Enhancement of optical transitions in graphene by attraction between electrons and holes.

M.V. Entin, M.M. Mahmoodian

Institute of Semiconductor Physics, Siberian Branch, Russian Academy of Sciences,
pr. Lavrent'eva 13, Novosibirsk, 630090 Russia
mahmood@isp.nsc.ru

Abstract

Graphene is known to have a remarkable optical absorption coefficient $\pi\alpha$ determined by the fine-structure constant α. This value is found in the Born approximation and it does not take into account the single-electron spectrum reconstruction due to the interaction.

Electron-hole interaction is important factor mediating on the optical transitions. In bulk gapped semiconductors with central c and v bands the influence of e-h interaction is connected with the Sommerfeld factor $Z = |\psi(0)|^2$ which is determined by the electron-hole envelope function $\psi(r)$ at zero distance between electron and hole. The attraction between them strongly enhances the probability of transition near the absorption threshold. The absorption threshold behavior proportional to electron-hole DOS $\nu(\hbar\omega - E_g) \propto \sqrt{\hbar\omega - E_g}$ is replaced by $Z\nu(\hbar\omega - E_g)$, where

$$Z = \frac{2\pi}{q(1 - e^{-2\pi/q})}, \quad q = \frac{\hbar\chi}{e^2}\sqrt{2(\hbar\omega - E_g)/m},$$

m is a e-h pair reduced mass, χ is a dielectric constant of medium, e is an electron charge, ω is the light frequency, E_g is the bandgap. As a result, the absorption at the threshold has a gap, instead vanishing. The parameter $2\pi/q$ is a dimensionless interaction constant which determines the interaction correction value. The Bohr energy $me^4/(\chi^2\hbar^2)$ plays role of a characteristic energy: at large detuning from the threshold the transition probability goes to the Born result for non-interacting particles.

The purpose of the present study is to find the e-h-interaction-induced correction to the absorption coefficient κ of graphene. The conic gapless electron spectrum of graphene determines energy-independent dimensionless constant of e-h interaction $g = e^2/(\chi\hbar s)$, where s is an electron velocity. Besides, in free-suspended graphene this constant has large order. We found that κ obtains the additional Sommerfeld factor $Z = |\psi(0)|^2$ originating from e-h interaction of the unbounded pair, that essentially enhances the absorption at small frequencies. The consideration is limited by the case $g \ll 1$. The enhancement of the exciton effect results from singular behavior of the envelope wave function at small interparticle distance.

The two-particle problem for electron and hole pair can be transformed to the basis of free electron and hole wave functions:

$$|\mathbf{p}_e\rangle = \begin{pmatrix} p_{ex} + ip_{ey} \\ -p_e \end{pmatrix} \frac{1}{\sqrt{2}p_e} e^{i\mathbf{p}_e\mathbf{r}_e}, \tag{1}$$

$$|\mathbf{p}_h\rangle = \begin{pmatrix} p_{hx} - ip_{hy} \\ p_h \end{pmatrix} \frac{1}{\sqrt{2}p_h} e^{i\mathbf{p}_h\mathbf{r}_h}. \tag{2}$$

Matrix element of e-h interaction potential $V(\mathbf{r}) = -e^2/(\chi r), \mathbf{r} = \mathbf{r}_e - \mathbf{r}_h$, in the basis of $|\mathbf{p}_e, \mathbf{p}_h\rangle = |\mathbf{p}_e\rangle|\mathbf{p}_h\rangle$ is

$$V_{\mathbf{p}_e, \mathbf{p}_h, \mathbf{p}'_e, \mathbf{p}'_h} = \langle \mathbf{p}'_e, \mathbf{p}'_h | V(\mathbf{r}_e - \mathbf{r}_h) | \mathbf{p}_e, \mathbf{p}_h \rangle. \tag{3}$$

For zero summary momentum $\mathbf{p}_e = -\mathbf{p}_h = \mathbf{p}$

$$V_{\mathbf{p},\mathbf{p}'} = \frac{B(\mathbf{p}, \mathbf{p}')}{4p^2 p'^2}, \quad B(\mathbf{p}, \mathbf{p}') = (\mathbf{p}\mathbf{p}' + pp')^2 + [\mathbf{p} \times \mathbf{p}']^2. \tag{4}$$

The integral Schrödinger equation $(\hat{H}_0 + \hat{V})\psi = \varepsilon\psi$ for the envelope function of the relative motion in the momentum representation takes form:

$$2sp\psi(p) + \int \frac{d^2p'}{(2\pi)^2} V(\mathbf{p} - \mathbf{p}')B(\mathbf{p}, \mathbf{p}')\psi(p') = \varepsilon\psi(p). \tag{5}$$

Here $V(\mathbf{q}) = \frac{2\pi}{q}\frac{e^2}{\chi}$. Integrating over polar angle in Eq. (5) we get

$$2sp\psi(p) - \frac{gsp}{2} \int w(x)\psi(xp)dx = \varepsilon\psi(p), \tag{6}$$

where

$$w(x) = \frac{1}{2\pi|x-1|}\left\{(x+1)^2 K\left[-\frac{4x}{(x-1)^2}\right] - (x-1)^2 E\left[-\frac{4x}{(x-1)^2}\right] + \right.$$

$$\left. |x^2-1|\left(K\left[\frac{4x}{(x+1)^2}\right] - E\left[\frac{4x}{(x+1)^2}\right]\right)\right\} \simeq \left\{\begin{array}{ll} x, & x \ll 1, \\ 1, & x \gg 1, \end{array}\right.$$

$K(x)$ and $E(x)$ are the complete elliptic integrals. If $2sp \gg \varepsilon$ we can rewrite Eq. (6) as

$$\psi(p) = \frac{g}{4}\int\limits_{\varepsilon/2sp}^{1} w(x)\psi(xp)dx \qquad (7)$$

and solve it in an iterative manner with zero order approximation $\psi^{(0)}(p) = \delta(2sp - \varepsilon)$. The result reads

$$\psi(p) = \psi^{(0)}(p) + \frac{g}{4\varepsilon}\left(\frac{2sp}{\varepsilon}\right)^{g/4-2}, \qquad (8)$$

and

$$\psi(r) = \psi^{(0)}(r)\left[1 + \left(\frac{2s}{\varepsilon r}\right)^{g/4}\right]. \qquad (9)$$

The wave function goes to infinity at $r \to 0$. To limit the divergency, we set $r = a$, where a is the lattice constant. Hence, $Z = |\psi(0)/\psi^{(0)}(0)|^2 = \left(1 + \left(\frac{4s}{\hbar\omega a}\right)^{g/4}\right)^2$ and the absorption coefficient is $\pi\alpha Z$. If $g\ln\frac{4s}{\hbar\omega a} \gg 1$, the absorption coefficient is much larger than α.

Note, that there is another interaction-induced contribution to the absorption coefficient caused by the renormalization of single-electron energy [1]. In our opinion, if $g\ln\frac{4s}{\hbar\omega a} \gg 1$ this contribution is less essential than e-h-attraction-induced. At the same time our result differs from that of [1], may be due non-correct collection of powers of $g\ln\frac{4s}{\hbar\omega a}$ made in [1]. As a result, the absorption coefficient grows at $\omega \to 0$, instead dropping predicted in [1].

We should emphasize that the singularity of the absorption coefficient results from the singularity of the conic spectrum. In analogy with the electron-electron scattering [2] and exciton formation [3], one could expect that the trigonal correction to the single-electron spectrum essentially corrects the absorption coefficient behavior. In fact, it is not the case. One can show that just conic character of the spectrum makes trigonal corrections inessential near the threshold.

References

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