Optical conductivity calculation of a k, p model semiconductor GaAs incorporating first-order electron-hole vertex correction

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Abstract. The role of excitons in semiconducting materials carries potential applications. Experimental results show that excitonic signals also appear in optical absorption spectra of semiconductor system with narrow gap, such as Gallium Arsenide (GaAs). While on the theoretical side, calculation of optical spectra based purely on Density Functional Theory (DFT) without taking electron-hole (e-h) interactions into account does not lead to the appearance of any excitonic signal. Meanwhile, existing DFT-based algorithms that include a full vertex correction through Bethe-Salpeter equation may reveal an excitonic signal, but the algorithm has not provided a way to analyze the excitonic signal further. Motivated to provide a way to isolate the excitonic effect in the optical response theoretically, we develop a method of calculation for the optical conductivity of a narrow band-gap semiconductor GaAs within the 8-band k, p model that includes electron-hole interactions through first-order electron-hole vertex correction. Our calculation confirms that the first-order e-h vertex correction reveals excitonic signal around 1.5 eV (the band gap edge), consistent with the experimental data.

1. Introduction

Semiconductor responds to light in a wide variety of ways, including the formation of short-lived quasiparticles which can affect the optical response of the material. Excitonic signals may appear in optical absorption spectra of semiconductors not only those with wide band gap, but also in narrow gap semiconductors, such as Gallium Arsenide (GaAs) [1]. GaAs is a promising material due to its superior properties, including high electron mobility and good opto-electrical transfer efficiency [2]. The formation of excitons inside GaAs also has an important role in increasing solar cell efficiency and light formation in LED and lasers.

There is much interest in the characterization of GaAs crystal over the past decades, mostly in its optical properties. Despite that excitonic signals have been observed in the GaAs optical spectra experimentally, the optical properties of GaAs have not yet been much explored theoretically. Calculation based purely on Density Functional Theory (DFT) without taking electron-hole interactions into account does not lead to the appearance of any excitonic signal [3]. Meanwhile, existing DFT-based algorithms that include a full vertex correction through Bethe-Salpeter equation may reveal an excitonic signal, but the algorithm has not provided a way to analyze the excitonic signal further [4]. In this study, we develop a method of calculation for the optical conductivity of a narrow band gap semiconductor GaAs within the 8-band k, p model, which includes electron-hole (e-h) interactions through first-order electron-hole vertex correction. By this method we could isolate the excitonic effect in the optical response theoretically. Our calculation confirms that the first order e-h vertex correction reveals excitonic signal around the band gap edge.
2. Model

We construct our model Hamiltonian using the following basis states: \(|s\rangle|t\rangle\) (forming the conduction band), and \(|p_x\rangle|l\rangle\), \(|p_y\rangle|l\rangle\), \(|p_x\rangle|l\rangle\), \(|p_y\rangle|l\rangle\), \(|p_x\rangle|l\rangle\) (forming the three degenerated valence band, known as the heavy hole, light hole, and split off bands [5]. By operating the Hamiltonian \(H = \frac{p^2}{2m_0} + V + \frac{\hbar}{4m_0} \mathbf{V} \times \mathbf{p} \cdot \boldsymbol{\sigma}\) on the above basis states, following Bahder [6], we obtain our 8-band model Hamiltonian matrix as

\[
H(k) = \begin{bmatrix}
0 & 0 & \sqrt{2}(W - U) & 0 & -\sqrt{2}(T - U) & -\sqrt{2}(T - V) & \sqrt{2}(T' - V') \\
0 & 0 & -\sqrt{2}(W - U) & 0 & -\sqrt{2}(T - U) & -\sqrt{2}(T - V) & \sqrt{2}(T' - V') \\
\sqrt{2}(W - U) & -\sqrt{2}(T - V) & -p - q & -p - q & -p - q & -\sqrt{2}R' & \sqrt{2}Q \\
-\sqrt{2}(W - U) & -\sqrt{2}(T - V) & -p - q & -p - q & -p - q & -\sqrt{2}R' & \sqrt{2}Q \\
0 & 0 & \sqrt{2}R' & \sqrt{2}Q & \sqrt{2}Q & \sqrt{2}Q & \sqrt{2}Q \\
0 & 0 & \sqrt{2}R' & \sqrt{2}Q & \sqrt{2}Q & \sqrt{2}Q & \sqrt{2}Q \\
0 & 0 & \sqrt{2}R' & \sqrt{2}Q & \sqrt{2}Q & \sqrt{2}Q & \sqrt{2}Q \\
0 & 0 & \sqrt{2}R' & \sqrt{2}Q & \sqrt{2}Q & \sqrt{2}Q & \sqrt{2}Q \\
\end{bmatrix}
\]

for which

\[
A = E_c + \left[ A' + \frac{\hbar^2}{2m_0} \right] (k_x^2 + k_y^2 + k_z^2) \\
U = \frac{1}{\sqrt{3}} P_0 k_x \\
V = \frac{1}{\sqrt{6}} P_0 (k_x - ik_y) \\
W = \frac{i}{\sqrt{3}} B k_x k_y \\
T = \frac{i}{\sqrt{6}} B k_x (k_x + ik_y) \\
P = -E_0 + \frac{1}{2} \gamma_1 \left( k_x^2 + k_y^2 + k_z^2 \right)
\]

with the empirical parameter values taken from Ref. [7] as: \(A=5.65 \text{ Å}, A'=0.314 \text{ eV}, E_c=1.519 \text{ eV}, A'=0 \text{ eVÅ}^2, B=4.19 \text{ eVÅ}^2, E_p=22.827 \text{ eV}, \gamma_1=6.672, \gamma_2=1.866, \text{ and } \gamma_3=2.669.\)

3. Calculation Method

To perform 0-5 eV optical conductivity which reveals excitonic signal, we calculate bare optical conductivity and add it up with the corresponding first order electron-hole vertex correction. We first calculate the retarded Green functions, density of states (DOS), and chemical potential. Then by using the obtained Green functions and chemical potential, we calculate the corresponding optical conductivity. The bare optical conductivity formula is derived using the Kubo formula [8]. As \(\sigma_{ab}\) is a retarded quantity then it is more convenient to first defined it in Matsubara frequency \(\omega_n = \frac{2\pi nk_B T}{\hbar}\) is the “bosonic” Matsubara frequencies, with \(T\) being the temperature and \(n\) being an integer running from \(-\infty\) to \(\infty\) [9].

![Figure 1](image1.png) **Figure 1.** Bubble diagram of bare optical conductivity.

![Figure 2](image2.png) **Figure 2.** Bubble diagram of first order vertex correction.
Figure 1 and 2 display the Feynman diagrams of the current-current correlation function. The diagram in Fig. 2 can be translated into the bare optical conductivity formula in Matsubara frequency domain as

$$ \sigma_{\alpha\beta}(\omega_n) = e^2 \frac{1}{\hbar v_F^2} \sum_{n=-\infty}^{\infty} \sum_{k} \text{Tr} \left[ v^\alpha(k) [g_0(k, \omega_n)] [v^\beta(k)] [g_0(k, \omega_n + i\omega_n)] \right]. \tag{2} $$

Because physical properties need to be extracted from retarded optical conductivity in real frequencies, we do analytical continuation through the Hilbert transformation to take optical conductivity from Matsubara to real frequency domain. The real part of bare optical conductivity could then be expressed by

$$ \text{Re} \sigma_{\alpha\beta}(\omega) = \frac{\pi e^2}{\hbar \omega} \int_{-\infty}^{\infty} dv \left( f(v, \mu, T) - f(v + \omega, \mu, T) \right) \sum_{k} \text{Tr} \left[ v^\alpha(k) [A_0(k, \nu)] [v^\beta(k)] [A_0(k, \nu + \omega)] \right]. \tag{3} $$

with

$$ [A_0(k, \nu)] = \frac{1}{2\pi i} \left( [g_0(k, \nu + i0^+)] - [g_0(k, \nu - i0^+)] \right), \tag{4} $$

and the velocity matrix

$$ v_{\lambda_1\lambda_2}^\alpha(k) = \frac{\partial}{\partial k_{\lambda_1}} H_{\lambda_1\lambda_2}(k). \tag{5} $$

As the attractive Coulomb interaction between electron in the conduction band and hole created in the valence band is incorporated, we then deal the diagram in Fig. 2, where the electron-hole interaction is represented by a wavy line connecting the electron and the hole propagators. This diagram translates mathematically as

$$ \sigma_{\alpha\beta}^{(1)}(\omega_n) = e^2 \frac{1}{\hbar v_F^2} \sum_{n=-\infty}^{\infty} \sum_{k} \sum_{\nu \omega} \sum_{\lambda_1} \sum_{\lambda_2} \sum_{\lambda_3} \sum_{\lambda_4} \left( \sum_{\alpha \beta} \sum_{\lambda_5} \sum_{\lambda_6} g_0(k, \nu + \omega) v_{\lambda_5\lambda_6}^\alpha(k) g_0(k, \nu + \omega + i\omega_n) \right) u(q) \left( \sum_{\lambda_7} \sum_{\lambda_8} \sum_{\nu \omega} g_0(k + q, \nu + \omega + i\omega_n) v_{\nu \omega}^\beta(k) g_0(k + q, \nu + \omega_n) \right). \tag{6} $$

For this formula, it is rather tedious to implement the Hilbert transformation, as it will generate many-many integrals over real frequency variables, resulting in expensive computation. To overcome this problem, we choose to use Padé approximant technique [10] to do the analytic continuation to transform the optical conductivity from Matsubara- to real-frequency domain.

4. Results and Discussion

Figure 3 shows the bare optical conductivity. Here we don’t have anisotropy as all the three curves corresponding to diagonal components of optical conductivity tensors overlay each other. The optical conductivity remains zero up to 1.4eV. At the frequency 1.4eV, it starts to rise and undergoes a significant change at 3eV until it reaches its highest peak at 4.4eV. This means that, below 1.4eV all electrons are confined in valence band and none in the conduction band, thus no carrier contributes to conduct the material. As the photon frequency exceeds the band gap value, photons start to excite electrons to the conduction band. The higher the photon energy, more free electrons are produced, and more conducting the material becomes.
To see how electron–hole interaction affects the optical response of GaAs, we add up the two corresponding curves, the bare optical conductivity and the corresponding first order correction. The results are displayed in Fig. 4.

**Figure 3.** Calculation result of bare optical conductivity.

**Figure 4.** Optical conductivity calculation including first-order e-h vertex correction. Left figures: first order vertex correction; right figures: bare optical conductivity added with its first order vertex correction.
The excitonic signal appears in all directions of optical conductivity $\sigma_{xx}$, $\sigma_{yy}$ and $\sigma_{zz}$. It appears slightly below the band gap energy. Our calculated first-order correction optical conductivity reveals excitonic signals starting at 1.27 eV for $\sigma_{xx}$, $\sigma_{yy}$ and 1.36 eV for $\sigma_{zz}$. The first order highest peak strikes at 1.4 eV for both $\sigma_{yy}$ and $\sigma_{zz}$, while for $\sigma_{xx}$, the peak strikes at frequency 1.75 eV. The excitonic signal from measurements also appear at about these frequencies. As to compare with the bare optical conductivity curve, a little discrepancy occurs at the first-order electron-hole vertex correction calculation which does not preserve isotropic behavior as the bare one does. We conjecture that such a discrepancy results from the uncontrollable error occurring in the use of Padé approximant technique.

5. Conclusion
In conclusion, we have developed a $k.p$ based model for GaAs and the method to calculate optical conductivity up to first order e-h vertex correction and obtained optical conductivity spectrum up to 18 eV. Our results for the first order e-h vertex correction reveals excitonic signal around 1.5 eV (the band gap edge), consistent with the experimental data. Overall, we assess that our model and method works pretty well. Despite some lack of accuracy in the Padé approximation that needs to be improved.

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