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Attractive electron correlation in wide band gap semiconductors by electron–photon interaction

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Abstract

We theoretically demonstrate attractive electron correlation in wide band gap semiconductors by electron–photon interaction. At low temperature, wavevectors of electromagnetic waves absorbed in wide band gap semiconductors cannot be neglected for wavevectors of electron waves; that is, electromagnetic waves affect the movements of electrons. In particular, attractive interaction occurs between two electrons when one electron changes from a valence band to a conduction band and the other electron changes from a conduction band to a valence band.

1. Introduction

In semiconductors, the absorption of electromagnetic waves caused by electron–photon interaction has attracted much attention from practical and fundamental viewpoints for many years [1–3]. This property has been used for electronic devices such as lasers and diodes, and has provided various valuable applications. Thus far, optical properties of semiconductors resulting from electron–photon interaction have mainly been studied, disregarding the effects of electromagnetic waves on the movements of electrons. Since a wavevector of electromagnetic waves is approximately $q = 5.07 \times 10^6\ \mathrm{m}^{-1}$ for band gaps approximately 1 eV in conventional semiconductors, q can be neglected for the wavevector of electron waves $k = 4.8 \times 10^8\ \mathrm{m}^{-1}$ at $T = 100$ K.

Recently, however, wide band gap semiconductors have also been studied from experimental and theoretical viewpoints. A research target of wide band gap semiconductors is to obtain electromagnetic waves with short wavelengths. For example, AlN ($E_g = 6.2$ eV) and $KBeF_3$ ($E_g = 8.1$ eV) have been reported experimentally and theoretically, respectively [4, 5]. Since the wavevector of electromagnetic waves at $E_g = 10$ eV is approximately $q = 5.07 \times 10^7\ \mathrm{m}^{-1}$, for example, q cannot be neglected for wavevectors of electron waves with $k = 4.8 \times 10^7\ \mathrm{m}^{-1}$ at $T = 1$ K. Therefore, we must consider the effects of the electromagnetic waves on the movements of electron waves. An impact of the photon wavevector transferred to photogenerated carriers has been proposed and studied [6, 7].

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In this paper, therefore, we investigate electron–photon interaction in wide band gap semiconductors, considering the effects of wavevectors of electromagnetic waves on those of electron waves. As is well known, electron–phonon interaction has attracted great interest since superconductivity can be explained by attractive interaction of electrons on the basis of electron–phonon interaction [8–10]. However, it should be noted that electron–photon interaction is similar to electron–phonon interaction, since photons and phonons are both bosons. Therefore, we explore the possibility of attractive electron–photon interaction.

In metals, electron correlation by electron–photon interaction depends on the wavevectors of electrons, and therefore, effective attractive interaction cannot be achieved. In wide band gap semiconductors, on the other hand, electron correlation exists independently of the wavevectors of electrons. We theoretically demonstrate electron–photon interaction by the same method as used in the BCS theory. This method is appropriate to discuss electron–photon interaction.

Although electron–electron interaction is generally repulsive, the repulsive interaction decreases under the influence of attractive electron correlation by electron–photon interaction, which means the tuning of electron correlation by photons. Moreover, superconductivity by electron–photon interaction may be expected in the case that attractive electron correlation exceeds repulsive electron interaction, although Bose condensation must be considered. In this paper, however, we do not discuss the possibility of superconductivity by electron–photon interaction.

2. Nonperturbation and perturbation Hamiltonians of electron–photon interaction

By using creation and annihilation operators, the vector potential of electromagnetic waves is represented as

$$\mathbf{A}(\mathbf{r}) = \tfrac{1}{2}\sum_{\mathbf{q},\lambda} A_{\mathbf{q},\lambda}\mathbf{e}_{\mathbf{q},\lambda}\{a_{\mathbf{q},\lambda} + a^{\dagger}_{-\mathbf{q},\lambda}\}\exp(\mathrm{i}\mathbf{q}\cdot\mathbf{r}), \tag{1}$$

where

$$A_{\mathbf{q},\lambda} = \sqrt{\frac{2\hbar}{\varepsilon\Omega\omega_{\mathbf{q}}}}. \tag{2}$$

$\mathbf{q}$ and λ indicate a wavevector and one of two polarizations of electromagnetic waves. $A_{\mathbf{q},\lambda}$ and $\mathbf{e}_{\mathbf{q},\lambda}$ are a coefficient and a polarized unit vector of a vector potential, respectively. $a_{\mathbf{q},\lambda}$ and $a^{\dagger}_{\mathbf{q},\lambda}$ are the annihilation and creation operators of electromagnetic waves, respectively. ε, Ω and $\omega_{\mathbf{q}}$ are the dielectric index, the volume of crystals and the frequency of electromagnetic waves, respectively. $\mathbf{A}(\mathbf{r})$ is assumed to satisfy the Coulomb gauge, $\nabla\cdot\mathbf{A}(\mathbf{r}) = 0$.

The nonperturbation Hamiltonian is

$$H_0 = H_{\text{electron}} + H_{\text{photon}} = \sum_{i=c,v}\sum_{\mathbf{k},\sigma}\varepsilon^{(i)}_{\mathbf{k}}c^{(i)\dagger}_{\mathbf{k},\sigma}c^{(i)}_{\mathbf{k},\sigma} + \sum_{\mathbf{q},\lambda}\hbar\omega_{\mathbf{q}}a^{\dagger}_{\mathbf{q},\lambda}a_{\mathbf{q},\lambda}. \tag{3}$$

H_{electron} and H_{photon} are Hamiltonians of electrons and photons, respectively. $\mathbf{k}$ and σ are the wavevector and the spin of electrons. $c^{(i)}_{\mathbf{q},\lambda}$ and $c^{(i)\dagger}_{\mathbf{q},\lambda}$ are annihilation and creation operators of electrons, respectively. $\varepsilon^{(i)}_{\mathbf{k}}$ is the energy of electrons, and c and v indicate conduction and valence bands, respectively.

By Bloch's theorem, the wavefunction of electrons is

$$\psi(\mathbf{r}) = \sum_{i=c,v}\sum_{\mathbf{k},\sigma}c^{(i)}_{\mathbf{k},\sigma}u^{(i)}_{\mathbf{k},\sigma}(\mathbf{r})\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r}). \tag{4}$$

The interaction Hamiltonian is represented as

$$H_{\rm int} = H_{\rm electron-photon} = \int_\Omega {\rm d}\mathbf{r}\, \psi^\dagger(\mathbf{r}) \frac{e}{m}\mathbf{A}(\mathbf{r})\cdot\mathbf{p}(\mathbf{r})\psi(\mathbf{r})$$
$$= \sum_{i,j}\sum_{\mathbf{k}',\sigma'}\sum_{\mathbf{k},\sigma}\sum_{\mathbf{q},\lambda}\frac{e}{2m}A_{\mathbf{q},\lambda}c^{(j)\dagger}_{\mathbf{k}',\sigma'}(a_{\mathbf{q},\lambda}+a^\dagger_{-\mathbf{q},\lambda})c^{(i)}_{\mathbf{k},\sigma}$$
$$\times \int_\Omega {\rm d}\mathbf{r}\, \exp\{{\rm i}(-\mathbf{k}'+\mathbf{k}+\mathbf{q})\cdot\mathbf{r}\}u^{(j)*}_{\mathbf{k}',\sigma'}(\mathbf{r})\mathbf{e}_{\mathbf{q},\lambda}\cdot\{\mathbf{p}(\mathbf{r})+\hbar\mathbf{k}\}u^{(i)}_{\mathbf{k},\sigma}(\mathbf{r}). \tag{5}$$

Let us consider the normal process; that is, $\mathbf{k}' = \mathbf{k}+\mathbf{q}$ and $\sigma' = \sigma$. Then we focus our attention on the integral term in equation (5).

$$M^{j,i}_{\mathbf{k},\sigma;\mathbf{q},\lambda} = \int_\Omega {\rm d}\mathbf{r}\, u^{(j)*}_{\mathbf{k}+\mathbf{q},\sigma}(\mathbf{r})\mathbf{e}_{\mathbf{q},\lambda}\cdot\{\mathbf{p}(\mathbf{r})+\hbar\mathbf{k}\}\, u^{(i)}_{\mathbf{k},\sigma}(\mathbf{r})$$
$$\approx \int_\Omega {\rm d}\mathbf{r}\, u^{(j)*}(\mathbf{r})\mathbf{e}_{\mathbf{q},\lambda}\cdot\mathbf{p}(\mathbf{r})u^{(i)}(\mathbf{r}) + \mathbf{e}_{\mathbf{q},\lambda}\cdot\hbar\mathbf{k}\int_\Omega {\rm d}\mathbf{r}\, u^{(j)*}(\mathbf{r})u^{(i)}(\mathbf{r})$$
$$= \langle j|\mathbf{e}_{\mathbf{q},\lambda}\cdot\mathbf{p}(\mathbf{r})|i\rangle(1-\delta_{i,j}) + \mathbf{e}_{\mathbf{q},\lambda}\cdot\hbar\mathbf{k}\delta_{i,j}. \tag{6}$$

$\delta_{i,j}$ is Kronecker's delta. For simplicity, we neglect dependences of $u^{(i)}_{\mathbf{k},\sigma}$ on $\mathbf{k}$ and σ, similarly to absorption of electromagnetic waves in conventional semiconductors. The first term in equation (6) is zero at $i = j$, while the second term in equation (6) is zero at $i \neq j$. Therefore, $H_{\rm int}$ is represented as

$$H_{\rm int} = \sum_{i,j}\sum_{\mathbf{k},\sigma}\sum_{\mathbf{q},\lambda} D^{j,i}_{\mathbf{k},\sigma;\mathbf{q},\lambda}c^{(j)}_{\mathbf{k}+\mathbf{q},\sigma}(a_{\mathbf{q},\lambda}+a^\dagger_{-\mathbf{q},\lambda})c^{(i)}_{\mathbf{k},\sigma}, \tag{7}$$

where

$$D^{j,i}_{\mathbf{k},\sigma;\mathbf{q},\lambda} = \frac{eA_{\mathbf{q},\lambda}M^{j,i}_{\mathbf{k},\sigma;\mathbf{q},\lambda}}{2m}. \tag{8}$$

This interaction Hamiltonian is similar to that of electron–phonon interaction although $D^{j,i}_{\mathbf{k},\sigma;\mathbf{q},\lambda}$ is independent of $\mathbf{k}$ in electron–phonon interaction, in contrast to electron–photon interaction.

3. Effective electron–photon interaction

The Hamiltonian of the electron–photon interaction is represented as

$$H = H_0 + H_{\rm int}. \tag{9}$$

By the method used in the BCS theory, we obtain the following effective Hamiltonian:

$$\tilde{H} = e^{-S}He^S = H_0 + \tfrac{1}{2}[H_{\rm int}, S] + {\rm O}(S^3), \tag{10}$$

where

$$H_{\rm int} = [S, H_0]. \tag{11}$$

The second term in equation (10) corresponds to the effective electron–photon interaction. By the same method as used in the BCS theory, the electron correlation by electron–photon interaction is

$$H_{\rm eff} = \tfrac{1}{2}\langle 0|[H_{\rm int}, S]|0\rangle = -\tfrac{1}{2}\sum_{i',j'}\sum_{i,j}\sum_{\mathbf{k}',\sigma'}\sum_{\mathbf{k},\sigma}\sum_{\mathbf{q},\lambda} D^{j',i'}_{\mathbf{k}',\sigma';\mathbf{q},\lambda}D^{j,i}_{\mathbf{k},\sigma;-\mathbf{q},\lambda}$$
$$\times\left\{\frac{\hbar\omega_{\mathbf{q}}}{(\hbar\omega_{\mathbf{q}})^2-(\varepsilon^{(i)}_{\mathbf{k}}-\varepsilon^{(j)}_{\mathbf{k}-\mathbf{q}})^2}+\frac{\hbar\omega_{\mathbf{q}}}{(\hbar\omega_{\mathbf{q}})^2-(\varepsilon^{(i)}_{\mathbf{k}'}-\varepsilon^{(j)}_{\mathbf{k}'+\mathbf{q}})^2}\right\}$$
$$\times c^{(j')\dagger}_{\mathbf{k}'+\mathbf{q},\sigma'}c^{(i')}_{\mathbf{k}',\sigma'}c^{(j)\dagger}_{\mathbf{k}-\mathbf{q},\sigma}c^{(i)}_{\mathbf{k},\sigma}. \tag{12}$$

At $i = j$ or $i' = j'$, $D^{j,i}_{\mathbf{k},\sigma;-\mathbf{q},\lambda}$ and $D^{j',i'}_{\mathbf{k}',\sigma';\mathbf{q},\lambda}$ depend on $\mathbf{k}$ and $\mathbf{k}'$, respectively, as shown in equation (6). That is, it depends on $\mathbf{k}$ and $\mathbf{k}'$ whether H_{eff} is attractive or repulsive. Therefore, sums of such interactions become very small. For metals, only the second term exists in equation (6) since there are no differences in the conduction and valence bands. Therefore, effective electron–photon interaction cannot be achieved in metals.

At $i \neq j$ and $i' \neq j'$, on the other hand, $D^{j,i}_{\mathbf{k},\sigma;-\mathbf{q},\lambda}$ and $D^{j',i'}_{\mathbf{k}',\sigma';\mathbf{q},\lambda}$ are independent of $\mathbf{k}$ and $\mathbf{k}'$, as shown in equation (6). Particularly at $i = j'$ and $j = i'$,

$$D^{i,j}_{\mathbf{k}',\sigma';\mathbf{q},\lambda} D^{j,i}_{\mathbf{k},\sigma;-\mathbf{q},\lambda} = \left(\frac{e}{2m}\right)^2 |A_{\mathbf{q},\lambda}|^2 \left|\langle i|\mathbf{e}_{\mathbf{q},\lambda}\cdot\mathbf{p}(\mathbf{r})|j\rangle\right|^2 \geqslant 0. \tag{13}$$

This term is positive regardless of $\mathbf{k}$, $u^{(i)}$ or $u^{(j)}$, and therefore, we focus our attention only on this interaction. Then, the electron correlation is represented as

$$\begin{aligned} H_{\mathrm{eff}} = -\frac{1}{2}\sum_{i\neq j}\sum_{\mathbf{k}',\sigma'}\sum_{\mathbf{k},\sigma}\sum_{\mathbf{q},\lambda}\left(\frac{e}{2m}\right)^2 |A_{\mathbf{q},\lambda}|^2 \left|\langle i|\mathbf{e}_{\mathbf{q},\lambda}\cdot\mathbf{p}(\mathbf{r})|j\rangle\right|^2 \\ \times \left\{\frac{\hbar\omega_{\mathbf{q}}}{(\hbar\omega_{\mathbf{q}})^2 - (\varepsilon^{(i)}_{\mathbf{k}'} - \varepsilon^{(j)}_{\mathbf{k}'+\mathbf{q}})^2} + \frac{\hbar\omega_{\mathbf{q}}}{(\hbar\omega_{\mathbf{q}})^2 - (\varepsilon^{(i)}_{\mathbf{k}} - \varepsilon^{(j)}_{\mathbf{k}-\mathbf{q}})^2}\right\} \\ \times c^{(i)\dagger}_{\mathbf{k}'+\mathbf{q},\sigma'} c^{(j)}_{\mathbf{k}',\sigma'} c^{(j)\dagger}_{\mathbf{k}-\mathbf{q},\sigma} c^{(i)}_{\mathbf{k},\sigma}. \end{aligned} \tag{14}$$

This interaction occurs between two electrons when one electron changes from a valence band to a conduction band and the other one changes from a conduction band to a valence band. This could be realized by a strong inversion population of electrons from a valence band to a conduction band. Since electrons near band gaps affect electronic properties, $(\varepsilon^{(i)}_{\mathbf{k}} - \varepsilon^{(j)}_{\mathbf{k}\pm\mathbf{q}})^2 \approx E_{\mathrm{g}}^2$ is satisfied. Moreover,

$$\langle i|\mathbf{e}_{\mathbf{q},\lambda}\cdot\mathbf{p}(\mathbf{r})|j\rangle = \mathrm{i}\frac{m}{\hbar}\left\{\varepsilon^{(j)} - \varepsilon^{(i)}\right\}\langle i|\mathbf{e}_{\mathbf{q},\lambda}\cdot\mathbf{r}|j\rangle \approx \pm\mathrm{i}\frac{m}{\hbar}E_{\mathrm{g}}\langle i|\mathbf{e}_{\mathbf{q},\lambda}\cdot\mathbf{r}|j\rangle. \tag{15}$$

By inserting equations (2) and (15) into equation (14),

$$H_{\mathrm{eff}} = -\sum_{i\neq j}\sum_{\mathbf{k},\sigma}\sum_{\mathbf{k}',\sigma}\sum_{\mathbf{q},\lambda} V_{\mathrm{electron-photon}} c^{(i)\dagger}_{\mathbf{k}'+\mathbf{q},\sigma'} c^{(j)}_{\mathbf{k}',\sigma'} c^{(j)\dagger}_{\mathbf{k}-\mathbf{q},\sigma} c^{(i)}_{\mathbf{k},\sigma}, \tag{16}$$

where

$$\begin{aligned} V_{\mathrm{electron-photon}} &= \frac{1}{2}\left(\frac{e}{2m}\right)^2 |A_{\mathbf{q},\lambda}|^2 \left|\langle i|\mathbf{e}_{\mathbf{q},\lambda}\cdot\mathbf{p}(\mathbf{r})|j\rangle\right|^2 \\ &\times \left\{\frac{\hbar\omega_{\mathbf{q}}}{(\hbar\omega_{\mathbf{q}})^2 - (\varepsilon^{(i)}_{\mathbf{k}'} - \varepsilon^{(j)}_{\mathbf{k}'+\mathbf{q}})^2} + \frac{\hbar\omega_{\mathbf{q}}}{(\hbar\omega_{\mathbf{q}})^2 - (\varepsilon^{(i)}_{\mathbf{k}} - \varepsilon^{(j)}_{\mathbf{k}-\mathbf{q}})^2}\right\} \\ &\approx \frac{e^2\left|\langle i|\mathbf{e}_{\mathbf{q},\lambda}\cdot\mathbf{r}|j\rangle\right|^2}{2\varepsilon\Omega}\frac{E_{\mathrm{g}}^2}{(\hbar\omega_{\mathbf{q}})^2 - E_{\mathrm{g}}^2}. \end{aligned} \tag{17}$$

Although the electron–photon interaction is attractive at $\hbar\omega_{\mathbf{q}} > E_{\mathrm{g}}$, effective attractive interaction cannot be achieved at $\hbar\omega_{\mathbf{q}} \gg E_{\mathrm{g}}$ since $V_{\mathrm{electron-photon}}$ becomes small, as is evident in equation (17). In order to achieve effective attractive interaction, therefore, wide band gaps are necessary for $\hbar\omega_{\mathbf{q}} \approx 10$ eV.

Even if this attractive electron correlation were weak, it could be amplified artificially by using photonic crystals with dielectric periodic structures. Photonic crystals have photonic band gaps in which electromagnetic waves with certain frequencies cannot propagate [11–13]. The lattice constants of the photonic crystals are of the order of the wavelength of electromagnetic waves. Moreover, group velocities of electromagnetic waves become zero at frequencies of photonic band gap edges since the gradient of frequency for wavevectors

of electromagnetic waves is zero. In photonic crystals composed of wide band gap semiconductors, therefore, electron–photon interaction can be amplified at the frequencies of band gaps edges because of the very long interaction time between electrons and photons resulting from the zero group velocities, as is well known in photonic crystals. Two- and three-dimensional photonic crystals composed of semiconductors have already been reported [14, 15]. Therefore, effective electron–photon interaction may be achieved in photonic crystals composed of wide band gap semiconductors.

4. Conclusion

We have theoretically demonstrated attractive electron correlation in wide band gap semiconductors by electron–photon interaction. The attractive interaction occurs between two electrons when one electron changes from a valence band to a conduction band and the other one changes from a conduction band to a valence band. Even if this attractive electron correlation were weak, it could be amplified by using photonic crystals with dielectric periodic structures composed of wide band gap semiconductors.

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