Monte Carlo simulation of the photon drag effect in black phosphorene

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Using Monte Carlo simulation, the photon drag effect in black phosphorene is numerically investigated in the approximation of a constant relaxation time. The influence of the anisotropy of the energy spectrum on the manifestation of the effect is shown. According to the calculation data, inelastic electron scattering plays a decisive role in the occurrence of the drag current.

Keywords: phosphorene, photon drag effect, Monte Carlo simulations.

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Black phosphorene, experimentally obtained in 2014 has an anisotropic energy spectrum [1]:

$$\varepsilon = \sqrt{v_F^2 p_x^2 + (\Delta + u p_y^2)^2}. \qquad (1)$$

Here Δ — half-width of the band gap; depending on the method of preparing the phosphorene sample this parameter takes the values $\Delta = 0.15-1.0$ eV [2]. The parameters v_F and u are associated with the components of the effective mass tensor: $v_F = \sqrt{\Delta/m_x}$, $u = 1/(2m_y)$. According to calculations [2], for black phosphorene the effective mass tensor is

$$m = \begin{pmatrix} 1.2854 & 0 \\ 0 & 0.1255 \end{pmatrix} m_c,$$

m_e — free electron mass. Black phosphorene is a semiconductorwith direct band and belongs to the so-called Dirac-like materials: along one direction (axis OX) the movement of charge carriers is similar to the movement in graphene, the dependence of energy on the corresponding momentum component is linear, and the dependence of energy on the perpendicular component of the quasi-momentum (in the direction of the axis OY) is quadratic. It is interesting to study the manifestations of the anisotropy of the energy spectrum of the material under consideration in kinetic effects, one of which is the effect of dragging current carriers by photons [3,4]. This effect, caused by the transfer of photon momentum to the electronic subsystem, is explained within the framework of the semiclassical approach as a result of action of the Lorentz force that occurs when an electron moves in the alternating electric and magnetic fields of the wave. In the paper [5] the infrared and terahertz spectra of photocurrents in topological insulators are experimentally studied, and it is shown that the cause of photocurrents is the linear photogalvanic effect. The paper [6] relates to the experimental study of the circular and linear photovoltaic effect in the so-called vertically grown graphene based on the data analysis of terahertz emission spectroscopy. The paper [7] relates to the study of the mechanical stress influence on the amplitude of the photovoltaic effect in two-dimensional photodetector nickel−phosphorene−nickel; a strong dependence of the photocurrent value on the asymmetry of the sample is reported. The paper [8] reports the creation of a polarimeter built on the basis of stacked several samples of two-dimensional materials, one of which is black phosphorene. The polarimeter demonstrates reliable detection of light with linear and elliptical polarization due to the manifestation of the linear and circular photovoltaic effect in the phosphorene layer. In this paper an attempt is made to study the linear photovoltaic effect in the quasi-classical approximation based on direct modeling using the Monte Carlo method. In comparison with the quantum mechanical consideration used, for example, in [7], the quasi-classical approach will allow, in principle, to consider large amplitudes of radiation incident on sample, as well as to study the influence of various mechanisms of charge carrier scattering on inhomogeneities of the crystal lattice.

Let us consider a situation where an electromagnetic wave propagates along the surface of black phosphorene, so that the magnetic field strength vector $\mathbf{H} = \mathbf{H}_0 \cos\omega t$ is perpendicular to the sample plane, and the electric field strength vector $\mathbf{E} = \mathbf{E}_0 \cos\omega t$ is directed arbitrarily in the sample plane (Figure 1).

The classical equations of electron motion take the form

$$\frac{dp_x}{dt} = eE_0 \sin\alpha \cos t + \frac{e}{c} v_y H_0 \cos\omega t,$$

$$\frac{dp_y}{dt} = eE_0 \cos\alpha \cos t - \frac{e}{c} v_x H_0 \cos\omega t. \qquad (2)$$

Here α — the angle between the positive direction of the axis OY and the vector $\mathbf{E}$,

$$v_x = v_F^2 p_x \Big/ \left(\sqrt{v_F^2 p_x^2 + (\Delta + up_y^2)^2}\right),$$

$$v_y = 2up_y(\Delta + up_y^2) \Big/ \sqrt{v_F^2 p_x^2 + (\Delta + up_y^2)^2}$$

— components of the electron velocity vector.

The quasi-classical kinetic Boltzmann equation in the general case has the form

$$\frac{\partial f}{\partial t} + \mathbf{F}\frac{\partial f}{\partial \mathbf{p}} + \mathbf{v}\frac{\partial f}{\partial \mathbf{r}} = I(f), \tag{3}$$

where $f(\mathbf{p})$ — distribution function, $\mathbf{F}$ — resultant force, $\mathbf{v}$ — speed, $I(f)$ — collision integral. In the case of a non-degenerate electron gas, the collision integral takes the form

$$I(f) = -\int \left[W(\mathbf{p}, \mathbf{p}')f(\mathbf{p}, t) - W(\mathbf{p}', \mathbf{p})f(\mathbf{p}', t)\right] d\mathbf{p}', \tag{4}$$

where $W(\mathbf{p}, \mathbf{p}')$ — the probability of electron scattering per unit time from a state with momentum $\mathbf{p}$ to state with momentum $\mathbf{p}'$, $f(\mathbf{p})$ — distribution function.

The numerical solution of the integro-differential Boltzmann equation (3) is associated with great mathematical difficulties and is difficult for paralleling. One of the frequently used approximations is the use of the simplest model collision integrals, for example, in Bhatnagar–Gross–Krook form [9]:

$$I(f) = -\big(f(\mathbf{p}, t) - f_0(\mathbf{p})\big)/\tau, \tag{5}$$

where $f_0(\mathbf{p})$ — equilibrium distribution function, τ — relaxation time. However, even in this case it is necessary to solve the partial differential equation numerically using various grid methods.

Due to the nonlinearity of the equations of motion (2), it is convenient to use the Monte Carlo method to solve the kinetic equation (see, for example, [10–12]). The idea of the Monte Carlo method is to assume that in the intervals between collisions the electron moves according to the equations of motion (3), and the moment of collision is determined based on the probabilities of charge carrier scattering on acoustic and optical phonons, charged and uncharged impurities [11]. The Monte Carlo method in the specified formulation is successfully used to calculate kinetic coefficients, and when considering the integral term of collisions in the kinetic equation, but often for a qualitative consideration of transfer phenomena it is sufficient to use the constant relaxation time approximation. In this case, it is necessary to determine such a form of the function $W(\mathbf{p}, \mathbf{p}')$ that expression (4) turns into the Bhatnagar–Gross–Krook collision integral (5). By direct calculation it is easy to make sure that the required form is given by the expression

$$W(\mathbf{p}, \mathbf{p}') = f_0(\mathbf{p}')/\tau. \tag{6}$$

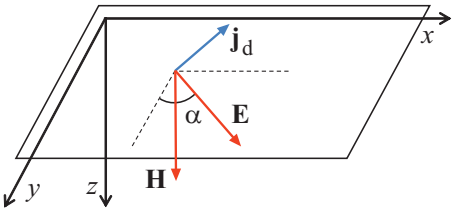

Figure 1. Configuration of electromagnetic fields applied to the sample.

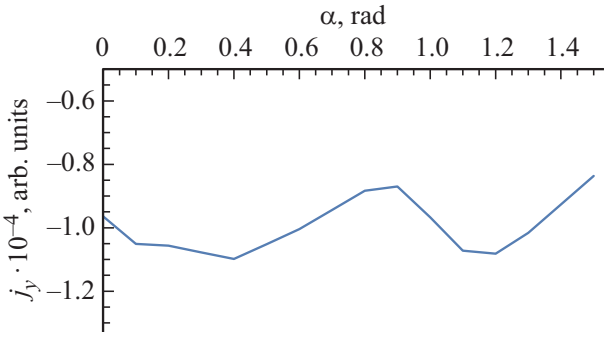

Figure 2. Current density along the axis OY vs. angle α between the wave polarization plane and the axis OY.

Indeed, after substituting (6) into (4), taking into account the normalization

$$\int f(\mathbf{p}, t)d\mathbf{p} = 1, \quad \int f_0(\mathbf{p})d\mathbf{p} = 1 \tag{7}$$

the collision integral (4) takes the form (5).

Simulation showed that a necessary condition for the drag current occurrence is the inelasticity of electron scattering on inhomogeneities of the crystal lattice. Generally speaking, the approximation of the constant relaxation time is derived for elastic scattering; however, with some stipulations, the average relaxation time can also be introduced for the processes of inelastic electron scattering on optical phonons (see, for example, [13]). In the paper [11] devoted to the study of the direct current occurrence in graphene perpendicular to the pulling field under conditions of normal incidence of elliptically polarized wave on the sample, the need to take into account the inelasticity of current carrier scattering for effect occurrence was also noted. Figure 2 shows the dependence of the drag current density along the axis OY on the angle α (Figure 1) in relative units. In the case of a material with parabolic energy spectrum, this dependence shall be sinusoidal, and in the case under study it is clear that the drag current weakly depends on the angle between the wave polarization plane and the axis OY, which is due to the large difference in components of the effective masses tensor and non-additivity of the energy spectrum (1).

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Conflict of interest

The authors declare that they have no conflict of interest.

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