Skipping and snake orbits of electrons: singularities and catastrophes

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Near the sample edge, or a sharp magnetic field step the drift of two-dimensional electrons in a magnetic field has the form of skipping/snake orbits. We show that families of skipping/snake orbits of electrons injected at one point inside a 2D metal generically exhibit caustics folds, cusps and cusp triplets, and, in one extreme case, a section of the butterfly bifurcation. Periodic appearance of singularities along the ±B-interface leads to the magneto-oscillations of nonlocal conductance in multi-terminal electronic devices.

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Skipping orbits have been introduced into physics of metals by Niels Bohr in the early studies of diamagnetism [1]. Skipping orbits also play a special role in the two-dimensional (2D) electron systems, where they determine the chiral current-carrying properties of the electron edge states [2] important for the formation of the quantum Hall effect [3]. Snake orbits have been discussed, first, in the context of the electrons propagation along domain walls in ferromagnetic metals [9, 10] and, later, used for channeling ballistic electrons in 2D semiconductors in a spatially alternating magnetic field [11–16], $B = B_{z} \sin \theta$. In isotropic 2D metals, where all electrons with energies close to the Fermi level revolve along cyclotron circles with the same radius, $R = pF/eB$, skipping and snake orbits have the form of consecutive circular segments matched by the specular reflection at the edge, or by the smooth continuity on the opposite sides of the ±B-interface, see Fig. 1. A close relation between these two families can be established [17] by folding a sheet of a 2D material (graphene [18] or hexagonal transition-metal dichalcogenide [19, 20] which can sustain sharp bends with the radius much smaller than the electron cyclotron radius) in a homogeneous magnetic field. Then, the electron path near the fold looks like a skipping orbit with circular segments alternating between the top and bottom layers, but when projected onto an unfolded sheet, the electron motion resembles the motion near a ±B-interface.

Below, we study bunching in the families of skipping and snake orbits of electrons injected into a 2D metal and singularities in the spatial distribution of electronic trajectories. Mathematically, such features originate from the singularities in the differentiable maps in Thom’s catastrophe theory [21, 22]. The list of stable singularities in 2D dynamical systems includes caustic folds (caustics) and cusps, whereas focus is the most famous unstable singularity. All of those are often encountered in ray optics [23]. While focusing of light is one of the widest-implemented physical phenomena, one often encounters optical caustics when observing sunlight sparkling on the sea, or starlight twinkling [25]. In electronics, observations of caustics and focusing are less common. In 2D systems, electron focusing requires designing potential lenses [26] and electrostatic mirrors [27] by tailoring semiconductor heterostructures. Caustics and fo-
cusing of surface-band electrons have also been observed in ‘corals’ built by the STM manipulation of atoms on noble metal surfaces [28]. Focusing has also been realised using a magnetic field. Magnetic focusing of electrons in the three-dimensional space has facilitated studies of Fermi surfaces of pure metals and semimetals [29–31]. Later, this magnetic focusing technique has lent its name to the nonlocal magnetotransport effect observed near the edge of a 2D electron gas in semiconductors [18, 19], where, inspirationally for this work, one family of caustics has been identified [5] for skipping orbits of electrons injected from the edge of a ballistic 2D electron system. Here, we demonstrate that caustic bunching is generic for snake/skipping orbits of electrons injected into a 2D metal at any distance $X_0 < 2R$ near the $\pm B$-interface/sample edge. As shown in Fig. 1, for $X_0 > R > \frac{1}{2}X_0$, the networks of caustics display a periodic appearance of individual cusps, which split into cusp triplets when $R > X_0$. In general, such crossover would happen via the formation of swallowtail singularities [23], but, uniquely for a sharp field step/sample edge, these two regimes are separated at $X_0 = R$ by the butterfly bifurcation [23] seen as a higher-intensity unstable singularity of the intensity.

For electrons isotropically injected into a 2D metal with an isotropic dispersion of electrons, at a point $(-X_0, 0)$ near the $\pm B$-interface/edge at $x = 0$, their trajectories can be parametrised using the angle $\theta$ (counted in the anticlockwise direction) between the initial velocities and $x$-axis. In Figure 1, these trajectories are drawn for $0 < \theta < 2\pi$, with a step of 0.1. For the orbits near the $\pm B$-interface/edge, these are the sequences of semicircles with the coordinates $r_n = (x_n, y_n)$, $x_n = \zeta_n + R \sin \varphi$, $\zeta_n = b^n (R \sin \theta - X_0)$, $y_n = \eta_n + R \cos \varphi$, $\eta_n = 2n \sqrt{R^2 - \zeta_0^2} - R \cos \theta$, where $n = 0, 1, 2, \ldots$ labels the number of times the trajectory arrived at the interface/edge at $x = 0$, angle $\varphi$ counted from the $y$-axis allows to describe all points on a single segment $(b^n R \sin \varphi < -\zeta_0$, for $n > 0)$, and $b = \pm 1$ for skipping/snake orbits. A sheet density, $\rho = \int \delta(r - r_n) d\varphi d\theta$, of such trajectories can be evaluated (using a sequence of substitutions), as

$$
\rho(r) = [1 - b^n \text{sign} x] \left| \frac{\partial F}{\partial \theta} \right|^{-1} \bigg|_{F=0},
$$

$$
F(x, y; \theta) \equiv (x - \zeta_n)^2 + (y - \eta_n)^2 - R^2.
$$

This density is singular along caustics $R_n = (u_n, v_n)$, where, simultaneously,

$$
\frac{\partial F}{\partial \theta} = 0; F = 0.
$$

This determines the equations for caustics,

$$
u_n = \zeta_n + R - \frac{c_n s}{\sqrt{1 + c_n^2}}, \quad c_n = \frac{2n - \tan \theta}{\sqrt{R^2 - \zeta_0^2}} - \tan \theta,
$$

$$
v_n = \eta_n + R - \frac{b^n s}{\sqrt{1 + c_n^2}}, \quad s = \text{sign}(\cos \theta),
$$

(3)

where we choose the sign ‘±’ and permitted range of $\theta$ using the requirement that

$$
\zeta_0 \sqrt{1 + c_n^2} \pm b^nc_n sR < 0.
$$

The density of trajectories is most singular in the vicinity of cusps $(u_c^n, v_c^n)$, which are characterised by the condition $\frac{\partial^2 F}{\partial \theta^2} = 0$, additional to Eq. (4). For strong magnetic fields, such that $X_0 > R > \frac{1}{2}X_0$, the periodically appearing cusps are illustrated in Fig. 1(a), with $u_c^n = X_0$ and the universal curving of caustics near the cusps,

$$
u_n - u_c^n \propto (v_n - v_c^n)^{3/2}.
$$

(4)

A very typical for cusps calculated semiclassically interference pattern is shown in the top inset. The y-positions of the cusps, $v_c^n$, are plotted in Fig. 1(c) against the ratio $R/X_0$. The top/bottom parts of Fig. 1(c) distinguish between the cusps appearing on the left/right from the magnetic field step. For skipping orbits, the latter should be folded onto the same half-plane. When $R < \frac{1}{2}X_0$, all the extended caustics disappear, leaving only one limiting caustic of the closed orbits: a circle with a $2R$-radius centred at the source. The inset in Fig. 1(c) shows the limiting positions of the cusps at $R \rightarrow \frac{1}{2}X_0$ (spaced with the period of $\approx 0.4X_0$) before their final disappearance.

The second regime in the formation of catastrophes of snake/skipping orbits is characteristic for the weak magnetic fields, such that $R > X_0$. In the latter case, the singularities form cusp triplets shown in Fig. 1(b). The semiclassically calculated interference pattern of the electron waves in the vicinity of the cup triplets is illustrated in the top inset in Fig. 1(b), and their positions are shown on the r.h.s. of Fig. 1(c). Note that for $X_0/R \rightarrow 0$ caustics in Fig. 3(b) transform into caustics of skipping orbits originated from a point source exactly at the edge of a 2D system [5].

Finally, the form of caustics and cusps at the transition point between these two regimes, i.e., for $X_0 = R$, is shown in Fig. 2. In this case, new higher-order singularities are formed - the butterfly bifurcation, for which In this case higher order singularities are formed out of two merging pieces of caustics,

$$
u_n - u_c^n = \pm (\frac{4}{5})^{\frac{3}{4}} n^{-\frac{1}{4}} R^{-\frac{1}{4}} (v_c^n - v_n)^{\frac{3}{4}},
$$

(5)

Such a singularity is characterized by two additional constraints, $\frac{\partial^N F}{\partial \theta^N} = 0$ with $N = 1, 2, 3, 4$, and it represents a section of the $A_5$ butterfly bifurcation [24]. According to the mathematical catastrophe theory [21, 22, 25], such
higher-order singularities are not stable, so that their formation is uniquely specific to the infinitely sharp ±B-interface. Any weak smearing of the interface, or an effective gauge field created for electrons by lattice deformations in, e.g., the bended region of folded graphene sheet replaces this transition by a precursive formation of the third-order singularity near the already existing cusp: a 'swallowtail' catastrophe consisting in the nucleation of a pair of cusps, followed by a gradual separation of the latter until the three singularities form the triplets shown in Fig. 1(b). All of the above results are also applicable to the electron skipping orbits, by folding caustics in Fig. 1 onto a single half-plane as shown on the r.h.s. of Fig. 2.

Periodic appearance of cusps of snake/skipping orbits suggests that they can generate magneto-oscillation of non-local conductance in ballistic multi-terminal devices incorporating a ±B-interface (or graphene fold in a magnetic field). Figure 3 shows the calculated magneto-oscillations of the current $I_{SD}$ in the three-terminal geometry (for $W = \pi^2 X_0$). Here, the injected current is registered in the drain placed on the right from the ±B field step. The marks $\alpha, \alpha'/\beta, \beta'$ relate maxima/minima of $I_{SD}$ to the cusps reaching the upper edge of the sample on the right/left from the field step, as marked on Fig. 1(c).

(b) Bunching of trajectories and magneto-oscillations of the source-drain current in a four-terminal device with a ±B-interface and width $W$. Two top panels illustrate families of trajectories for the conditions corresponding to the maximum/minimum ($\alpha/\beta$) of $I_{SD}$, with positions of the cusps pointed by arrows. The oscillations in $I_{SD}$ are the result of singularities in the ensemble of electron trajectories: each time when a cusp/focus on the right from the interface reaches the upper sample edge, $I_{SD}$ experiences a maximum, and when a singularity on the left reaches the sample edge - a minimum. Such oscillatory behavior persist both in the regime of individual cusps formation and the regime of cusp triplets. However, for the lowest magnetic fields, such that $R/X_0 \ll 1$, the cusps in each of triplet get separated so much that one of those crosses the ±B-interface; after that, the magneto-oscillations of $I_{SD}$ become rather irregular and loose in the amplitude. Figure 3(b) gives an example of magneto-oscillations of the current $I_{SD}$ in a 4-terminal device incorporating a ±B-interface. Here, current is injected from an isotropic side.

FIG. 2. Snake orbits (left) and skipping orbits (right) for electrons injected at a distance $X_0 = R$ from the ±B-interface/edge, with caustics (blue) merging at a higher-order singularity: a section of the so called butterfly bifurcation.

FIG. 3. (a) Bunching of trajectories (for $X_0 = R$) and the calculated magneto-oscillations of the current $I_{SD}$ in the three-terminal geometry (for $W = \pi^2 X_0$). Here, the injected current is registered in the drain placed on the right from the ±B field step. The marks $\alpha, \alpha'/\beta, \beta'$ relate maxima/minima of $I_{SD}$ to the cusps reaching the upper edge of the sample on the right/left from the field step, as marked on Fig. 1(c). (b) Bunching of trajectories and magneto-oscillations of the source-drain current in a four-terminal device with a ±B-interface and width $W$. Two top panels illustrate families of trajectories for the conditions corresponding to the maximum/minimum ($\alpha/\beta$) of $I_{SD}$, with positions of the cusps pointed by arrows.
contact at the lower edge (biased against the electrode on the l.h.s. at the upper edge) and registered using a drain contact placed at the r.h.s. at the upper edge. Similarly to Fig. 3(a), oscillations of $I_{SD}$ in Fig. 3(b) reflect periodic appearance (on the left and right hand side from the $\pm B$-interface) of cusps in the family of sequentially linked skipping and snake orbits.

To summarise, we show that snake/skipping orbits of electrons injected at one point into in a 2D metal (at the distance $X_0$ from the $\pm B$-interface/edge) generically display caustic bunching and formation of intense local singularities - cusps, with two characteristic regimes of cusp formation: (i) periodic appearance of individual cusps (for $2R > X_0 > R$) and (ii) cusp triplets (for $R > X_0$). Singularities in the distribution of trajectories, which are most intense when $R = X_0$, can lead to the magneto-oscillations in the non-local conductance of multi-terminal devices made, e.g., of a bi-folded graphene flake. Alternatively, one can employ near-field optics source to generate electron-hole pairs in the heterostructure, with electrons placed at the energy close to the Fermi level, and, then, detecting the presence of singularities by measuring magnetic-field and source-position dependences of a voltage drop between a fixed point contact and a massive contact placed further up along the edge.

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