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 SPIN RELATED PHENOMENA IN NANOSTRUCTURES

Non-Abelian Properties of Charge Carriers in a Quasirelativistic Graphene Model

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Abstract—Charge carrier transport peculiarities stipulated by non-trivial topology of a quasi-relativistic graphene model are investigated. It has been demonstrated that the model predicts additional topological contributions such as Majorana-like mass-term correction to ordinary Ohmic component of current, spin-orbital-coupling and “Zitterbewegung”-effect corrections to conductivity in space and time dispersion regime. Phenomena of negative differential conductivity for graphene have been interpreted based on the proposed approach.

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1. INTRODUCTION

Currently, the progress in the development of quantum devices on the graphene-like material platform is connected with the so-called “valleytronics direction” utilizing the valley Hall effect (VHE). VHE for graphene reveals itself as an appearance of an electrical current in the direction orthogonal to an applied electric field (applied bias) \mathbf{E} in the absence of a magnetic field. The existence of VHE signifies that charge transport for graphene can be topologically nontrivial. Suggested explanations of VHE are model dependent. The effect for monolayer graphene could be due to a non-zero Berry curvature which is non-vanishing at breaking inversion symmetry or(and) time reversal symmetry. But, the gap opening which should accompany such a breaking inversion symmetry has not been confirmed experimentally. Up to now there is no consistent theory of topologically nontrivial graphene conductivity.

Graphene belongs to strongly correlated many-body systems, where topologically non-trivial effects, such e.g., as Majorana fermion states can manifest themselves. Experimental signatures of graphene Majorana states in graphene-superconductor junctions without need for spin-orbital coupling (SOC) have been established in [1].

In this paper, we investigate quantum transport of charge carriers with vortex dynamics in a quasi-relativistic graphene model using a high-energy $\mathbf{k} \times \mathbf{p}$ -Hamiltonian. The Wilson non-closed loop method

will be used to prove dichroism of the band-structure which leads to valley Hall conductivity.

2. FUNDAMENTALS

Quasi-relativistic graphene model has been derived (see, \cite{symmetry2020}) and reference therein) as a consequent account of the effects of relativistic exchange interaction on the ground of truly secondary quantized relativistic consideration of the problem within the known Dirac–Hartree–Fock self-consistent field approximation. It has been established that the model admits a form as Majorana-like system of equations as well as two-dimensional Dirac-like equation with an additional “Majorana-force correction” term [2], and it reads

$$v_F [\boldsymbol{\sigma}_{2D}^{AB} \times \mathbf{p}_{BA} - c^{-1} M_{BA}] |\psi_{BA}^*\rangle = E |\psi_{BA}^*\rangle \quad (1)$$

and the same equation with labels (AB, BA) exchanged for another sublattice. Here (AB, BA) are related to sublattices and refer to the quantities which are obtained by similar transformations with a relativistic exchange matrix Σ_{rel}^x e.g., for the momentum operator \mathbf{p} one gets $\mathbf{p}_{BA} = \Sigma_{BA} \mathbf{p} \Sigma_{BA}^{-1}$; v_F is the Fermi velocity.

The vector of 2D Pauli matrixes comprises of two matrixes $\boldsymbol{\sigma}_{2D} = (\sigma_x, \sigma_y)$. The term $M_{BA} = -\frac{1}{c v_F} \Sigma_{BA} \Sigma_{AB}$ is a Majorana-like mass term, where c is the speed of light. It turns out to be zero in the Dirac point $K(K')$

and gives a very small momentum dependent correction outside of $K(K')$. The relativistic exchange operator for tight-binding approximation and accounting of nearest lattice neighbors is given by as

$$\Sigma_{rel}^x = \begin{pmatrix} 0 & \Sigma_{AB} \\ \Sigma_{BA} & 0 \end{pmatrix} \quad (2)$$

so that its action on secondary quantized wave functions on sublattices $A(B)$ of the system reads

$$\begin{aligned} \Sigma_{AB} \hat{\chi}_{\sigma_i^B}^\dagger(\mathbf{r})|0, \sigma\rangle &= \sum_{i=1}^{N_v N} \int d\mathbf{r}_i \hat{\chi}_{\sigma_i^B}^\dagger(\mathbf{r})|0, \sigma\rangle \Delta_{AB} \\ &\times \langle 0, -\sigma_i | \hat{\chi}_{-\sigma_i^A}^\dagger(\mathbf{r}_i) V(\mathbf{r}_i - \mathbf{r}) \hat{\chi}_{-\sigma_i^B}(\mathbf{r}_i) |0, -\sigma_i\rangle, \end{aligned} \quad (3)$$

$$\begin{aligned} \Sigma_{BA} \hat{\chi}_{-\sigma_i^A}^\dagger(\mathbf{r})|0, \sigma\rangle &= \sum_{i'=1}^{N_v N} \int d\mathbf{r}_{i'} \hat{\chi}_{-\sigma_{i'}^A}^\dagger(\mathbf{r})|0, -\sigma\rangle \Delta_{BA} \\ &\times \langle 0, \sigma_{i'} | \hat{\chi}_{\sigma_{i'}^B}^\dagger(\mathbf{r}_{i'}) V(\mathbf{r}_{i'} - \mathbf{r}) \hat{\chi}_{-\sigma_{i'}^B}(\mathbf{r}_{i'}) |0, -\sigma_{i'}\rangle. \end{aligned} \quad (4)$$

Here interaction (2×2) -matrices Δ_{AB} and Δ_{BA} are gauge fields (or components of a gauge field). Vector-potentials for these gauge fields are introduced by the phases α_0 and $\alpha_{\pm, k}$, $k = 1, 2, 3$ of $\pi(p_z)$ -electron wave functions $\psi_{p_z}(\mathbf{r})$ and $\psi_{p_z, \pm \delta_k}(\mathbf{r})$ attributed to a given lattice site and its three nearest neighbors (see detail in [2]), $V(\mathbf{r})$ is the three-dimensional (3D) Coulomb potential, summation is performed on all lattice sites and number of electrons. The introduction of these non-abelian gauge fields was stipulated by a requirement of reality of eigenvalues of the Hamiltonian operator as gauge conditions. In this case, the operator of relativistic exchange gains an additional implicit \vec{k} -dependence upon momentum in the case of non-zero values of gauge fields.

A global characterization of all Dirac touching with non-abelian Zak phases Φ_1, \dots, Φ_4 as arguments of Wilson-loop operator for our model predict the

homotopy group Z_{12} with generator $\pi/6$ in the Dirac points $K(K')$ [2]. It is naturally to assume that such peculiarities would lead also to observable consequences in charge transport in such a system.

3. NON-ABELIAN CURRENTS IN QUASI-RELATIVISTIC GRAPHENE MODEL

Conductivity can be considered as a coefficient linking the current density with an applied electric field in linear regime of response. To reach the goal, several steps should be performed. First, one has to subject the system by an electromagnetic field, this can be implemented by standard change to canonical momentum $\mathbf{p} \rightarrow \mathbf{p} - \frac{e}{c} \mathbf{A}$ in the Hamiltonian where \mathbf{A} is a vector-potential of the field. Then, one can find a quasi-relativistic current of charge carriers in graphene as:

$$j_i^{SM} = c^{-1} j_i \equiv j_i^O + j_i^{Zb} + j_i^{so}, \quad i = 1, 2; \quad (5)$$

$$\begin{aligned} j_i &= e \chi_{+\sigma_B}^\dagger(x^+) v_{x^+}^i \chi_{+\sigma_B}(x^-) - \frac{e^2 A_i}{c M_{AB}} \chi_{+\sigma_B}^\dagger(x^+) \chi_{+\sigma_B}(x^-) \\ &+ \frac{e \hbar}{2 M_{AB}} [\nabla \times \chi_{+\sigma_B}^\dagger(x^+) \sigma \chi_{+\sigma_B}(x^-)]_i. \end{aligned} \quad (6)$$

Here $x^\pm = x \pm \epsilon$, $x = \{\mathbf{r}, t_0\}$, $\mathbf{r} = \{x, y\}$, $t_0 = 0$, $\epsilon \rightarrow 0$; $v_{x^+}^i$ is the velocity operator determined by a derivative of the Hamiltonian (1), $\chi_{\sigma_B}(x^+)$ is the secondary quantized fermion field, the terms j_i^O , j_i^{Zb} , j_i^{so} , $i = x, y$ describe an ohmic contribution which satisfies the Ohm law and contributions of the polarization and magneto-electric effects respectively. Potential energy operator V for interaction between the secondary quantized fermionic field $\chi_{\sigma_B}(x^+)$ with an electromagnetic field reads

$$\begin{aligned} V &= \chi_{+\sigma_B}^\dagger \left[-c \sigma_{BA} \times \frac{e}{c} \mathbf{A} - M_{BA}(0) - \sum_i \frac{dM_{BA}}{dp_i} \Big|_{p_i=0} \left(p_i^{AB} - \frac{e}{c} A_i \right) \right. \\ &\left. - \frac{1}{2} \sum_{i,j} \frac{d^2 M_{BA}}{dp_i dp_j} \Big|_{p_i, p_j=0} \left(p_i^{AB} - \frac{e}{c} A_i \right) \left(p_j^{AB} - \frac{e}{c} A_j \right) + \dots \right] \chi_{+\sigma_B}. \end{aligned} \quad (7)$$

To perform quantum-statistical averaging for the case of non-zero temperature, we use a quantum field method developed in [3]. After tedious but simple algebra one can find the conductivity in our model:

$$\begin{aligned} \sigma_{ii}^O(\omega, k) &= \frac{ie^2 \beta^2}{(2\pi c)^2} \text{Tr} \\ &\times \int \left(1 - M_{BA}(\mathbf{p}) \frac{\partial^2 M_{BA}}{\partial p_i^2} \right) (M \mathbf{v}^i(p) N \mathbf{v}^i(p)) d\mathbf{p}, \end{aligned} \quad (8)$$

$$\sigma_{ii}^{Zb}(\omega, k) = \frac{ie^2\bar{\beta}^2}{(2\pi c)^2} \text{Tr} \times \int M_{BA}(\mathbf{p}) \frac{1}{2} \sum_{i=1}^2 \frac{\partial^2 M_{BA}}{\partial p_i^2} (M\mathbf{v}^i(p), N\mathbf{v}^i(p)) d\mathbf{p}, \quad (9)$$

$$\sigma_{12(21)}^{so}(\omega, k) = (-1)^{l(2)} \frac{1}{2} \frac{ie^2\bar{\beta}^2}{(2\pi c)^2} \text{Tr} \times \int M_{BA}(\mathbf{p}) \frac{\partial^2 M_{BA}}{\partial p_1 \partial p_2} (M\mathbf{v}^{1(2)}(p), N\mathbf{v}^{1(2)}(p)) \sigma_z d\mathbf{p}, \quad (10)$$

for the currents j_i^O , j_i^{Zb} , j_i^{so} respectively. Here matrices M , N are given by the following expressions:

$$M = \frac{f[\bar{\beta}((H(p^+) - \mu)/\hbar)] - f[\bar{\beta}(H^\dagger(-p^-) - \mu/\hbar)]}{\bar{\beta}(z - \bar{\beta}(H(p^+)/\hbar) + \bar{\beta}(H^\dagger(-p^-)/\hbar))}, \quad (11)$$

$$N = \frac{\delta(\hbar\omega + \mu)}{(\hbar z + H(p^+) - H^\dagger(-p^-))\bar{\beta}}. \quad (12)$$

Here f is the Fermi–Dirac distribution, $z = \omega + i\epsilon$, $\mathbf{p}^\pm = \mathbf{p} \pm \mathbf{k}$, ω is a frequency, μ is a chemical potential, $\bar{\beta}$ is an inverse temperature divided by c . Total current \mathbf{J} in graphene are determined by two currents of valleys K, K' as $\mathbf{J} = \mathbf{J}_K - \mathbf{J}_{K'}$. $\mathbf{J}_K, \mathbf{J}_{K'}$ are orthogonal to each others due to the homotopy group \mathbf{Z}_{12} of graphene Brillouin zone. Therefore the current directed along an applied electrical field $\mathbf{E} = (E_x, E_y)$ can be presented as $\mathbf{J} = \mathbf{J}_x - \mathbf{J}_y + \sum_{i=1}^2 (-1)^{i-1} (\sigma_{ii}^O + \sigma_{ii}^{Zb}) \mathbf{E}_i$.

Let us denote the first and the second terms in σ_{ii}^O through σ_{ii}^o and σ_{ii}^{add} respectively: $\sigma_{ii}^O = \sigma_{ii}^o + \sigma_{ii}^{add}$. σ_{ii}^{add} and σ_{ii}^o depends and does not depend on the Majorana-like mass term M_{AB} . through respectively. Then, one can determine conductivity σ_{ii}^{tp} for topological currents as $\sigma_{ii}^{tp} = \sigma_{ii}^{add} + \sigma_{ii}^{Zb}$, $\sigma_{xx}^{tp} = -\sigma_{yy}^{tp}$.

Figure 1 demonstrates the negative differential conductivity for the topological current $j^{tp} = \Re e \sigma_{ii}^{tp}(\omega) U$ assuming the increase of the system energy in a form $\hbar\omega \sim U^2$, where U is a bias voltage.

A total spin-orbital valley current $\mathbf{J}_{VHE} = \sigma_{xy}^{so} \mathbf{B}_y - \sigma_{yx}^{so} \mathbf{B}_x$ is produced under an action of a magnetic field \mathbf{B}_\parallel parallel to \mathbf{E} . One can note that \mathbf{J}_{VHE} is always directed orthogonally to the bias \mathbf{E} and, accordingly compensates the current \mathbf{j}^{tp} . The current in the direction of the vector \mathbf{E} increases because of the decrease of “topological current” of leakage $\mathbf{j}^{tp} - \mathbf{J}_{VHE}$ in orthogonal to \mathbf{E} direction signifying that a negative magnetoresistance (NMR) appears at weak magnetic fields parallel to electric ones.

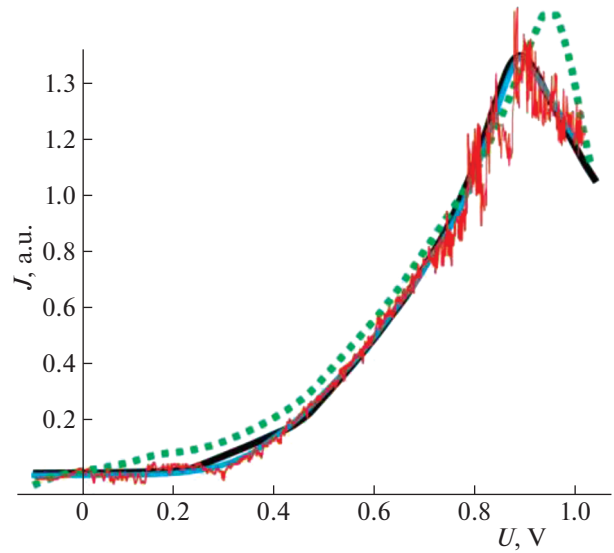


Fig. 1. Dependencies of topological current J on bias voltage U : simulation results (red solid curve) and their fitting (blue solid curve) for negative differential conductivity (NDC) in our quasirelativistic graphene model at temperature $T = 3$ K, chemical potential $\mu = 135$ K; black solid and green dashed curves present experimental data and theoretical calculation for NDC in two graphene flakes twisted approximately at 90° to each other at 1.8° misalignment angle [4]. The bias voltage U is given in volts.

NMR is a specific feature of topological materials and presents a phenomenon of chiral anomaly [5].

4. CONCLUSIONS

To summarize our findings, we have demonstrated that the \mathbf{Z}_{12} semimetal model as an effective controlling tool due to dichroism of the band structure offers a new class of topological gapless materials. Device construction based on topological currents existing in such materials would provide robust quantum computing.

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CONFLICTS OF INTEREST

Authors declare no conflict of interests in preparation of this paper.

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