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Fourier Grid Hamiltonian applied in the study of optical and transport properties of intermediary band solar cells computationally simulated using the *Julia* language

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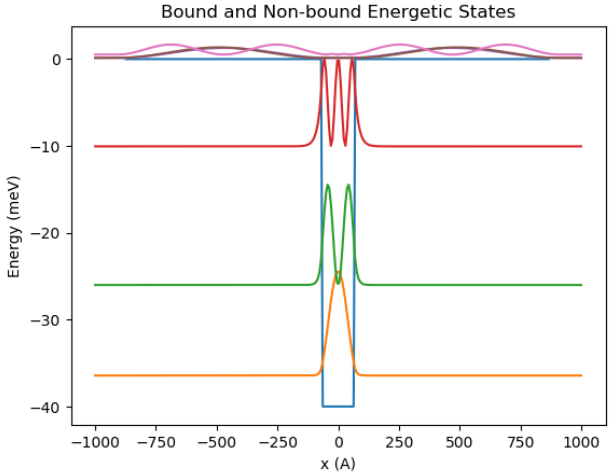
Graphical Abstract

Bound and non-bound eigenstates in the finite quantum well described by the diagonalization of Hamiltonian operator

$$H_{ij} = \frac{1}{\Delta x}\left\{\frac{2}{N}\sum_{l=1}^{n} cos\left(\frac{l2\pi(i-j)}{N}\right)T_l + Vx_i\delta_{ij}\right\}$$



Abstract

The technological advances in the area of opto-electronic semiconductor devices has increased significantly in the last decades due the great demand for clean and renewable energy fonts. Thus, the search for clean energetic fonts demands a continuous attention on the efficiency of electric current generation of these devices. Among these advances we can highlight the utilization of clean and renewable energy by means of solar cells. They can be optimized as intermediate band solar cells, that present greater efficiency in comparison to the usual ones. For the quantum analysis of the optical and electronic transport properties of intermediate band solar cells, we developed a numerical algorithm for the Schroedinger equation using the Fourier Grid Hamiltoninan method, using as tool the high-level computational language Julia. We obtained the eigenstates of the Hamiltonian describing the cell's architecture and we were able to evaluated the transition probabilities, giving us clues of the transport and optical properties of intermediate band solar cells.

Introduction

Solar cells are photovoltaic devices that produces electric current when their charge carriers interact with light, more precisely, light in the visible area of the electromagnetic solar spectrum. The matter-radiation interaction in these devices generate electron-hole pairs that, in a presence of a potential difference generated by the built-in field of the cell, are spatially separated and collect by the electric contacts, generating electric current [1, 2].

Aiming to increase the cell's efficiency, and make them feasible to the large-scale use, the scientific community has been mobilized in order to optimize the cell through the utilization of quantum wells that simulate intermediate bands for optical transition. The bound states of the quantum well act as news absorption channels to the sun-light, increasing the cell's absorption and, consequently, its efficiency.

The improvement of these solar cells has quantum origin, and for this kind of analysis, is necessary a computational treatment. For that, a numerical algorithm was developed for the resolution of time-independent Schroedinger equation, using the programing language *Julia* [3], developed by MIT (*Massachusetts Institute of Technology*). For the equation resolution it was used the method *Fourier Grid Hamiltonian*, in order to find the eigenvalues and the eigenfunctions of Hamiltonian, that describe the electronic dynamics in solar cells.

Methods

In order to accomplish the presented objectives, the solution of the time-independent Schroedinger equation was obtained by the numerical simulation of a *p-i-n* junction containing a quantum well on its intrinsic region. To solve the equation it was used the method *Fourier Grid Hamiltonian* [4], that allows us to put the Schroedinger equation in a dual representation of the positions and the momenta. In this representation, the kinetic and potential operators are projected in their specific eigenvector basis. The method allow us to directly obtain the matrix elements of the Hamiltonian and, the diagonalization of the matrix returns its respective eigenvectors and eigenvalues [5].

A particle subjected to an unidimensional potential is described by the time-independent Schroedinger equation,

$$\hat{H} = \hat{T} + \hat{V}(\vec{x}) = \frac{\hat{P}^2}{2m} + \hat{V}(\vec{x}), \tag{1}$$

where $\hat{T}$ and $\hat{V}(\vec{x})$ are the kinetic and potential operators, respectively.

To turn the equation resolution simpler, in the method we define each operator in their own representation. With the changes done for the operators, we got the analytic equation to the set of Hamiltonian elements of matrix

$$\langle x|\hat{H}|x'\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ik(x-x')} T_k dk + V(x)\delta(x'-x). \tag{2}$$

Such equations are laborious or impossible to solve analytically. Hence, it is required a numerical implementation, and the equation can be solved computationally. Discretizing the subspaces and describing the variables numerically, the following equation is obtained

$$H_{ij} = \frac{1}{\Delta x} \left\{ \frac{2}{N} \sum_{l=1}^{n} cos\left(\frac{l2\pi(i-j)}{N} \right) T_l + V x_i \delta_{ij} \right\}. \tag{3}$$

The eigenvectors and eigenvalues in discrete form are found from the diagonalization of Hamiltoninan operator

$$det\left[H_{ij} - \frac{E_n \delta_{ij}}{\Delta x} \right] = 0. \tag{4}$$

To solve the solar cells problem, the potential of p-i-n junction with quantum wells is described numerically in a grid with the same quantity of points of the Hamiltoninan matrix. Therefore, the matrix is then diagonalized returning its eigenvectors and eigenvalues, namely, the eigenstates and eigenenergies of solar cells. The solution was implemented using the programing language *Julia*, which is very useful with problems that require high computational cost.

Results and Discussion

Once built the algorithm, the parameters were adjusted for the program generate an acceptable approximation compared to intermediate band semiconductors. The material utilized for the numerical implementation of the quantum well was the Gallium Arsenide (GaAs) with the effective electron mass $m = 0,067$, constant for all points of the grid.

Defining the initial parameters and generated the quantum well, the Hamiltonian matrix was written. The matrix was diagonalized returning the eigenvectors and the eigenenergies. With these values we can analyze the bounded and the non-bounded states in the quantum well. The figure 1 shows three energetic states.

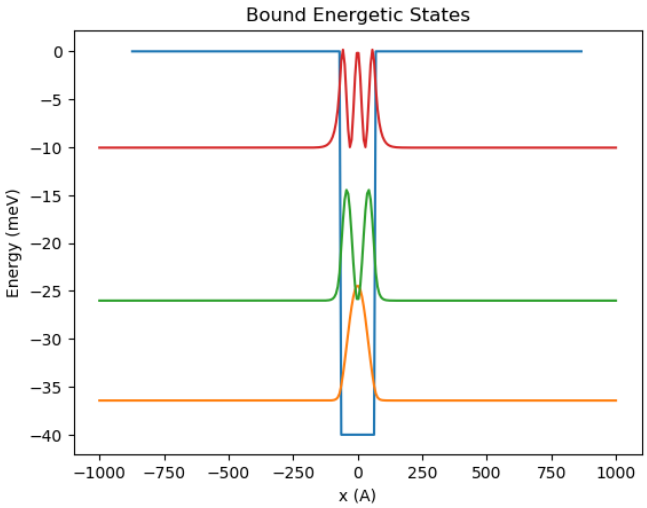


Figure 1: Three bound states in a potential well

With the states defined, it was possible to calculate the transition probability by means of the Fermi's Golden Rule. This rule define the photonic energy needed to the electronic excitation, being proportional to the square root of the overlap between the ground state eigenvector and the excited ones. The figure 2 shows the absorption probability of the electron being excited from ground to excited states within the conduction band of the solar cell. The most intense peaks define a higher probability of transition between eigenstates with that energy difference.

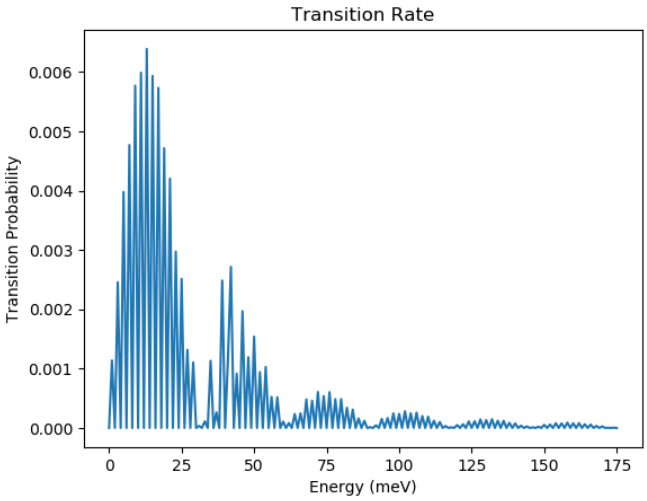


Figure 2: Absorption probability given by the Fermi's Golden Rule

Conclusion

The method *Fourier Grid Hamiltonian* is straightforward and relatively simple to numerically evaluate the physical properties of intermediate band solar cells. The obtained results from this method are coherent and, based on this, we can conclude that the algorithm, just like the language, are functional and efficient, demonstrating results of quantum phenomena impossible to reach analytically. This work have as principal intent complement the range of tools required to the improvement of intermediate band solar cells.

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