Quantum wire-dot-wire photovoltaic junction in the Keldysh formalism

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CONTEXT AND OBJECTIVE

Quantum nanostructures, like dots, wires or wells, shall be integrated for future solar cell generations to improve efficiency compared to conventional cells [1], but also to devise novel operating concepts. The functioning of this new kind of cells crucially needs to be analyzed via quantum simulations. However, still very isolated works were carried out on this burning topic [2].

In this work, we examine the functioning of a quantum wire-dot-wire photovoltaic junction within the Keldysh formalism. We aim to deeper understand one crucial issue that strongly affects quantum solar cell's behavior: here the quantum dot-wire contact.

NANODEVICE MODEL

We developed a one-dimensional tight-binding scheme to model a quantum dot connected to two infinite non-interacting wires at each side shown Fig. 1. The dot is given by two energy levels. So are described the wires but using a different gap value and wide bands. Two hopping parameters (here identical), one for each level, characterize contacts to left and right reservoirs (here identical). The cell we modelled works using heterogeneous working functions to control electron/hole selectivity, which results in band offsets at each dot-wire contact. The band diagram is represented Fig. 2.

The photovoltaic properties of the junction were determined within the Keldysh formalism. Numerical calculations were performed on MERLIN cluster of the IM2NP, Marseille

RESULTS

The present study put the focus on the effect of the dot-wire(reservoir) hopping parameter h that characterizes the junction for a fixed monochromatic light resonant with the gap of the isolated dot. But contacts induce resonance shifting and broadening enhanced with h, as illustrated Fig. 3, via the amplitude of the reservoir self-energies that similarly shifts and broadens the discrete levels of the dot. In this out-of-resonance configuration, the electron-photon interaction creates a double peak in the spectral responses as shown Fig. 4 for the left current, localized inside the conduction mini-band. We observe the same for the right current, but localized inside the valence mini-band (not shown). This double peak directly arises within the self-consistent structure of interaction self-energies from the energy difference between photon energy and centered mini-band gap of the connected dot in the dark that is the resonance photon energy. This energy difference gives the energy separation between the two peak maxima, it decreases when h decreases until it cancels at resonance. When h increases, peaks decrease and broaden, as the energy levels of the connected dot. The total current produced hence decreases for all voltages when h increases (see Fig. 5). The two I-V characteristics moreover reveal that both the shunt resistance and the series resistance of the equivalent cell circuit increase when h increases. Similarly, the electrical power supplied by the cell decreases when h increases (see Fig. 6). Higher hopping increase current and power supplied by the cell, but decrease the contact selectivity. More, curves exhibit a peculiar shape. A bias translates the overlap window between the narrow bands of the dot and the wide bands of reservoir. We analyze that current as power cancel when overlap disappears, and that the singularity point occurs when partial overlap starts, giving rise to these peculiar working behavior.

CONCLUSION

The dot-wire hopping parameter shows a strong and intricate impact on the functioning of the quantum photovoltaic cell and the proposed architecture can thus be designed in order to optimize it. This first model must be seen as a building block for future investigations that will include electron-electron interaction as well as relaxation processes.

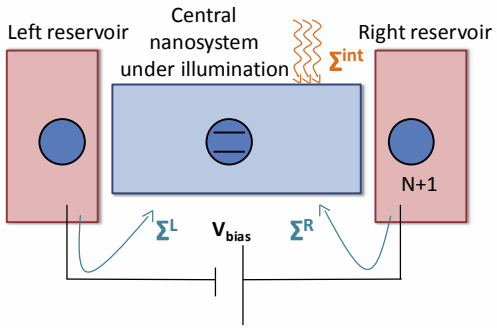

Fig. 1. Modeling of the quantum wire-dot-wire junction

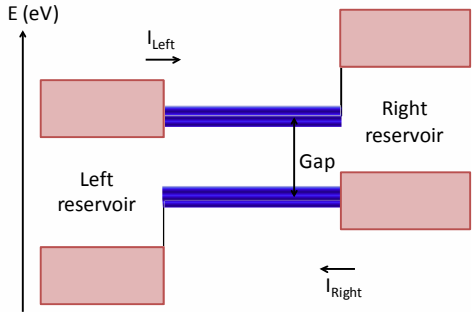

Fig. 2. Band diagram of the quantum wire-dot-wire junction

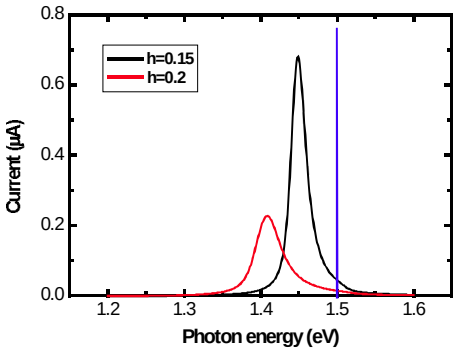

Fig. 3. Left current at zero bias voltage as a function of the photon energy. The initial gap values 1.5eV (vertical line)

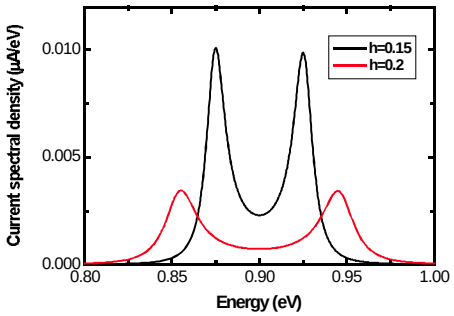

Fig. 4. Left current spectral density at zero bias voltage as a function of the electron energy

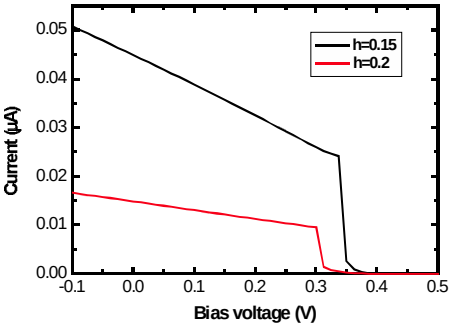

Fig. 5. Left current as a function of the bias voltage

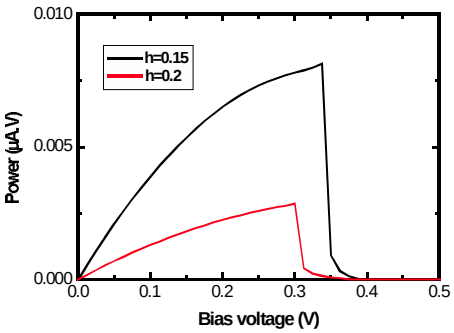

Fig. 6. Left electrical power as a function of the bias voltage

REFERENCES

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[2] U. Aeberhard, "Theory and simulation of quantum photovoltaic devices based on the non-equilibrium Green's function formalism", *J Comput Electron*, 2011, 10.1007/s10825-011-0375-6.