INVESTIGATION OF NONLINEAR ABSORPTION OF STRONG ELECTROMAGNETIC WAVE IN TWO - DIMENSIONAL GRAPHENE BY USING QUANTUM KINETIC EQUATION METHOD

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Abstract: *Quantum theory of nonlinear absorption of strong electromagnetic wave (EMW) by confined electrons in two - dimensional (2D) graphene without magnetic field has been studied by using the quantum kinetic equation in assumption of electron - optical phonon scattering. The analytic expression of absorption coefficient is obtained in 2D graphene. The results in this case are compared with the case of the bulk semiconductors show the difference and the novelty of the results. The results numerically calculated and plotted show the dependence of absorption coefficient on the photon energy of the electronmagnetic wave and the temperature of the system in 2D graphene.*

Keywords: *Absorption coefficient, Quantum kinetic equation, 2D Graphene, confined electron, Electron - phonon scattering, Electromagnetic wave.*

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1. INTRODUCTION

Quite recently, there has been considerable interest in the behavior of low-dimensional systems, in particular, new two dimensional electron gas (2DEG) systems such as quantum wells, superlattices, silence,… Specially, graphene, as a perfect two-dimensional electron gas (2DEG) system, has been extensively studied both experimentally and theoretically . Since the discovery in 2004 [1] Graphene , it is composed of a single layer of carbon atoms in two dimensional (2D) honeycomb lattice and a unit cell that contains two carbon atoms. Futhermore, electrons in Graphene show relativistic behavior and can be viewd as massless charged fermions in 2D space [1, 2] such as photons or neutrinos. We are aware that although many efforts have been reported to explain different properties of Graphene using a linear response method [3], a detailed consideration of the EMW absorption in Graphene is still

lacking. Therefore, studying the absorption effect is timely and expected to increase our understanding of this new interesting 2D material.

In this paper we theoretically study the nonlinear absorption of strong electromagnetic wave (EMW) in 2D Graphene without magnetic field by using quantun kinetic equation method. We will consider the problem in case of the system is subjected to an EMW with the electric field vector $E = E_0 \sin \Omega t$ (E_0 and Ω are the amplitude and the frequency, respectively). The results show that the 2D Graphene has various characteristic behaviors different from traditional 2D systems such as quantum well, doped superlattice, … [4, 5]. The purpose of this paper is to give clearity expression of nonlinear absorption coefficient EMW in 2D Graphene.

The paper is organized as follows: In the next section we outline a quantum kinetic equation for electrons confined in 2D Graphene. The analytical expression for the nonlinear absorption coefficient in the case of the electron – optical phonon interaction is obtained in Sec. III. The numerical results and brief review are presented in Sec. IV. Finally, conclusions are given in Sec. V.

2. QUANTUM KINETIC QUATION FOR ELECTRONS IN 2D GRAPHENE

2.1. Electron structure and Hamiltonian of the electron – phonon system in 2D Graphene without magnetic field

In this report, we use quantum kinetic equation method to obtain nonlinear absorption coefficient in 2D Graphene in the presence of electromagnetic wave. We consider a 2D Graphene subjected to plane (x – y). The wave function and the corresponding energy [3] are given by the formula below:

$$\Psi_{n,\mathbf{k}}(\mathbf{r}) = \frac{1}{L\sqrt{2}} \begin{bmatrix} e^{-i\theta_{\mathbf{k}}} \\ n \end{bmatrix} \exp(i\mathbf{k}\cdot\mathbf{r}) \tag{1}$$

With L^2 is the area of the system, $n = +1$, and -1 denote the conduction and valence bands, respectively, and

$$k_x = k\cos\theta_{\mathbf{k}} \quad k_x = k\sin\theta_{\mathbf{k}} \quad k = \sqrt{k_x^2 + k_y^2} \tag{2}$$

The corresponding energy is given by

$$\varepsilon_{n,\mathbf{k}} = n\gamma k \tag{3}$$

With $\gamma = 6.46\text{eV}.\overset{0}{\text{A}}$ is a band parameter.

The Hamiltonian of the electron – optical phonon system in 2D Graphene in the second quantization presentation can be written as:

$$\mathrm{H} = \sum_{n,\mathbf{k}} \varepsilon_{n,\mathbf{k}} \left(\mathbf{k} - \frac{e}{c}\mathbf{A}(t) \right) a^{+}_{n,\mathbf{k}} a_{n,\mathbf{k}} + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \left(b^{+}_{\mathbf{q}} b_{\mathbf{q}} + \frac{1}{2} \right) + \sum_{n,n'} \sum_{\mathbf{k},\mathbf{q}} C(\mathbf{q}) a^{+}_{n,\mathbf{k}+\mathbf{q}} a_{n,\mathbf{k}} \left(b^{+}_{\mathbf{q}} + b_{\mathbf{q}} \right) \tag{4}$$

where: $\varepsilon_{n,\mathbf{k}}$ is energy of electron (3), $\mathbf{k},\mathbf{q}$ respectively are wave vectors of electron, phonon, $|n,\mathbf{k}\rangle, |n',\mathbf{k}+\mathbf{q}\rangle$ are electron states before and after scattering, respectively. $a^+_{n,\mathbf{k}}, a_{n,\mathbf{k}}\left(b^+_{\mathbf{q}}, b_{\mathbf{q}}\right)$ are the creation and annihilation operators of electron (phonon).

$|C(\mathbf{q})|^2 = \frac{\hbar D^2_{op}}{2\rho L^2 \omega_{\mathbf{q}}}$ is the electron - optical phonon interaction constant, $\rho = 7.7\times10^{-8}\text{g/cm}^2$ is mass density of 2D Graphene, $D_{op} = 1.4\times10^{-9}\text{eV/cm}$ is deformed potential of optical phonon.

2.2. Quantum kinetic equation for electrons in 2D Graphene

When a high-frequency electromagnetic wave is applied to the system in the y direction with electric field vector $\mathbf{E} = \mathbf{E}_0 \sin\Omega t$ (where $\mathbf{E}_0$ and Ω are the amplitude and the frequency of the electromagnetic wave), the quantum kinetic equation of average number of electron $f_{n,\mathbf{k}} = \left\langle a^+_{n,\mathbf{k}} a_{n,\mathbf{k}} \right\rangle_t$ is:

$$i\hbar \frac{\partial f_{n,\mathbf{k}}(t)}{\partial t} = \left\langle \left[a^+_{n,\mathbf{k}} a_{n,\mathbf{k}}, \mathrm{H} \right] \right\rangle_t . \tag{5}$$

Starting from the Hamiltonian (4) and using the commutative relations of the creation and the annihilation operators, we obtain the quantum kinetic equation for electrons in 2D Graphene :

$$\begin{aligned}\frac{\partial f_{n,\mathbf{k}}(t)}{\partial t} = -\frac{1}{\hbar^2}\sum_{n,n'}\sum_{\mathbf{k},\mathbf{q}}|C(\mathbf{q})|^2 \Big\{ & \Big[f_{n,\mathbf{k}}(t_1) N_{\mathbf{q}} - f_{n',\mathbf{k}+\mathbf{q}_y}(t_1)\left(N_{\mathbf{q}}+1\right)\Big] \\ & \times \exp\left[\frac{i}{\hbar}\left(\varepsilon_{n',\mathbf{k}+\mathbf{q}} - \varepsilon_{n,\mathbf{k}} - \hbar\omega_{\mathbf{q}}\right)(t-t_1) - \frac{ie}{m_e c}\int_{t_1}^{t} \mathbf{q}\cdot\mathbf{A}(t_2)\,dt_2 \right] \\ & - \Big[f_{n',\mathbf{k}+\mathbf{q}}(t_1)(t_1) N_{\mathbf{q}} - f_{n,\mathbf{k}}\left(N_{\mathbf{q}}+1\right)\Big] \\ & \times \exp\left[\frac{i}{\hbar}\left(\varepsilon_{n',\mathbf{k}+\mathbf{q}} - \varepsilon_{n,\mathbf{k}} - \hbar\omega_{\mathbf{q}}\right)(t-t_1) - \frac{ie}{m_e c}\int_{t_1}^{t} \mathbf{q}\cdot\mathbf{A}(t_2)\,dt_2 \right] \Big\}\end{aligned} \tag{6}$$

Where $\mathbf{A}(t) = \frac{\mathbf{E}_0 c}{\Omega}\cos\Omega t$ is vector potential, c being light velocity.

Obtaining explicit solutions from Eq. (6) is seen to be very difficult. In this paper, the first-order tautology approximation method is used to solve this equation. In detail, in Eq. (6), we use the approximation:

$$f_{n,\mathbf{k}}(t_1) \approx \overline{f}_{n,\mathbf{k}} \quad f_{n,\mathbf{k}+\mathbf{q}}(t_1) \approx \overline{f}_{n,\mathbf{k}+\mathbf{q}} \quad f_{n,\mathbf{k}-\mathbf{q}}(t_1) \approx \overline{f}_{n,\mathbf{k}-\mathbf{q}}$$

where $\overline{f}_{n,\mathbf{k}}$ is the time - independent component of the electron distribution function. The approximation is also applied for a similar exercise in bulk semiconductor [6, 7]. As the result, the expression for the unbalanced electron distribution function can be obtained :

$$f_{n,\mathbf{k}}(t)=\frac{1}{\hbar\Omega}\sum_{n,n'}\sum_{\mathbf{k},\mathbf{q}}\left|C(\mathbf{q})\right|^2\sum_{k,\ell=-\infty}^{+\infty}J_{k+\ell}\left(\frac{e\mathbf{E}_0\cdot\mathbf{q}}{m\Omega^2}\right)J_k\left(\frac{e\mathbf{E}_0\cdot\mathbf{q}}{m\Omega^2}\right)\frac{\exp\left(-i\ell\Omega t\right)}{\ell}$$
$$\times\left[\frac{\overline{f}_{n,\mathbf{k}}N_{\mathbf{q}}-\overline{f}_{n',\mathbf{k}+\mathbf{q}}\left(N_{\mathbf{q}}+1\right)}{\varepsilon_{n',\mathbf{k}+\mathbf{q}}-\varepsilon_{n,\mathbf{k}}-\hbar\omega_{\mathbf{q}}-\ell\hbar\Omega+i\hbar\delta}+\frac{\overline{f}_{n,\mathbf{k}}\left(N_{\mathbf{q}}+1\right)-\overline{f}_{n',\mathbf{k}+\mathbf{q}}N_{\mathbf{q}}}{\varepsilon_{n',\mathbf{k}+\mathbf{q}}-\varepsilon_{n,\mathbf{k}}+\hbar\omega_{\mathbf{q}}-\ell\hbar\Omega+i\hbar\delta}\right.$$
$$\left.+\frac{\overline{f}_{n',\mathbf{k}-\mathbf{q}}N_{\mathbf{q}}-\overline{f}_{n,\mathbf{k}}\left(N_{\mathbf{q}}+1\right)}{\varepsilon_{n,\mathbf{k}}-\varepsilon_{n',\mathbf{k}-\mathbf{q}}-\hbar\omega_{\mathbf{q}}-\ell\hbar\Omega+i\hbar\delta}-\frac{\overline{f}_{n',\mathbf{k}-\mathbf{q}}\left(N_{\mathbf{q}}+1\right)-\overline{f}_{n,\mathbf{k}}N_{\mathbf{q}}}{\varepsilon_{n,\mathbf{k}}-\varepsilon_{n',\mathbf{k}-\mathbf{q}}+\hbar\omega_{\mathbf{q}}-\ell\hbar\Omega+i\hbar\delta}\right] \quad (7)$$

where $N_{\mathbf{q}}$ is the time-independent component of the phonon distribution function, $J_k\left(x\right)$ is the Bessel function and the quantity δ is infinitesimal and appears due to the assumption of an adiabatic interaction of the electromagnetic wave.

2.3. The nonlinear absorption coefficient of strong electromagnetic wave in 2d graphene

The carrier current density formula in 2D Graphene takes the form :

$$\mathbf{J}\left(t\right)=\frac{e\hbar}{m}\sum_{n,\mathbf{k}}\left[\mathbf{k}-\frac{e}{\hbar c}\mathbf{A}\left(t\right)\right]f_{n,\mathbf{k}}\left(t\right) \quad (8)$$

Because the motion of electrons is confined along the z direction in a 2D Graphene, we only consider the in plane (x, y) current density vector of electrons $\mathbf{J}\left(t\right)$. Substituting Eq. (7) into Eq. (8), we find the expression for current density vector:

$$\mathbf{J}\left(t\right)=-\frac{e^2\mathbf{E}_0n_0}{m_e\Omega}\cos\Omega t+\mathbf{J}_0\left(t\right) \quad (9)$$

here:

$$\mathbf{J}_0\left(t\right)=-\frac{e}{m_e\Omega}\sum_{n,n'}\sum_{\mathbf{k},\mathbf{q}}\left|C(\mathbf{q})\right|^2\mathbf{q}\cdot N_{\mathbf{q}}\sum_{k,\ell=-\infty}^{+\infty}J_{k+\ell}\left(\frac{e\mathbf{E}_0\cdot\mathbf{q}}{m\Omega^2}\right)J_k\left(\frac{e\mathbf{E}_0\cdot\mathbf{q}}{m\Omega^2}\right)\frac{\exp\left(-i\ell\Omega t\right)}{\ell}$$
$$\times\left[\frac{\overline{f}_{n',\mathbf{k}+\mathbf{q}}}{\varepsilon_{n',\mathbf{k}+\mathbf{q}}-\varepsilon_{n,\mathbf{k}}-\hbar\omega_{\mathbf{q}}-k\hbar\Omega}+\frac{\overline{f}_{n',\mathbf{k}+\mathbf{q}}}{\varepsilon_{n',\mathbf{k}+\mathbf{q}}-\varepsilon_{n,\mathbf{k}}+\hbar\omega_{\mathbf{q}}-k\hbar\Omega}\right.$$
$$\left.+\frac{\overline{f}_{n',\mathbf{k}-\mathbf{q}}}{\varepsilon_{n,\mathbf{k}}-\varepsilon_{n',\mathbf{k}-\mathbf{q}}-\hbar\omega_{\mathbf{q}}-k\hbar\Omega}-\frac{\overline{f}_{n',\mathbf{k}-\mathbf{q}}}{\varepsilon_{n,\mathbf{k}}-\varepsilon_{n',\mathbf{k}-\mathbf{q}}+\hbar\omega_{\mathbf{q}}-k\hbar\Omega}\right] \quad (10)$$

And $\sum_{n,\mathbf{k}} f_{n,\mathbf{k}}(t) = n_0$ is electron density of 2D Graphene.

By using the electron - optical phonon interaction factor in Eq. (4) and the Bessel function [8, 9], from the expression for the current density vector Eq. (10) we establish the nonlinear absorption coefficient of the electromagnetic wave :

$$\begin{aligned}\alpha &= \frac{8\pi}{c\sqrt{\chi_\infty}E_0^2}\left\langle \mathbf{J}(t)\cdot\mathbf{E}_0 \sin\Omega t\right\rangle_t \\ &= \frac{8\pi^2\Omega}{c\sqrt{\chi_\infty}E_0^2}\sum_{\mathbf{q}}\left|C(\mathbf{q})\right|^2 N_{\mathbf{q}} \sum_k kJ_k^2\left(\frac{e\mathbf{q}\cdot\mathbf{E}_0}{m_e\Omega^2}\right)\sum_{n',n,\mathbf{k}}\overline{f}_{n,\mathbf{k}}(t)\delta\left(\varepsilon_{n',\mathbf{k}+\mathbf{q}}-\varepsilon_{n,\mathbf{k}}+\hbar\omega_{\mathbf{q}}-k\hbar\Omega\right)\end{aligned} \tag{11}$$

where $\langle X\rangle_t$ means the usual thermodynamic average of X at moment t, and χ_∞ is the high-frequency dielectric constants, $\delta(x)$ is the Dirac delta function. For simplicity, in this paper, we limit the problem to the cases of $k = 0, \pm 1$, this means that the processes with more than one photon are ignored:

$$J_{\pm1}\left(\frac{e\mathbf{q}\cdot\mathbf{E}_0}{m_e\Omega^2}\right) = \frac{1}{4}\left(\frac{e\mathbf{q}\cdot\mathbf{E}_0}{m_e\Omega^2}\right)^2 \tag{12}$$

When the temperature of the system is high (T > 50K), the electron – optical phonon interaction is higher than other interactions. In this case, electron gas is assumed that non-generated gas and abided by the Maxwell – Boltzmann distribution. Let assume that phonon is not dispersive means is the optical phonon frequency non-dispersion:

$$\hbar\omega_{\mathbf{q}} = \hbar\omega_0 \quad N_{\mathbf{q}} = \frac{k_B T}{\hbar\omega_0} \tag{13}$$

After some calculation, we find the expression for absorption coefficient:

$$\alpha = \frac{e^2 n_0 D_{op}^2 k_B T}{8c\sqrt{\chi_\infty}\rho\omega_0^2\Omega^3 m_e^2\gamma}\exp\left(\frac{\hbar\Omega-\hbar\omega_0}{2k_B T}\right)\int_0^{+\infty} q^2\exp\left(-\frac{\gamma q}{2k_B T}\right)dq \tag{14}$$

We use the integral results in [9]:

$$\int_0^{+\infty} x^n \exp(-\mu x)\,dx = n!\,\mu^{-n-1} \tag{15}$$

Finally, inserting (15) into (14) we find the explicit expression for the absorption coefficient is written as:

$$\alpha = \frac{16 n_0 e^2 D_{op}^2 (k_B T)^7}{c\sqrt{\chi_\infty}\rho\omega_0^2\Omega^3\gamma^7 m_e^2}\exp\left(\frac{\hbar\Omega-\hbar\omega_0}{2k_B T}\right) \tag{16}$$

As one can see, Eq. (16) is more simple than traditional two dimensional semiconductors, it depends only on the temperature of the system and the energy photon (

$\hbar\Omega$) of electromagnetic wave. In the following, we will give physical conclusions to above results by carrying out a numerical evaluation and a graphic consideration using a computational method.

2.3. Numerical results and discussion

In this section, we give a deeper insight to the absorption coefficient for the case of a special 2D Graphene. For this section, the parameters used in computational calculations are as follows [1, 5] in Table I:

Table 1. The parameters

Symbols	Units	Values
ρ	g/cm^2	7,7.10^{-8}
D_{op}	eV/cm	1,4.10^{-9}
k_B	J/K	1,3807.10^{-23}
$\hbar\omega_o$	meV	162
c	m/s	3.10^8
$\hbar$	J.s	1,05459.10^{-34}
χ_∞		10,9
γ	eV. $\overset{o}{A}$	6,46
n_0		10^{12}

2.4. The dependence of absorption coefficient on temperature

The effect of temperature on the absorption coefficient due to optical phonon scattering is illustrated in Fig. 1. As can be seen from this figure that the absorption coefficient α depends strongly and non-linearly on temperature of the system.

We can see that absorption coefficient reaches at the saturated value in the low-temperature regime and increases quickly when temperature is high (T > 100K). This is in good agreement with previous results by using similar method in other two-dimensional systems [11, 12, 13]. This coefficient absorption is the same as the results which gained in bulk semiconductors [6, 7]. In addition, we survey influent of EMW on absorption

coeffiecient in 3 diffient single values of photon energy, it can be obviously seen that when photon energy increases the absorption coefficient value move up as the same tendency [11].

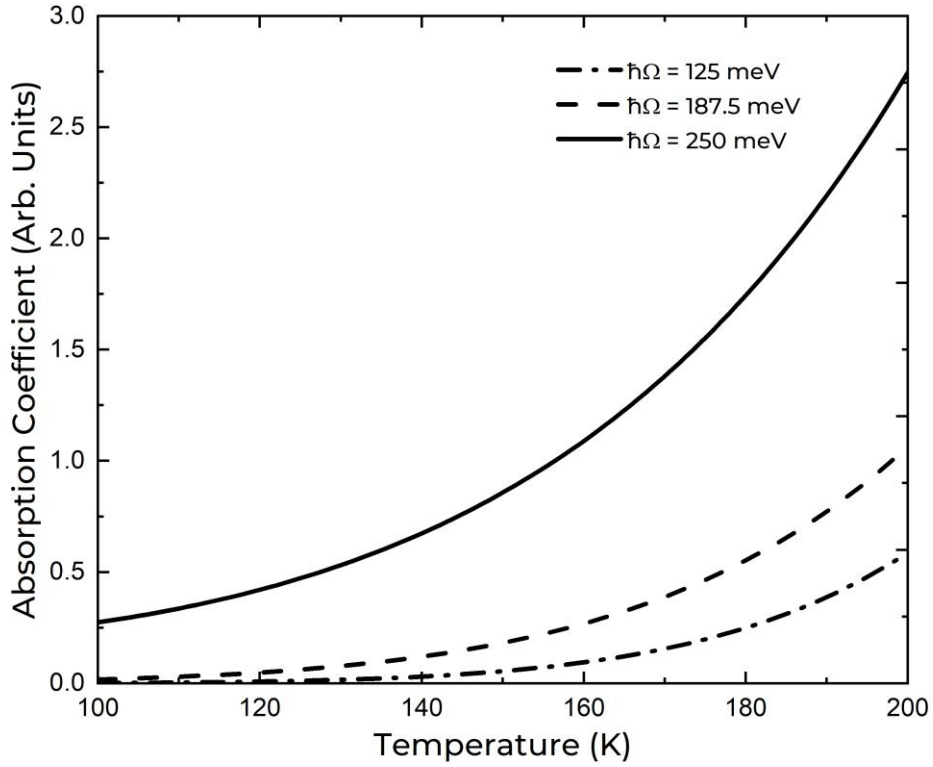

Fig. 1. The dependence of α on T at 3 diffirent values of photon energy $\hbar\Omega$

2.5. The dependence of absorption coefficient on photon energy

In order to analyse the physical expression of absorption coefficient in system parameters, we investigate and graph the influence of absorption coefficient on photon energy and 3 different cases of Temperture. The solid line means the highest temperature value case (T=220K), the dotted-line stands for the lowest temperature value case (T=180K) and the one case left is dashed-line (T=190K). We can easily obtain that the absorption coefficient goes up gradually as the Temperature rises. Then, when the photon energy stays in low value domain, the 3-line graph chance to one curve which mean the absorption coefficient is independent from the temperature when low photon energy.

Furthermore, also in considering of low photon energy regime, the absorption coefficient graph is almost linear line. The above analysis is the physical expression of absorption coefficient in photon energy and temperature. This is diffirent from that for Quantum Wells – another 2D system [11] (in Quantum Wells, the absorption coefficient reaches one maximun peak). This results from the difference between the electron structure of Graphene and Quantum Wells. This prediction would give a good suggestion for further experiments in the future. We can use this effect as one of the criteria for 2D Graphene

fabrication technology.

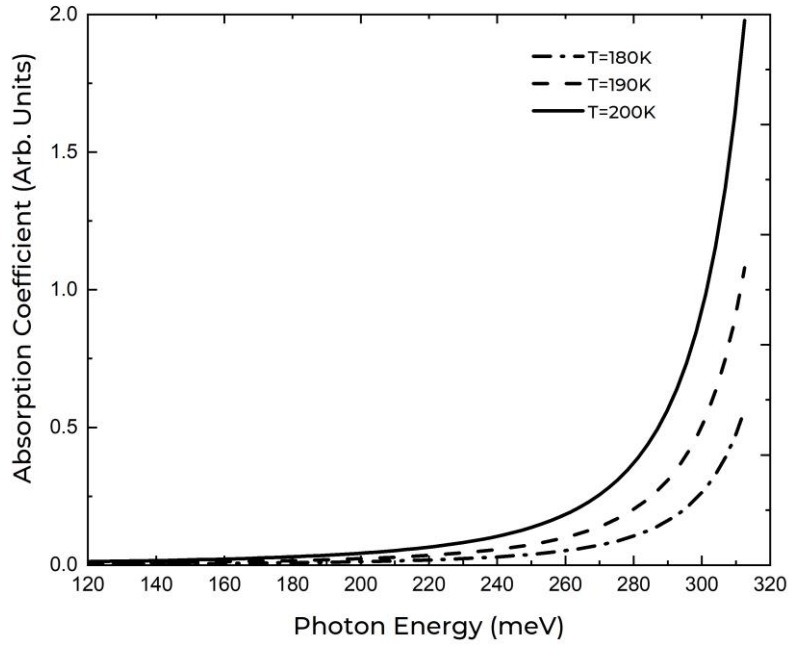

Fig. 2. The dependence of α on photon energy at 3 diffirent values of temperature.

3. CONCLUSION

In this work, we have studied the linear absorption coefficient, as well as the differences in monolayer Graphene in the presence of an external electromagnetic wave. By using Quantum Kinetic Equation method, we obtained the expression of the absorption coefficient due to the propagation of EMW in system, which can be changed by the photon energy of external EMW and the temperature of system. An strong increase of absorption coefficient towards higher temperature domain. In addition, the results show the dependence of the absorption coefficient on photon energy is quite strong in high temperature range. These theoretical results show a potential of 2D Graphene as a new two – dimensional material gas for designing nano-electronic and optical devices as a promising alternative to other traditional semiconductors.

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NGHIÊN CỨU VỀ HẤP THỤ PHI TUYẾN SÓNG ĐIỆN TỪ MẠNH TRONG GRAPHENE HAI CHIỀU BẰNG PHƯƠNG PHÁP PHƯƠNG TRÌNH ĐỘNG LƯỢNG TỬ

Tóm tắt: *Nghiên cứu lý thuyết lượng tử hấp thụ phi tuyến sóng điện từ mạnh (EMW) trong Graphene hai chiều (2D) bằng phương trình động lượng tử với giả thiết cơ chế tán xạ electron-phonon quang. Thu được biểu thức giải tích cho hệ số hấp thụ trong Graphene 2D. Các kết quả là mới mẻ và được so sánh với trường hợp trong bán dẫn thấp chiều truyền thống để thấy sự khác biệt. Kết quả thu nhận được tính toán số và vẽ đồ thị biểu thị sự phụ thuộc của hệ số hấp thụ vào năng lượng photon của sóng điện từ và nhiệt độ của hệ Graphene 2D.*

Từ khóa: *Hệ số hấp thụ, phương trình động lượng tử, 2D Graphene, electron giam cầm, tán xạ electron-phonon, sóng điện từ.*