $\mathcal{E}_\mathrm{F}$. This produces quantum oscillations of the density of states at the Fermi energy. They are seen in figure 4, showing $N(\mathcal{E}_\mathrm{F})/N_0$ versus the effective barrier strength $\mathcal{V}$.

The periodic change in the number of electron states near the Fermi level, increasing the barrier strength (e.g. by varying a gate voltage), necessarily results in quantum oscillations of the transport and thermodynamic properties of graphene. For example, the conductance of graphene along the barrier qualitatively mimics the quantum oscillations of the density of electron states.

Figure 4 shows the quantum oscillations of the density of electron states in e-type graphene (with a positive Fermi energy). For p-type graphene, with $E_\mathrm{F} < 0$, quantum oscillations of the density of states at the Fermi level can also be observed, if the (now opposite-bias) applied voltage forms a *potential well instead of a barrier*. Indeed, the Dirac equation (2) is invariant with respect to the transformation: $E \to -E$, $V \to -V$, $x \to -x$ and $y \to -y$.

4. Conclusions

In conclusion, we predict an unusual type of electron states in graphene localized *within a potential barrier*. For barriers with sufficiently high magnitude and width, the density of localized states has singularities. This feature of localized states can result in quantum oscillations of the thermodynamic and transport properties (e.g. the conductance along the barrier) of graphene when changing the barrier strength (e.g. by varying a gate voltage). These

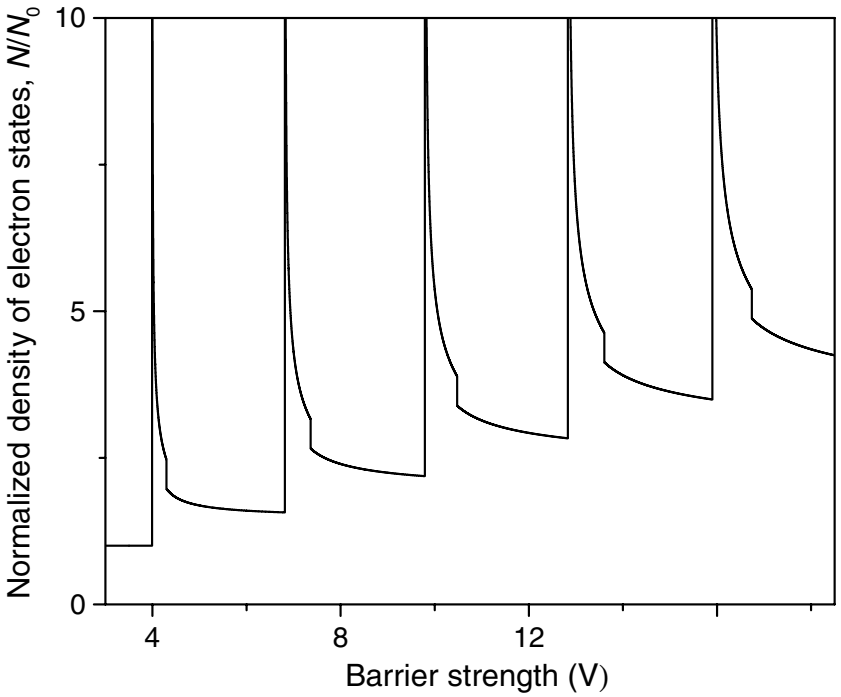

Figure 4. Dimensionless density of electron states $N(\mathcal{N})/N_0$ at the Fermi level versus the effective strength $\mathcal{V}$ of the potential barrier, for $D/L_x = 0.5$ and $\mathcal{E}_F = 1$.

electric-field driven quantum oscillations are similar to the SdH oscillations of conductivity, which are produced in standard metals when changing the external magnetic field.

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