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Electron Transport Peculiarities Expected in 2D Metals

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Abstract:
In the frames of simple Drude model, there are analytically treated the general features of electron transport in 2D metals. It is demonstrated that depending on the Fermi level position such materials can reveal a non-standard current–voltage characteristic opening wide perspectives of creating the novel functional 2D materials for superfast nanoelectronics.

Key Words*: 2D metal; Electron transport; Drude model; Electron-energy-surface.*

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I. Introduction

Graphene – monolayer carbon hexagonal sheet, the 2D material most known and most used in nanoelectronics, is a semimetal with conic electron-energy-surface (EES) and, consequently, linear energy–momentum dispersion relation. Among 2D materials predicted and synthesized after grapheme, borophene – monolayer boron triangular sheet is of special interest because most of its allotropes are metallic and reveal complex of unique physical properties [1] making them useful for application in the next-generation nanoelectronics.

Recently, one of authors *et al*. have numerically calculated [2] electronic structure of flat hexagonal-holeless boron sheet. The detailed topological analysis of the obtained EESs will be reported elsewhere. Here, we intend to consider one result, which seems to be of high academic interest and importance in view of applications as well. The point is that flat holeless boron sheet has been found to be metallic with conduction band, which in the vicinity of Fermi energy in good approximation can be represented by a quadric surface different from standard paraboloid characteristic of 3D metals.

Present paper aims studying theoretically the general features of electron transport in 2D metals with conduction band in form of all the possible quadric EESs.

II. Case of Non-Standard Current–Voltage Characteristic

Let us start with case of hyperboloidal conduction band. As hyperboloid is a quadric surface, it is defined by a polynomial of degree two in three variables. Among other quadric surfaces, hyperboloid – not being a double-cone – is characterized by having the symmetry center. In addition, hyperboloid has three pairwise perpendicular axes and also planes of symmetry.

If one chooses a Cartesian coordinate system (x, y, z) , whose axes are the axes of symmetry and origin is the center of symmetry of the given hyperboloid, it may be defined by the following equations:

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}-\frac{z^2}{c^2}=\pm 1 ,$$

where a , b , and c are given constants. Both of these surfaces are asymptotic to double-cone of equation:

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}-\frac{z^2}{c^2}=0 .$$

So, all the three surfaces can be expressed by general formula:

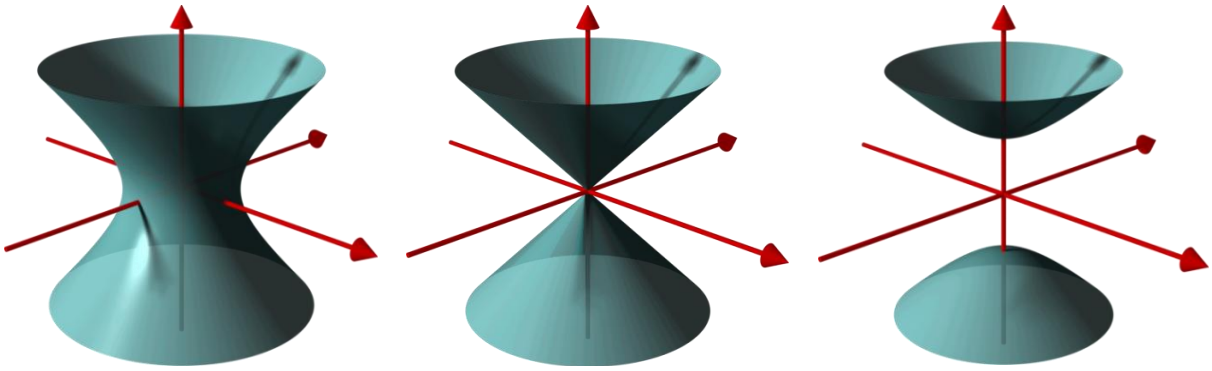
$$\frac{x^2}{a^2}+\frac{y^2}{b^2}-\frac{z^2}{c^2}=\eta$$

with parameter $\eta = +1, 0, -1$. Note, any equation with different η can be easily reduced to the standard form by dividing on $|\eta|$ and redefinition of constants: $a^2|\eta| \to a^2$, $b^2|\eta| \to b^2$, and $c^2|\eta| \to c^2$. For $\eta = +1$ and $\eta = -1$ hyperboloid has one or two sheets, respectively. Figure 1 shows one- and two-sheet hyperboloids, and double-cone between them.

When hyperboloid approximates an EES in 2D material, variables x and y , and z have to be replaced by the components p_x and p_y of charge carrier quasi-momentum, and its energy $\varepsilon = \varepsilon(p_x, p_y)$, respectively:

$$\frac{\varepsilon(p_x,p_y)}{\varepsilon_0}=\pm\sqrt{\frac{p_x^2}{p_{x0}^2}+\frac{p_y^2}{p_{y0}^2}-\eta} .$$

Here p_{x0} and p_{y0} , and ε_0 are constants of dimensions of momentum and energy. And signs "+" and "–" correspond to electron and hole energy-bands.



(a) **(b)** **(c)**

Figure 1: One-sheet hyperboloid (a), double-cone (b), and two-sheet hyperboloid (c).

From this dispersion relation, components v_x and v_y of group velocity of the wave-packet, which represents a charge carrier, are determined as:

$$v_x = \frac{\partial\varepsilon(p_x,p_y)}{\partial p_x} = \pm\frac{\varepsilon_0 p_x}{p_{x0}^2\sqrt{\frac{p_x^2}{p_{x0}^2}+\frac{p_y^2}{p_{y0}^2}-\eta}}$$

and

$$v_y = \frac{\partial\varepsilon(p_x,p_y)}{\partial p_y} = \pm\frac{\varepsilon_0 p_y}{p_{y0}^2\sqrt{\frac{p_x^2}{p_{x0}^2}+\frac{p_y^2}{p_{y0}^2}-\eta}}.$$

For simplicity, below we assume EES to be a hyperboloid of revolution – circular hyperboloid, which is generated by rotating a hyperbola around one of its principal axes, i.e. with $p_{x0} = p_{y0} \equiv p_0$. And for definiteness, we will consider upper part (with sign "+") of a two-sheet hyperboloid (with $\eta = -1$):

$$\frac{\varepsilon(\boldsymbol{p})}{\varepsilon_0} = \sqrt{\frac{\boldsymbol{p}^2}{p_0^2}+1}$$

and

$$\boldsymbol{v} = \frac{\partial\varepsilon(\boldsymbol{p})}{\partial\boldsymbol{p}} = \frac{v_0\boldsymbol{p}}{\sqrt{\boldsymbol{p}^2+p_0^2}},$$

where $\boldsymbol{p}$ and $\boldsymbol{v}$ are quasi-momentum and group-velocity vectors, respectively. Maximum or saturation velocity

$$v_0 = \frac{\varepsilon_0}{p_0}$$

is achieved asymptotically at $p>>p_0$.

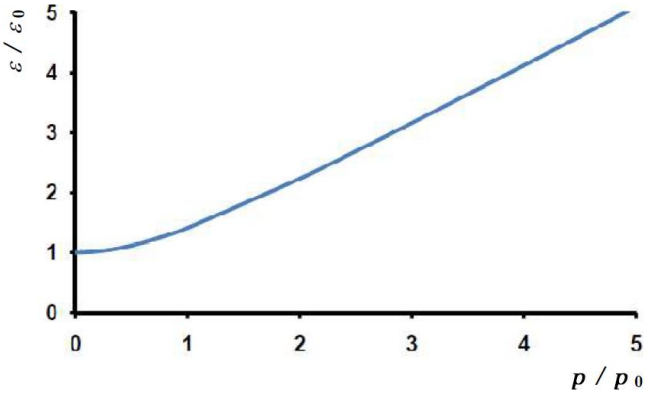


Figure 2: Energy dispersion relation in 2D metal with hyperboloidal conduction band.

For convenience, let rewrite above relation in the dimensionless form:

$$\frac{\boldsymbol{v}}{v_0} = \frac{\frac{\boldsymbol{p}}{p_0}}{\sqrt{\frac{\boldsymbol{p}^2}{p_0^2}+1}}.$$

Figure 2 shows $\varepsilon - p$ dependence according to derived relation.

For not having any credible information on momentum relaxation mechanism in 2D metals with possible hyperboloidal conduction band, it is expedient to approach problem of determining their current–voltage characteristics within frames of simple Drude model [3] of electron transport in metals with only single parameter of the material – relaxation time τ independent of momentum $\boldsymbol{p}$.

Dispute the model's simplicity, there are several factors making us believers that finally we will come to quite credible conclusions:

- Amazingly, the conductivity predicted by the Drude formula, which initially was derived by assuming that the charge carriers form a classical ideal gas, turns out to be the same when the theory is extended to the free quantum electrons model, where the carriers follow Fermi–Dirac statistics. Thus, calculated conductivity should not depend on the form of the electron momentum distribution.
- The Drude model provides a very good explanation of DC and AC conductivities in number of real materials with metallic properties, in particular, high-mobility 2D electron gases [4].
- In metallic conductance contribute only electrons with momentum near the Fermi momentum and thus momentum-dependence of relaxation time practically does not affect their conductivity.

According to the Drude model, the electronic equation of motion is:

$$\frac{d\boldsymbol{p}(t)}{dt} = -e\boldsymbol{E} - \frac{\boldsymbol{p}(t)}{\tau},$$

where t is the time, $\boldsymbol{p}(t)$ is the average momentum per electron, $\boldsymbol{E} = \text{const}$ is the strength of stationary uniform electric field applied, and e is the elemental charge.

Apparently, for free electron gas $\boldsymbol{E} = 0$ and $\boldsymbol{p}(t) \equiv 0$ as well. But when an external field applied, $\boldsymbol{E} \neq 0$ and $\boldsymbol{p}(t) \neq 0$. After the steady state is achieved, $d\boldsymbol{p}(t)/dt = 0$ and $\boldsymbol{p}(t) \equiv \boldsymbol{p}(\boldsymbol{E}) = \text{const}$ with

$$\boldsymbol{p}(\boldsymbol{E}) = -e\tau\boldsymbol{E}\ .$$

It is natural to relate average velocity in the electric field, i.e. drift velocity, $\boldsymbol{v}(\boldsymbol{E})$ to average momentum $\boldsymbol{p}(\boldsymbol{E})$ according to the general $\boldsymbol{v} - \boldsymbol{p}$ relation stated above:

$$\frac{\boldsymbol{v}(\boldsymbol{E})}{v_0} = -\frac{\frac{\boldsymbol{E}}{E_0}}{\sqrt{\frac{\boldsymbol{E}^2}{E_0^2}+1}}\ .$$

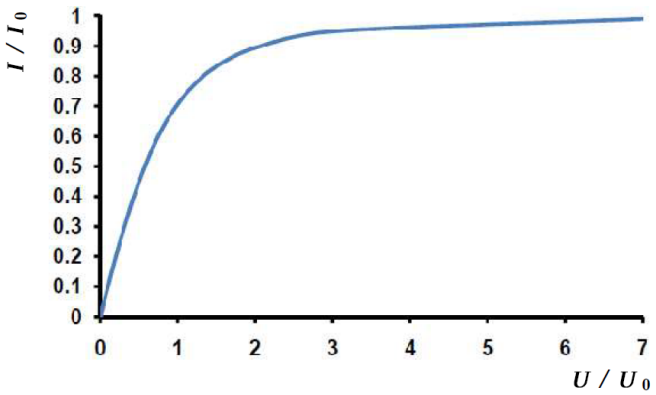


Figure 3: Current–voltage characteristics of 2D metal with hyperboloidal conduction band.

Here

$$E_0 = \frac{p_0}{e\tau}$$

is the constant of electric field strength dimension. If n is the electron sheet-concentration in 2D material, then electric current linear density $\boldsymbol{j}(\boldsymbol{E})$ at field $\boldsymbol{E}$ is:

$$\boldsymbol{j}(\boldsymbol{E}) = -en\boldsymbol{v}(\boldsymbol{E})\ .$$

Finally, introducing the parameter

$$j_0 = env_0\ .$$

of electric current density dimension, we obtain:

$$\frac{\boldsymbol{j}(\boldsymbol{E})}{j_0} = \frac{\frac{\boldsymbol{E}}{E_0}}{\sqrt{\frac{\boldsymbol{E}^2}{E_0^2}+1}}\ .$$

If l and w are 2D conductor's length and width, respectively, current $I = jw$ and voltage $U = El$ can be related by the following equation:

$$\frac{I}{I_0} = \frac{\frac{U}{U_0}}{\sqrt{\frac{U^2}{U_0^2}+1}},$$

where

$$I_0 = env_0w$$

and

$$U_0 = \frac{p_0 l}{e\tau}.$$

The obtained current–voltage characteristic is shown in Figure 3. Apparently, its shape is similar to the velocity dispersion curve $v - p$.

III. Case of Standard Current–Voltage Characteristic

Now we briefly discuss situations, when conduction band of a 2D material can be approximated by other quadric surfaces.

Obviously that in case of one-sheet hyperboloid, current–voltage characteristic takes the following form:

$$\frac{I}{I_0} = \frac{\frac{U}{U_0}}{\sqrt{\frac{U^2}{U_0^2}-1}}.$$

It has to be treated as an unphysical result because there is a non-zero threshold voltage U_0, only at which charge carriers start flow and that initial current is infinite: $I \to \infty$.

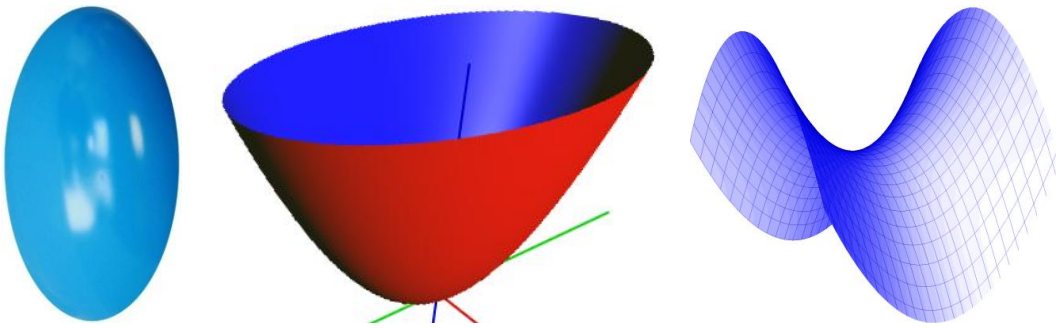
For ellipsoidal surface (see Figure 4**a**),

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}+\frac{z^2}{c^2} = 1,$$

the current–voltage characteristic should be as:

$$\frac{I}{I_0} = \frac{\frac{U}{U_0}}{\sqrt{1-\frac{U^2}{U_0^2}}}.$$

This form does not have a physical sense as well because at sufficiently high voltage, $U = U_0$, current again becomes infinite: $I \to \infty$.



(a) **(b)** **(c)**

Figure 4: Ellipsoid (a), elliptic (b), and hyperbolic paraboloids (c).

And finally, consider paraboloidal surfaces,

$$z = \frac{x^2}{a^2} \pm \frac{y^2}{b^2},$$

where signs "+" and "–" stand for elliptic (Figure 4b) and hyperbolic (Figure 4c) paraboloids, respectively. In particular, for an elliptic paraboloid of revolution (i.e. with sign "+" and at condition $a = b$) conduction band energy and velocity dispersion relations can be presented as:

$$\varepsilon(\boldsymbol{p}) = \frac{\boldsymbol{p}^2}{2m}$$

and

$$\boldsymbol{v} = \frac{\boldsymbol{p}}{m},$$

respectively. As it is well known, here constant m can be considered as effective mass of non-relativistic charge carriers in solid. These relations directly lead to the Ohm's law in its standard form:

$$I = \frac{U}{R}$$

where

$$R = \frac{ml}{e^2 n\tau w}$$

is the sheet-resistance of the conductor.

IV. Conclusion

Thus, among quadric surfaces useful to fit a 2D metal's conduction band EES in the vicinity of Fermi level only two-sheet hyperboloid leads to current–voltage characteristic with non-trivial form and at same time having a physical sense.

For conductor made from such a material, it can be introduced the critical voltage U_0, which is inversely proportional to the momentum relaxation time τ : $U_0 \sim 1/\tau$. Initially, i.e. at relatively low voltages of $U \ll U_0$, current is proportional to the applied voltage, $I \sim U$, in accordance to Ohm's law. However, at relatively high voltages of $U \gg U_0$, charge carriers' velocity v reaches its maximum value v_0 and, consequently, electric current saturates, $I \to I_0$. In this regard a 2D metal under the consideration differs from semimetalic graphene, where conduction band surface is conic. This means that $U_0 \equiv 0$ and charge carriers reach their maximum velocity even in infinitesimal voltage. In our case, $U_0 \neq 0$, but if material is structurally perfect and chemically pure the momentum relaxation time τ could be too high and, consequently, critical voltage U_0 too low.

These novel 2D metals are expected to be different from standard 3D conductors, where Fermi level is usually located in the lower part of the conduction band with EES very close to the paraboloid. There, as the vertical section is a parabola, the corresponding $\varepsilon - p$ curve has a squared slope. However, at higher energies the requirements of analyticity and periodicity of the dispersion function in the reciprocal space should lead to a gradual transition to the zero-slope to ensure smooth sewing with the second Brillouin zone. Consequently, there definitely exist energy regions, where the slope is approximately linear, which corresponds to a conic EES, and quasi-linear, $\sim\sqrt{p^2 + p_0^2}$, which corresponds to a hyperboloidal one.

Virtually, in common conductors Fermi level can be shifted in such hyperboloidal or conic (at $p_0 \equiv 0$) energy region if apply extreme high voltages. But, actually due to energy relaxation process drift velocity of electrons overheated in such strong electric field saturates at value significantly lower than maximum value v_0 .

As for the 2D metals, one can shift up Fermi level to locate it just in the hyperboloidal or conic regions more easily, e.g. by doping electrons from its substrate.

So, it is possible to induce electric current of charge carriers with hyperboloidal dispersion and then achieve their maximum velocity even at low applied voltages. It opens the door for future applications of 2D metals in superfast nanoelectronics.

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