Induced nonlinear cross sections of conductive electrons scattering on the charged impurities in doped graphene

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(Dated: September 9, 2018)

Relativistic quantum theory of induced scattering of 2D Dirac particles by electrostatic field of impurity ion (in the Born approximation) in the doped graphene at the presence of an external electromagnetic radiation field (actually terahertz radiation, to exclude the valence electrons excitations at high Fermi energies) has been developed. It is shown that the strong coupling of massless quasiparticles in the quantum nanostructures to a strong electromagnetic radiation field leads to the strongly nonlinear response of graphene, which opens diverse ways for manipulating the electronic transport properties of conductive electrons by coherent radiation fields.

PACS numbers: 42.50.Hz, 34.80.Qb, 32.80.Wr, 31.15.-p

I. INTRODUCTION

The physics of graphene [1, 2] with the current advanced technologies opens large research and applied fields including wide spectrum of investigations from low-energy condensed matter physics to quantum electrodynamic (QED) effects [3, 4] due to exotic features of quasiparticles in graphene that behave like massless "relativistic" Dirac fermions (with the Fermi velocity much less than the light speed in vacuum: \(v_F = 10^6\text{cm/s}\)) and obey a two-dimensional (2D) Dirac equation [3, 6]. These properties of quasiparticles lead to various applications of graphene to replicate the fundamental nonlinear QED processes in much weaker electromagnetic (EM) fields compared to common materials and vacuum where superintense laser fields of ultrarelativistic intensities are required for observation of nonlinear phenomena such as production of electron-positron pairs from the vacuum, nonlinear Compton scattering, multiphoton stimulated bremsstrahlung (SB) etc, proceeding actually in the current strong and superstrong laser fields [7-10].

Among the important processes induced by external radiation fields SB is one of the first stimulated effects at laser-matter interaction revealed immediately after the invention of lasers [11]. The latter is basic mechanism of energy exchange between the charged particles and plane monochromatic wave in plasma-like media to provide the energy-momentum conservation law for real absorption-emission processes. What concerns the electrons elastic scattering on impurity ions in graphene, there are many papers with consideration of this basic scattering effect which have been described mainly within the framework of perturbation theory by electrostatic potential (see, e.g., [12-18]). Regarding the SB process in graphene at moderate intensities of stimulated radiation, in case of its linear absorption by electrons (or holes), at the present time there are extensive investigations carried out in the scope of the linear theory, see, e.g. [19-22]. The linear absorbance of single layer graphene from infrared up to visible spectral range is \(\pi\alpha \approx 2.3\%\) which depends solely on the fine-structure constant \(\alpha = 1/137\) [24]. Consequently, taking into account the graphene thickness, the absorption coefficient will be \(10^6\text{cm}^{-1}\), which is a remarkably high value for absorption effect. On the other hand, high EM radiation absorption by ultrasmall volumes is a very challenging property for shielding materials used in nanoelectronics, aviation, and space industry, where strict requirements on lightness and smallness of materials exist. In this aspect, due to its unique properties graphene can act as a THz emitting device and/or shielding material for nanodevices, enabling to bridge so-called THz gap [25, 26]. Meanwhile, consideration of multiphoton SB process in graphene in moderately strong laser fields as a basic mechanism for radiation absorption towards the mentioned applications is absent up to now. The latter is given in the current paper.

In general, the interaction of a free electron with the EM wave is described by the dimensionless relativistic invariant parameter of intensity \(\xi = eE_0\lambda/(2\pi mc^2)\) [7], which represents the wave electric field (with amplitude \(E_0\)) work on a wavelength \(\lambda\) in the units of electron rest energy. Particularly for THz photons \(\hbar\omega \sim 0.01\text{eV}\), multiphoton effects take place at \(\xi \sim 1\) that corresponds to intensities \(I_\xi \sim 10^{14}\text{Wcm}^{-2}\), while the massless electron-wave interaction in graphene is characterized by the dimensionless parameter \(\chi = ev_FE_0/(\hbar\omega^2)\) [8], which represents the work of the wave electric field on a period \(1/\omega\) in the units of photon energy \(\hbar\omega\). Depending on the value of this parameter \(\chi\), three regimes of the wave-particle interaction may be established: \(\chi \ll 1\) – that corresponds to one-photon interaction regime [27, 28], \(\chi \ge 1\) – which is the static field limit of superpower fields in QED or Schwinger regime [30], and \(\chi \ge 1\) – is the multiphoton interaction regime [8] with the corresponding intensity \(I_\chi = \chi^2 \times 3.07 \times 10^{11}\text{Wcm}^{-2}[\hbar\omega/\text{eV}]^4\). Comparison of this intensity threshold with the analogous one for the free electrons or situation in common atoms shows the essential difference between the values of these thresholds: \(I_\xi/I_\chi \sim 10^{11}\). Thus, for realization of multiphoton
SB in graphene one can expect $10^{11}$ times smaller intensities than for SB in atoms [9, 10, 11, 31, 32].

In the present work, the influence of multiphoton effects in SB absorption process with moderately strong laser fields is considered. Here the selected frequency range of terahertz radiation excludes the valence electrons excitations at high Fermi energies.

In Sec. I the scattering rates and total multiphoton cross-sections for SB of conduction electrons in graphene have been obtained. The analytic formulas in case of screened Coulomb potential have been analyzed numerically in Sec. II. We have also present results for the angular dependence of scattered Fermi electrons on the laser radiation intensities. Conclusions are given in Sec. III.

II. MULTIPHOTON AMPLITUDES AND CROSS-SECTIONS OF SB IN GRAPHENE

Below we will develop the relativistic scattering theory for the 2D Dirac fermions on arbitrary electrostatic potential $U(r)$ of an impurity ion in doped graphene and interacting with an external EM wave field of moderate intensities. To exclude the valence electrons excitations at high Fermi energies in graphene, we will assume for a EM wave actually a terahertz radiation.

Let us determine the scattering Green function formalism in the Born approximation by potential $U(r)$. Note that the first nonrelativistic treatment of SB in the Born approximation has been carried out analytically in the work [11], and then this approach has been extended to the relativistic domain [31].

Transition amplitude of SB process in the EM wave field from the state with the canonical momentum $p_0(p_x, p_y)$ to the state with momentum $p$ $(p_x, p_y)$ in graphene plane $(x, y)$ can be written as:

$$C_{pp_0} = -\frac{i}{\hbar} \int \Psi^*_p(r, t)U(r)\Psi_{p_0}(r, t)dt d\tau,$$  

where $\Psi^+$ is the complex conjugation of $\Psi$.

The fermion particle wave function $\Psi_p(r, t)$ in the strong EM wave field may be presented in the form:

$$\Psi_p(r, t) = \exp \left(\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}\right)f_p(t),$$  

with the spinor wave function $f_p$ determined as follows:

$$f_p(t) = \frac{1}{\sqrt{2S}} \left(e^{i\Theta(p + \frac{S}{\hbar}A(\tau))}\right) e^{-i\Omega(p, t)},$$  

where the instantaneous temporal phase $\Omega(p, t)$ is defined as: $\Omega(p, t) = \frac{\tau}{\hbar} \int \sqrt{(p_x + \frac{S}{\hbar}A_x)^2 + p_y^2} dt$, the function $\Theta(p + \frac{S}{\hbar}A(\tau))$ is the angle between the vectors of particle kinematic momentum in the EM field $\mathbf{p} = p_x + \frac{S}{\hbar}A_x, p_y$ and the wave vector potential $\mathbf{A}(t) = -e \int_0^t \mathbf{E}(t')dt'$ (unit vector $\mathbf{e}$ is directed along the axis $OX$), and parameter $S$ is the quantization area - graphene layer surface area. In terms of these parameters, the graphene linear dispersion law for quasiparticles energy-momentum $E(p)$ defined by the characteristic Fermi velocity $v_F$, reads: $E = \pm v_F |p| = \pm v_F \sqrt{p_x^2 + p_y^2}$, where the upper sign corresponds to electrons and the lower sign - to holes.

As is known, the state of an electron in the field of a strong EM wave, and consequently, the cross section of SB essentially depends on the wave polarization. Hence we will consider the case of certain polarization of the wave, let a linear.

Let us first study a single electron scattering on charged impurity in graphene and interacting simultaneously with an EM radiation field $\mathbf{E}(t)$ (it is clear that at such small Fermi velocities of scattered particles the plane monochromatic wave field of frequency $\omega$ will turn into the uniform periodic electric field of frequency $\omega$: $E(t) = E_0 \cos \omega t$) polarized along the $OX$ axis.

For determination of spinor wave function $f_p$ we will use the results of the paper [33] with the obtained formula for transition amplitude:

$$C_{pp_0} = -\frac{i}{\hbar} \int f_p^*(t)U(r)f_{p_0}(t)\exp \left(\frac{i}{\hbar}(p - p_0)\cdot r\right) dt d\tau,$$  

or represented in the form:

$$C_{pp_0} = -\frac{i}{\hbar} \int f_p^*(t)\tilde{U} \left(\frac{p - p_0}{\hbar}\right) f_{p_0}(t)dt,$$  

i.e., the transition amplitude $C_{pp_0}$ is depended by the Fourier transform of the scattering potential:

$$\tilde{U} \left(\frac{p - p_0}{\hbar}\right) = \int \exp \left(\frac{i}{\hbar}(p - p_0)\cdot r\right)U(r)dr.$$  

For the impurity potential of the arbitrary form $\tilde{U} \left(\frac{p - p_0}{\hbar}\right)$ from the relation [52] we have:

$$C_{pp_0} = -\frac{i}{\hbar} \frac{1}{2S} \tilde{U} \left(\frac{p - p_0}{\hbar}\right)$$

$$\times \int \left(1 + e^{i\Theta(p_0 + \frac{S}{\hbar}A(\tau)) - \Theta(p + \frac{S}{\hbar}A(t))}\right)$$

$$e^{-\frac{\tau}{\hbar}v_F \int_0^\tau \sqrt{(p_x + \frac{S}{\hbar}A_x)^2 + p_y^2 - \sqrt{(p_{0x} + \frac{S}{\hbar}A_x)^2 + p_{0y}^2}}} dt d\tau.$$  

In accordance to the transition amplitude [7], impurity potential can be expressed in the following form:

$$C_{pp_0} = \int B(\tau)e^{-\frac{\tau}{\hbar}v_F (p - p_0)\cdot r} d\tau,$$  

$$B(\tau) = \frac{1}{\sqrt{2S}} \int e^{i\Theta(p_0 + \frac{S}{\hbar}A(\tau)) - \Theta(p + \frac{S}{\hbar}A(t))} e^{-i\Omega(p, t)} dt d\tau.$$
where
\[
B(\tau) = -\frac{i}{\hbar} \frac{1}{2S} \bar{U} \left[ \frac{P - P_0}{\hbar} \right]
\]
\[\times \left( 1 + e^{i[\Theta(p_0 + \tilde{\mathbf{A}}(t)) - \Theta(p + \tilde{\mathbf{A}}(t))] \cdot P} \right)
\]
\[\times e^{-i(v_F P_0) \int_0^T \left[ \sqrt{(p + \tilde{\mathbf{A}}(t))^2 + p_0^2} - \left( \sqrt{(p + \tilde{\mathbf{A}}(t))^2 + p_0^2} - P_0 \right) \right] dt}
\]
is the periodic function of time, and the time-depened modules of the "quasimomentums" $P_0, P$ are defined as:
\[
P_0 = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} B(t) \exp(-i\omega t) dt,
\]
\[
P = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} B(t) \exp(i\omega t) dt.
\]
Here making a Fourier transformation of the function $B(t)$ over $t$, using the known relations
\[
B(t) = \sum_{n=-\infty}^{\infty} \bar{B}_n \exp(-i\omega t),
\]
\[
\bar{B}_n = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} B(t) \exp(in\omega t) dt,
\]
and carrying out the integration over $t$ in the formula \[8\], we obtain:
\[
C_{pp_0}^{(n)} = 2\pi \hbar \bar{B}_n \delta \left( v_F P - v_F P_0 - n\hbar \omega \right).
\]

Within the Born approximation, the differential probability $W_{pp_0}$ of SB per unit time, from the electron or hole state with two-dimensional momentum $p_0$ to a state with momentum $p$ in the phase space $SdP/(2\pi\hbar)^2$ is described by the formula:
\[
W_{pp_0} = \lim_{t \to \infty} \frac{1}{t} |C_{pp_0}^{(n)}|^2 PdP d\theta \frac{S}{(2\pi\hbar)^2},
\]

where $d\theta$ is the differential scattering angle (linear).

Dividing the differential probability $W_{pp_0}$ of SB by initial flux density $v_F$ and integrating over $dP$, we obtain the differential cross-section of SB for quasiparticles in doped graphene:
\[
\frac{d\Lambda}{d\theta} = \sum_{n=-n_m}^{\infty} \frac{d\Lambda^{(n)}}{d\theta},
\]
where
\[
\frac{d\Lambda^{(n)}}{d\theta} = \frac{|P|}{v_F} \left| \bar{B}_n \right|^2 \frac{8\pi v_F \hbar}{|p_0|} \left( P - P_0 \right) \frac{d\theta}{8\pi v_F \hbar^2}.
\]
linearly polarized EM wave with the dimensionless vector dielectric (screening) function in random phase approximation in Eq. (16) at \( \mathbf{A}(\tau) = 0 \) is the overlap factor \( (1 + e^{-i\theta_q}) (1 + e^{i\theta_q}) = 2 (1 + \cos \theta_q) \),

\[
(1 + e^{-i\theta_q}) (1 + e^{i\theta_q}) = 2 (1 + \cos \theta_q),
\]

where \( \theta_q = \Theta(p_0) - \Theta(p) \). The term (19) known as a Berry phase term arising from the inherent sublattice symmetry, which with a graphene fourfold ground state degeneracy arising from the spin and valley factors, restricts the carriers from backscattering.

III. DIFFERENTIAL CROSS-SECTIONS OF SB ON THE SCREENED COULOMB POTENTIAL OF IMPURITY IONS IN GRAPHENE

Now we utilize Eq. (16) in order to obtain the differential cross-section in particular case of SB process on a screened Coulomb potential of impurity ions in graphene [15], [18], [34–37]. In accordance with [15], the Fourier transform \( \tilde{U}(\mathbf{q}) = \int U(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r} \) of a charged impurity center potential can be written as:

\[
\tilde{U}(\mathbf{q}) = \frac{2\pi e^2}{\kappa q c (q)},
\]

where \( \epsilon(q) \) (\( q = |\mathbf{q}| \)) is the 2D finite temperature static dielectric (screening) function in random phase approximation (RPA) appropriate for graphene [37], given by the formula

\[
\epsilon(q) = 1 + \frac{q_s}{q} \times \left\{ \begin{array}{ll}
\frac{\pi\xi_F}{2q} & q \leq 2k_F \\
1 - \frac{\pi\xi_F}{2q} - \frac{q\sin^{-1}(2k_F/q)}{4k_F} & q > 2k_F 
\end{array} \right.
\]

Here \( k_F = \epsilon_F/hv_F \) is 2D Fermi wave vector, \( q_s = 4\epsilon^2k_F/(\hbar\epsilon_F) \) is the effective graphene 2D Thomas-Fermi wave vector, and \( \kappa = \kappa(1 + \pi r_s/2) \) is the effective dielectric constant of a substrate. The ratio of the potential to the kinetic energy in an interacting quantum Coulomb system is measured by the dimensionless Wigner-Seitz radius \( r_s = \epsilon^2/k_F \hbar v_F \), where \( \kappa \) is the background lattice dielectric constant of the system, \( \epsilon^2/\hbar v_F \approx 2.18 \) is “effective fine-structure constant” in graphene (in the vacuum). Since we are interested in actual laser pulses for external EM radiation, at the consideration of numerical results it is convenient to represent the differential cross-sections of SB on the charged impurities in the form of dimensionless quantities.

Taking into account Eqs. (16), (10), and (20), we obtain the following form for the dimensionless partial differential cross-sections of SB process \( d\Lambda^{(n)}(\theta)/d\theta \) in the field of linearly polarized EM wave with the dimensionless vector potential \( \mathbf{A}(t) = -\mathbf{e} \sin(2\pi \tau) \) (unit vector \( \mathbf{e} \) is directed along the axis \( OX \) ):

\[
d\Lambda^{(n)}(\theta)/d\theta = \frac{1}{300} \left( \frac{r_s}{2 + \pi r_s} \right)^2 \frac{1}{\left| \mathbf{p} - \mathbf{p}_0 \right|^2} \epsilon^2 \left( \mathbf{p} - \mathbf{p}_0 \right) \times \int_0^1 d\tau \left\{ 1 + e^{i\Theta(p_0 - \mathbf{e}\sin(2\pi \tau) - \Theta(p_0 - \mathbf{e}\sin(2\pi \tau)))} \right\}
\]

\[
\times \exp \left\{ i2\pi n \tau - 2\pi i \int_0^\tau \left[ \left( \mathbf{p}_x - \mathbf{e}_x \sin(2\pi \tau') \right)^2 + \mathbf{p}_y^2 \right] d\tau' \right\}
\]
In Eq. (22) the dimensionless momentum, energy, time, and relativistic invariant intensity parameter of EM wave introduced as follows:

$$\overline{p}_{x,y} = \frac{v_F}{\hbar \omega} p_{x,y}, \overline{p} = \frac{E}{\hbar \omega},$$

$$\overline{t}_F = \frac{E}{\hbar \omega}, dt = \frac{\hbar \omega}{E} \overline{r}, \chi = \frac{e v_F}{\hbar \omega^2} E_0.$$

For numerical analysis of SB cross sections in graphene we assume Fermi energy $\varepsilon_F = 20 \hbar \omega$ ($\varepsilon_F \gg n \hbar \omega$), coherent EM radiation with energy of photons $\hbar \omega = 0.01$ eV ($\lambda = 1.24 \times 10^8 \text{Å}$), dielectric environment constant $\kappa = 2.5$ for an impurity strength in the presence of the SiO$_2$ substrate [23], Wigner-Seitz radius $r_s = 0.87592$, and effective Fermi temperature $T = 0.01 \varepsilon_F$.

In the Figs. 1-5, the envelopes of partial differential cross sections $d\Lambda^{(n)}/d\theta$ (22) of SB in graphene for a linearly polarized EM wave are shown as a function of the angle $\theta_0$ between the vectors of the electron initial momentum and electric field strengths of a EM wave, $\theta - \theta_0$ is the electron deflection angle. These figures illustrate SB at different intensities of stimulated wave. Thus, Fig. 1 illustrates elastic part of bremsstrahlung ($n = 0$), while Figs. 2-5 – SB for different number of absorbed photons (or emitted photons at $n < 0$): Fig. 2 – one-photon SB ($n = 1$), Fig. 3 – two-photon SB ($n = 2$), Fig. 4 – three-photon SB ($n = 3$), and Fig. 5 – four-photon SB ($n = 4$), respectively. The angular dependences of partial differential cross sections in these figures are displayed for intensities: in Fig. 1 (a) at $\chi = 0$, (b) $\chi = 1$ ($I_\chi = 3 \times 10^3$ Wcm$^{-2}$), (c) $\chi = 5$ ($I_\chi = 7.7 \times 10^4$ Wcm$^{-2}$), and (d) $\chi = 7$ ($I_\chi = 1.5 \times 10^5$ Wcm$^{-2}$), and in Figs. 2-5: (a) $\chi = 1$, (b) $\chi = 3$ ($I_\chi = 2.7 \times 10^4$ Wcm$^{-2}$), (c) $\chi = 5$, and (d) $\chi = 7$, respectively. As one can see, the angular distribution becomes more asymmetrical with the increasing of the wave intensity. The maximum values of the cross sections correspond to different values of the deflection angle $\theta - \theta_0$.

In Fig. 6 we plot the dependence of envelopes of partial cross sections $n \Lambda^{(n)}$ for a linearly polarized wave upon the number of emitted or absorbed photons. The envelopes are obtained via integrating of the partial differential cross section of SB process $d\Lambda^{(n)}/d\theta$ (22) over scattering angle of the outgoing electron for diverse laser intensities. The angle $\theta_0$ between the initial electron momentum and wave electric field is taken to be: 0, $\pi/6$ rad, and $\pi/2$ rad. As it was expected with the increasing of laser intensity the multiphoton effect becomes dominant compared to the one-photon scattering in linear theory [17]. For THz photons, the multiphoton interaction regime in graphene can be achieved already at the intensities $I_\chi \sim 10^3$ Wcm$^{-2}$. Thus, for these intensities multiphoton SB process opens new channels for the wave absorption, and we can expect strong deviation of absorbance of a single layer doped graphene from linear one, which for frequencies smaller than Fermi energy is zero [24].

In Fig. 7 we display laser-modified elastic cross section $\Lambda^{(0)}$ versus intensity parameter for several initial angle $\theta_0$ between the electron momentum and wave electric field. As is seen from this figure, in the presence of strong radiation field elastic cross section is essentially modified and decreases with the increase of induced radiation intensity. The latter opens up possibility for manipulating of electronic transport properties of the doped graphene by coherent radiation field.
theory it has been investigated the induced scattering of 2D Dirac particles on the charged impurity ions of arbitrary electrostatic potential in the Born approximation and in an external electromagnetic radiation field (actually terahertz radiation to exclude the valence electrons excitations at high Fermi energies). The obtained relativistic analytical formulas for SB at the linear polarization of EM wave have been analyzed numerically for screened Coulomb potential. The latter shows that SB in graphene in the presence of strong radiation field is essentially nonlinear, and the multiphoton absorption/emission processes play significant role already at moderate laser intensities. For these intensities multiphoton SB process opens new channels for the wave absorption, which will essentially modify absorbance of single layer doped graphene compared to the case of linear absorbance (this problem will be presented in the coming paper). Besides, the laser-modified elastic cross section is substantially modified and decreases with the increase of radiation field intensity. The latter opens up possibility for manipulating of electronic transport properties of the doped graphene by coherent radiation field.

**Acknowledgments**

The authors are deeply grateful to the Prof. Hamlet K. Avetissian and Dr. G.F. Mkrtchian for permanent discussions during the work on the present paper, for valuable comments and recommendations. This work was supported by the State Committee of Science MES RA, in the frame of the research project No. 15T-1C013.

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