Green functions for photovoltaic response of quantum wire-dot-wire junctions

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Abstract-To investigate the photovoltaic properties of quantum dot connected to quantum wire reservoirs we rely on numerical calculations using the non-equilibrium Green function formalism. We examine impacts of the hopping parameter that controls the dot-wire contact for a monochromatic light resonant with the isolated dot gap. Global current and power increase when the hopping decreases, in particular the short-circuit current and the open-circuit voltage.

I. Introduction

Thanks to intelligent integration of nanoscale structures, new generation of quantum solar cells are expected to exhibit higher efficiency than conventional photovoltaic solar cells [1]. The quantum functioning of such innovative architectures imperatively needs to be understood but still very isolated works have been carried out on the subject. In this work, we rely on a mesoscopic tight-binding model to deeper understand the photovoltaic properties of quantum dots (QD) solar cells. We use the non-equilibrium Green function formalism (NEGF), perfectly adapted to studies on open interacting systems [2,3]. In order to explain quantum solar cell's behavior, a crucial point is to determine the interplay between light absorption and transport and, hence to propose new architectures.

II. Model

We developed a meaningful one-dimensional model that consists in a quantum dot, referred as the central nanosystem, connected to two infinite non-interacting wire reservoirs at left and right sides. 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). While the electron/hole selectivity is controlled by heterogeneous doping in p-n junctions, it is provided by heterogeneous working functions in the proposed cell model, which results in band offsets at each dot-reservoir contact. Band diagram is represented Fig.1.

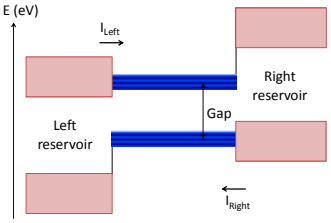

Fig1. Band diagram of the quantum wire-dot-wire junction

The photovoltaic properties of the central nanosystem were calculated within the self-consistent NEGF formalism in which self-energy functions account for contact to reservoirs, exactly, and interactions, generally in perturbation. This work only included the electron-photon interaction, operating in the dot, developed in the self-consistent Born approximation.
Numerical calculations were performed on MERLIN cluster of the IM2NP, Marseille.

III. Results

A. Device working

The presented study focuses on a wire/single-dot/wire unidirectional junction lighted with a single-mode monochromatic plane wave. Moreover, reference parameters of the tight-binding model have been chosen to cancel dark current and, hence, emphasize the photovoltaic conversion. Indeed, under illumination, electrons localized on down states of the central nanosystem may cross the gap and populate up ones. Radiative processes are modeled by the self-energies of the electron-photon interaction in the NEGF calculations. Effects of the self-energies of the electron-photon interaction are shown Fig.2. Due to band offsets, electrons can flow from the lowest band of the right reservoir to the highest band of the left reservoir, resulting in a net photocurrent shown Fig.3. By tuning the photon energy around the dot gap that is shifted and broadened by left and right contact self-energies, the system can evolve from a blocking state (dark current null) to a passing one (short-circuit current about 10^{-8}A) inside a resonance window of light energies which corresponds to a commutation window of the nanodevice. This resonance is

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shown Fig.4. Due to discrete energy levels in QDs, all responses of the nanodevice occur in narrow windows. The proposed architecture can thus be designed in order to understand and optimize how these cells operate.

B. Impact of hopping

We examine impacts of hopping to reservoirs. Contacts induce resonance shifting and broadening enhanced with *h*, 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. 5 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. We analyze that current cancels when overlap disappears, and that the singularity point occurs when partial overlap starts, giving rise to these peculiar working behavior.

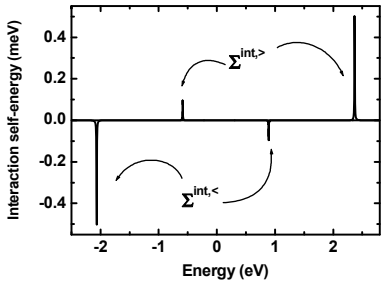

Fig2. . Real part of the self-energy of the electron-photon interaction at V_{bias}=0V. $\Sigma^{int,<}$ is plotted for the lowest level while $\Sigma^{int,>}$ is plotted for the highest level quantum

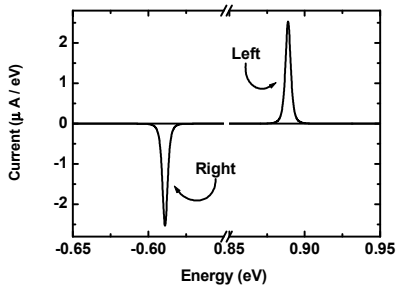

Fig3. .Left and right current spectral densities as a function of the electron energy at Vbias=0V

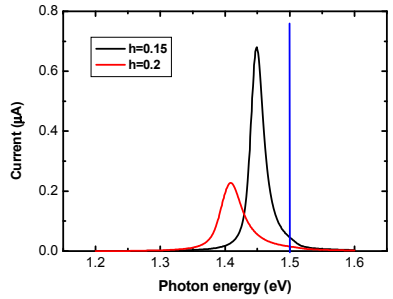

Fig4. . Left current at zero bias voltage as a function of the photon energy. The initial gap values 1.5eV (vertical line)

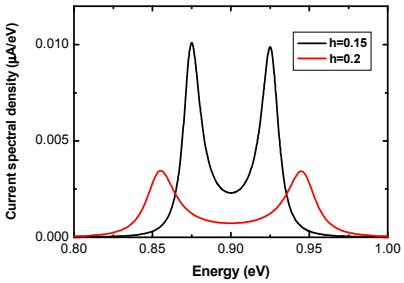

Fig5. . Left current spectral density at zero bias voltage as a function of the electron energy.

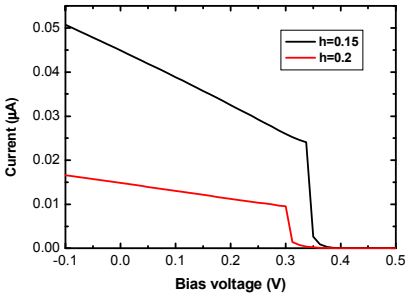

Fig6. . Left current as a function of the bias voltage.

IV. Conclusion

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

V. References

[1] Martin A. Green, "Third Generation Photovoltaics: Ultra-high Conversion Efficiency at Low Cost", *Prog. Photovolt: Res. Appl. 2001*, **9**: 123-135 .

[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.

[3] U. Aeberhard and R. H. Morf, "Microscopic nonequilibrium theory of quantum well solar cells", *Phys Rev B 77*, 2008, 125343.