



Joint density of states in low dimensional semiconductors



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HIGHLIGHTS

- Quantum well DOS is not a sharp steplike function.
- An accurately JDOS expression for direct transitions is proposed.
- Direct optical transitions are described by considering three spatial dimensions.
- In low dimensional semiconductors, DOS is calculated by convolution operation.
- Quantum well and superlattice absorption coefficients are accurately calculated.

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ABSTRACT

We present a different approach to evaluate density of states for quasi-bidimensional systems, which bonds density of states in the confinement direction with in-plane 2D density of states. Applying the convolution operation, we propose an accurately mathematical expression that combines directly the valence band and conduction band density of states functions to generate a joint density of states for direct transitions. When considering low dimensional semiconductors, another expression is found which shows that the density of states for electrons (holes) can be calculated by convolution operations between the confinement direction and in-plane electron (hole) density of states. Using both expressions, we have calculated the quantum well and superlattice absorption coefficient, resulting in positive alignment with experimental data. A more complete description of physical absorption is achieved with this new approach.

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1. Introduction

The optical absorption spectrum is a key requirement for many of the optoelectronic devices. The optical response of a semiconductor is described in terms of the spectral dependence of the optical absorption coefficient, $\alpha(\hbar\omega)$. The absorption process in direct gap semiconductors and therefore $\alpha(\hbar\omega)$, can be expressed as a function of the joint density of states (JDOS). The JDOS function provides a measure of the number of allowed optical transitions between the occupied valence band electronic states and the unoccupied conduction band electronic states separated by photon energy $\hbar\omega$.

Several attempts, relating the valence band and conduction band density of states (DOS) functions to JDOS have been reported in the literature [1–4]. However, all attempts were confined to

amorphous semiconductors where empirical expressions and simplified JDOS expressions were obtained. Moreover, to evaluate interband absorption coefficient in low dimensional semiconductors, quantum well and superlattice, JDOS has always been calculated through its in-plane component [5–7]. Besides, to describe excitonic absorption, it is generally assumed that each energy transition is broadened in a Lorentzian or Gaussian fashion with a broadening parameter. This approach disregards the contribution to JDOS of the dispersion relation between energy and the magnitude of its wave vector in the confinement direction.

In this study, we present for the first time a mathematical expression that links directly the valence band and conduction band density of states functions to a JDOS for direct transitions, which was proved in GaAs alloys including low dimensional systems like quantum wells and superlattices. Such expression is achieved by applying the convolution operation properties. A convolution is an operator which expresses the amount of overlap of one function as it is shifted over another function. It therefore blends one function with another.

In low dimensional semiconductors, we present a different

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approach to evaluate DOS for quasi-bidimensional systems, which bonds density of states in the confinement direction with in-plane 2D density of states. With this approach a mathematical expression was found which shows that the density of states for electrons (holes) can be calculated by the convolution operations on two functions: the confinement direction and in-plane electron (hole) DOS. We have accurately calculated the absorption coefficient for quantum wells and superlattices based on GaAs alloys, showing good agreement with experimental data.

2. Theory

Our research is focused on direct band semiconductors, where the absorption coefficient is given by [7]

$$\alpha(\hbar\omega) = \frac{\Lambda}{\hbar\omega} \sum_{i,f} \left| \hat{a} \cdot \vec{p}_{if} \right|^2 \delta(\varepsilon_f - \varepsilon_i - \hbar\omega) [f_i(\varepsilon_i) - f_f(\varepsilon_f)] \quad (1)$$

where factor $\Lambda = 4\hbar\pi^2 q^2 / n_r c m_0^2 \Omega$ is a material dependent constant, where n_r is the refractive index of the well material, m_0 is the free electron mass, q is the electron charge, c is the speed of light and Ω is the sample “volume” defined by Bastard [7]. The first term inside the element $\left| \hat{a} \cdot \vec{p}_{if} \right|^2$ represents the polarization unit vector, \hat{a} , while the second term represents the momentum matrix element, \vec{p}_{if} . The ε_i and ε_f , which depend on the wave vector \vec{k} , are the energy values for the initial valence band states $|i, \vec{k}, \vec{s}\rangle$ and the final conduction band states $|f, \vec{k}, \vec{s}\rangle$ which are involved in the transitions, where \vec{s} is the spin. The $f_i(\varepsilon_i)$ and $f_f(\varepsilon_f)$ are the occupation probability functions for initial and final states respectively which depend on the corresponding quasi-Fermi level.

Considering that interband transitions are “vertical” the interband matrix element becomes $\hat{a} \cdot \vec{p}_{if} = \langle u_{i\vec{k}} | \hat{a} \cdot \vec{p} | u_{f\vec{k}} \rangle$ where $u_{i\vec{k}}$ and $u_{f\vec{k}}$ represent the conduction band and valence band central cell states. For near bandedge transitions we will suppose that $u_{i\vec{k}}$ and $u_{f\vec{k}}$ are given by their zone center values. With these considerations we will assume that the matrix element is independent of \vec{k} and the term $\left| \hat{a} \cdot \vec{p}_{if} \right|^2$ may be moved out of the summation in Eq. (1):

$$\alpha(\hbar\omega) = \frac{\Lambda}{\hbar\omega} \sum_{i,f} \left| \hat{a} \cdot \vec{p}_{if} \right|^2 \sum_{\vec{k}, \vec{s}} \delta(\varepsilon_f - \varepsilon_i - \hbar\omega) [f_i(\varepsilon_i) - f_f(\varepsilon_f)] \quad (2)$$

In order to simplify Eq. (2), we restrict ourselves to a filled bottom band and an empty excited band. This is a good approximation as long as the separation of the two bands is greater than kT . Under this assumption $f_i(\varepsilon_i) \approx 1$ and $f_f(\varepsilon_f) \approx 0$, then

$$\alpha(\hbar\omega) = \frac{\Lambda}{\hbar\omega} \sum_{i,f} \left| \hat{a} \cdot \vec{p}_{if} \right|^2 J_{if}(\hbar\omega) \quad (3)$$

The JDOS function, $J_{if}(\xi)$, is conveniently rewritten, using Dirac delta properties, as:

$$J_{if}(\xi) = \sum_{\vec{k}, \vec{s}} \delta(\xi - \varepsilon_f(\vec{k}) - |\varepsilon_i(\vec{k})|); \xi = \hbar\omega \quad (4)$$

where the dispersion relations are given in the form

$$\begin{aligned} \varepsilon_f &= \varepsilon_f(\vec{k}) \\ \varepsilon_i &= -\varepsilon_i(\vec{k}) \end{aligned} \quad (5)$$

The JDOS function is related with the valence band and

conduction band density of states (DOS) which are linked with optical transitions. Our next goal is to redefine JDOS expression (Eq. (4)) as a straightforward dependence of DOS functions. For that, Fourier transform, with its linearity property, is applied to Eq. (4). Then,

$$\begin{aligned} \mathbf{F}\{J_{if}(\xi)\} &= 2 \sum_{\vec{k}} \mathbf{F}\{\delta(\xi - \varepsilon_f(\vec{k}) - |\varepsilon_i(\vec{k})|)\} \\ &= 2 \sum_{\vec{k}} e^{-2\pi i \xi (\varepsilon_f(\vec{k}) + |\varepsilon_i(\vec{k})|)} \\ &= 2 \sum_{\vec{k}} e^{-2\pi i \xi \varepsilon_f(\vec{k})} e^{-2\pi i \xi |\varepsilon_i(\vec{k})|} \\ \mathbf{F}\{J_{if}(\xi)\} &= 2 \sum_{\vec{k}} \mathbf{F}\{\delta(\xi - \varepsilon_f(\vec{k}))\} \mathbf{F}\{\delta(\xi - |\varepsilon_i(\vec{k})|)\} \end{aligned} \quad (6)$$

where the factor 2 has accounted for the spin degeneracy of each energy state and ξ corresponds to the domain of the Fourier transform. Here, we have assumed that both functions, $\delta(\xi - \varepsilon_f(\vec{k}))$ and $\delta(\xi - |\varepsilon_i(\vec{k})|)$, are Lebesgue integrable. After algebraic operations ($\sum_i A(k_i)B(k_i) = \sum_i \sum_j A(k_i)B(k_j)\delta_{ij}$, A and B arbitrary functions) and using properties of the Fourier Transform the Eq. (6) transforms into:

$$\begin{aligned} \mathbf{F}\{J_{if}(\xi)\} &= 2\mathbf{F}\left\{ \sum_{\vec{k}_2} \delta(\xi - \varepsilon_f(\vec{k}_2)) \right\} \mathbf{F}\left\{ \sum_{\vec{k}_1} \delta(\xi - |\varepsilon_i(\vec{k}_1)|) \right\} \delta_{\vec{k}_1 \vec{k}_2} \\ &= \frac{1}{2} \mathbf{F}\{ \mathbf{D}_f^e(\xi) \} \mathbf{F}\{ \mathbf{D}_i^h(\xi) \} \delta_{\vec{k}_1 \vec{k}_2} \end{aligned} \quad (7)$$

where $\delta_{\vec{k}_1 \vec{k}_2}$ assigns the conservation of the wave vector in the direct optical transitions and $\mathbf{D}_f^e(\xi)$ and $\mathbf{D}_i^h(\xi)$ denote the density of states for electrons and holes in the f and i bands.

In order to reach our goal, that is, to define JDOS as a straightforward dependence of DOS functions, the convolution theorem is applied to Eq. (7), then

$$J_{if}(\xi) = \beta \frac{1}{2} \mathbf{D}_f^e(\xi) * \mathbf{D}_i^h(\xi) \delta_{\vec{k}_1 \vec{k}_2} \quad (8)$$

where $*$ denotes the convolution operation. The normalization factor β is introduced because convolution operator leads to overestimated optical states number. Mathematical convolution involves multiplication between the linked states in valence (occupied states) and conduction bands (final empty states) and therefore it disregards that each optical state is related with an electron–hole pair generation. Such as, for the same k value, only two optical transitions are possible when there are two occupied states in the valence band and two empty states in the conduction band. Instead, the discrete convolution operation multiplies states in both bands, resulting in four possible optical transitions for the same k value. Then, only a fraction of the possible calculated optical states, represented by the β factor, are optical states due to real electronic transitions.

Then, the number of states, which can be optically linked, depends on either the available electronic states in the valence band or the final states in the conduction band for accommodating the excited electrons, whichever is the smaller [1]. The β factor is evaluated under the assumption that, in the first Brillouin zone (B. Z.), the number of optical states is equal to the number of linked states in each band. That is, the JDOS must be normalized to the number of linked states in each band. Then, normalization is given by

$$\int_{\text{B.Z.}} J_{if}(\xi) d\xi = \int_{\xi \in \text{B.Z.}} \mathbf{D}(\xi) d\xi \quad (9)$$

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