MOL2NET, International Conference Series on Multidisciplinary Sciences

Study of the optical properties of midband solar cells using the Split Operator method

Silva, Y. L.[a], *Almeida, J. V.*[a], *Macedo, G. S.* [a], *Bezerra, A. T.* [a]

[a] *UNIFAL-MG*

Abstract.

The solar cells consist of semiconductor devices that use quantum, optical and transport processes of charge carriers, and have as fundamental source of energy the light coming from of the Sun. They are destined to the conversion of solar energy into electric energy. The maximum efficiency of the silicon based commercial solar cells is 30%, defined by the thermodynamical theoretical model of Shockley-Queisser. Our proposal is to optimize the efficiency of these devices by means of the engineering of intermediate band solar cell (IBSC). In this kind of structure, the proposal is to add an intermediate band to the optical transition between valence and the conduction bands of a p-i-n junction, either by doping it or through bound states of quantum well structures. We based our study on the latter. We used the Split Operator method for the numerical solution of the time-dependent Schrodinger equation described by the solar cell's potential. Thus, we obtained the eigenfunctions and eigenenergies of the system, and from this it was possible to obtain the absorption rate applying the Fermi's Golden-rule. As the computational tool we use the Julia programming language. With the results obtained from the optical and transport properties it was possible to start understanding the processes by which the efficiency of IBSC can be increased.

Introduction

The consumption of electric energy in the post-Industrial Revolution world is a necessity for most people. However, the processes of obtaining energy are still highly dependent on fossil fuels burning and consequently are highly polluting. Meanwhile, about 1.7×10^5 TW [1, 2] per hour arrives at the top of the Earth's atmosphere, and solar cells (SC) are the devices designed to perform the conversion of such solar energy into electrical one by means of quantum, optical and transport processes.

However, commercial CSs made with a simple p-i-n junction, have a maximum theoretical limit to their efficiency of around 30%, defined by the Shockley-Queisser model [3]. In order to increase the cell's efficiency intermediate band solar cells (IBSC) are proposed, which can increase efficiency up to 60% [4].

The inclusion of the intermediate band (IB), as a band added between the valence band (VB) and the conduction band (CB), can be obtained by doping procedures or through self-stacks of a quantum well within the intrinsic region of the device. The quantum well potential profile is a result of the band gap difference between the different materials stacked together. Thus, our work consisted in modeling this quantum well within the cell profile and calculating the temporal evolution of the wave function,

using the numerical method Split Operator [5]. To do that, we used the high-level computer language Julia Language developed and distributed for free by MIT [6].

Materials and Methods

The problem of this work took into account the analysis of quantum properties, so it was necessary to solve the Schrodinger equation describing the IBSC quantum properties. More specifically we have dealt with the time-dependent equation. The Schrodinger equation is a second order differential equation, and we need a numerical method to solve it. We use the Split Operator method [5], which consists of the splitting of the time evolution operator, since the kinetic energy and potential energy operators are not commutative.

In evolving a wave function in time, we have

$$\Psi(x,t) = e^{\frac{-iH(t-t_0)}{\hbar}}\Psi(x,t_0) \quad (1)$$

where $\Psi(x,t_0)$ is the initial wave function and $\Psi(x,t)$ is the evolved wave function, H is the Hamiltonian and $\hbar$ is the normalized Planck constant. Applying the Zassenhaus expression and expliciting the separation between kinetic energy and potential energy operators, the time evolution operator is described as

$$e^{\frac{-i(T+V)\Delta t}{\hbar}} = e^{\frac{-iV\Delta t}{2\hbar}} + e^{\frac{-iT\Delta t}{\hbar}} + e^{\frac{-iV\Delta t}{2\hbar}} + O(\Delta t^3)\,, \quad (2)$$

where V is the potential energy, T is the kinetic energy, and $O(\Delta t^3)$ is the error. Being the increase of femtosecond order, it is a rather small error. In this way, we get the time evolved wave functions, but we need the eigenfunctions and the eigenenergies. For that we make the evolution with imaginary time.

To calculate the excited states, we need a method of ortonormalization and for this we use the Gram-Schmidt method. With the excited states it was possible to calculate the absorption rate of the system using the Fermi Gold rule [7] given by

$$\alpha(E) = \sum \frac{f_{if}\Gamma}{2\pi\left((E-E_i)^2+\frac{1}{4}\Gamma^2\right)} \quad (3)$$

where E is the energy of the incident photon, which causes the transition between the self-states with the energies E_i and E_f. The term f_{if} is the force of oscillator and Γ a broadening constant.

Results and Discussion

We started by modeling a potential well that describes the quantum well within the cell. We used as material host to the well Gallium Arsenide, as well as barriers of Gallium Aluminum Arsenide. The band gaps difference gave rise to the desired potential profile.

We applied the time evolution operator in a guessed initial wave function for the first eigenstate of the well, according to Figure 1. As we can see, the program realizes the evolution in time and the wave function is collapsed as the system eigenstate.

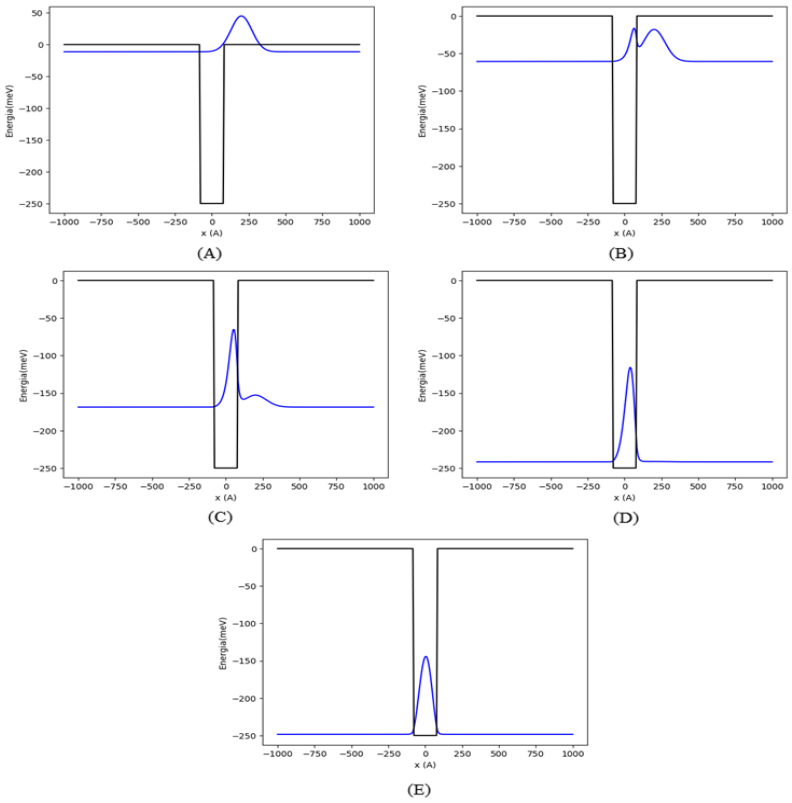

Figure 1: Representation of the temporal evolution of the wave function for the potential well being (A) evolution after 3 steps, (B) 278 steps, (C) 570 steps, (D) 1121 steps and (E) finally completely collapsed inside the well after 4685 time evolution steps.

From this, it was also possible to calculate other eigenfunctions that collapse as the excited states of the well, as we can see in Figure 2. The program also calculates extended states above the potential barriers, that is, states outside the well.

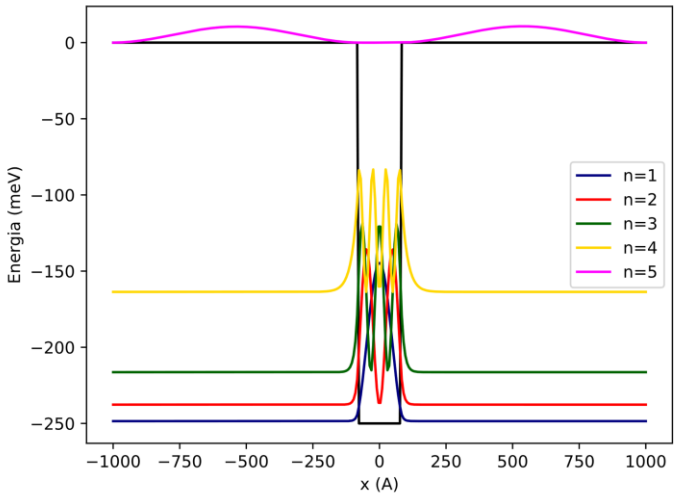

Figure 2: Probability density of several bound eigenstates in the quantum well.

With the calculation of the excited states we were able to calculate the absorption rate through the Fermi's Golden-rule. This calculation returns the rate of an electron being excited from ground state to higher energy levels. The results are shown in Figure 3, in which we can see that the selection rules are preserved, since there is a greater possibility of transport to certain levels than to another. The higher probability is represented by the more intense peak, this occurs due to the parity preservation of the wave functions of the system.

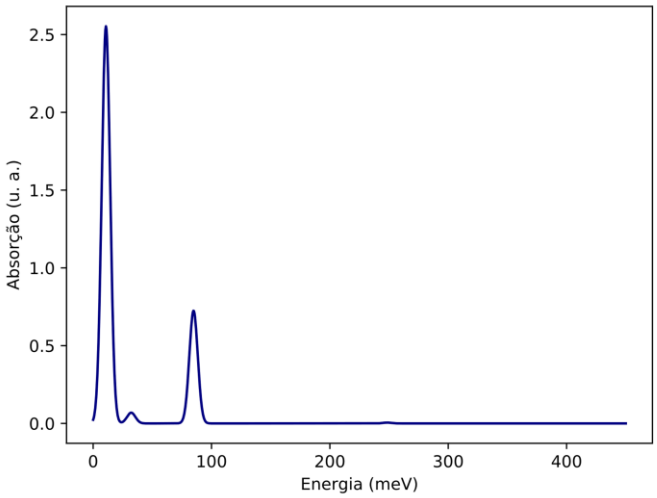

Figure 3: Absorption rate calculated using Fermi Golden rule.

Conclusions

Our work consisted of a study of optical and transport properties of the IBSC. For its realization we used the numerical method Split Operator to solve the time-dependent Schrodinger equation by means of the Julia high level programming language. With the evolution of several states of our system, we calculate the absorption rate through the Fermi's Golden-rule, which will be important in the future to calculate the dynamic properties, such as obtaining current from a IBSC.

References

[1] A. J. Nozik, "Exciton Multiplication and Relaxation Dynamics in Quantum Dots: Applications to Ultrahigh-Efficiency Solar Photon Conversion †," **Inorg. Chem.**, vol. 44, no. 20, pp. 6893–6899, 2005.

[2] K. Tanabe, "A Review of Ultrahigh Efficiency III-V Semiconductor Compound Solar Cells: Multijunction Tandem, Lower Dimensional, Photonic Up/Down Conversion and Plasmonic Nanometallic Structures. Energies, 2009, 2, 504-530.," **Energies**, vol. 2, no. 3, pp. 695–696, 2009.

[3] W. Shockley, H. J. Queisser, "Detailed balance limit of efficiency of p-n junction solar cells," *J. Appl. Phys.*, vol. 32, no. 3, pp. 510–519, 1961.

[4] A. Luque and A. Martí, "Increasing the Efficiency of Ideal Solar Cells by Photon Induced Transitions at Intermediate Levels," **Phys. Rev. Lett.**, vol. 78, no. 26, pp. 5014–5017, 1997.

[5] M. H. Degani, M. Z. Maialle, "Numerical calculations of the quantum states in semiconductor nanostructures," **J. Comput. Theor. Nanosci.**, vol. 7, no. 2, pp. 454–473, 2010.

[6] M. I. of Technology, "The Julia Language." [Online]. Disponível em: <http://julialang.org/>. Acesso em: 10/11/2018.

[7] N. W. Ashcroft, N. M. David. "Física do estado sólido". **Cengage Learning**, 2011.