STSM REPORT

STSM Application number: COST-STSM-BM1205-27414

STSM Grantee: Professor Mauro Pereira

Early Stage Researcher? No

STSM title: Nonequilibrium Green\`s Functions Approach to THz Generation by Frequency Multiplication in

Semiconductors

Home Institution: Sheffield Hallam University, Sheffield (UK)

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Host Institution: Lund University, Lund, (SE)

STSM period: 2015-05-19 to 2015-05-25

STSM purpose: The goal of this STSM is to adapt a Nonequilibrium Green\`s Functions (NEGF) computer code, which has been primarily developed at ULUND with now a module contribution from SHU for electron-electron scattering to the study of harmonic generation in semiconductor superlattices.

Working Group: WG 3: Tissue characterisation at terahertz frequencies using THz QCLs SMI.

Tissue characterization at THz frequencies. The THz emission from the nonlinear superlattices has potential to replace at lower cost the THz QCLs. The devices can also be integrated in detection schemes.

Description of the work carried out during the STSM: The ULUND simulator with an electron-electron subroutine developed jointly with SHU has been adapted to investigate the generation of THz radiation using the nonlinear voltage-current response of a semiconductor superlattice and the results have been compared with experimental data available in the literature.

Description of the main results obtained: See the file in Appendi**x.**

Mutual benefits for the Home and Host institutions: Both SHU and ULUND will benefit from this cooperation in terms of joint publications and possibilities for joint grant applications to use the numerical solutions for the predictive simulation of generation and detection of THz radiation using nonlinearities in superlattices which are far less expensive to fabricate then quantum cascade lasers and have potential for room temperature operation.

Future collaboration with the Host institution (if applicable): We plan to continue the cooperation between SHU and ULUND to solve the current difficulties related to the dynamical solution to obtain numerically stable results for lower frequencies (around 330 GHz) that can then be multiplied to around 1 THz through the third harmonic.

Foreseen publications or conference presentations expected to result from the STSM (if applicable):

- Conference: a paper has been submitted to ITQW 2015.

Publication: A detailed report is expected to be submitted to Optics Express in 2015.

Nonequilibrium Green`s Functions Approach to THz Generation by Frequency Multiplication in Semiconductors

Introduction

The starting point for the project was the inclusion of one of the versions of the electron-electron scattering subroutine in the ULUND simulator, following a simplification scheme jointly developed by SHU and ULUND, in order to adapt the fully frequency and momentum dependent approach of SHU to the more complete simulator at ULUND, which can deliver nonlinear responses of QCL media to the specific case of nonlinear multiplication in superlattices.

The electron-electron scattering selfenergy in second Born approximation reads,

$$\Sigma^{\gtrless}_{\mu\nu}(k,E) = \frac{1}{2}\sum_{k',\pm}(\pm)\, M_{\mu\nu}(k-k')\, b^{\gtrless}\left(\Omega_{\mu\nu}(\mathrm{k}-\mathrm{k}')\right) \mathrm{G}^{\gtrless}_{\mu\nu}\left(\mathrm{k}',\mathrm{E} \mp \Omega_{\mu\nu}(\mathrm{k}-\mathrm{k}')\right).$$

(1)

The first step in this long term project is to check how far we can use a series of approximations that allow for a qualitative analysis which can be a starting point for more complete simulations. We have thus started by calculating the static output to compare and contrast with the experiments of Ref. [2]. Figure 1 shows the superlattice multiplier of Ref. [2].

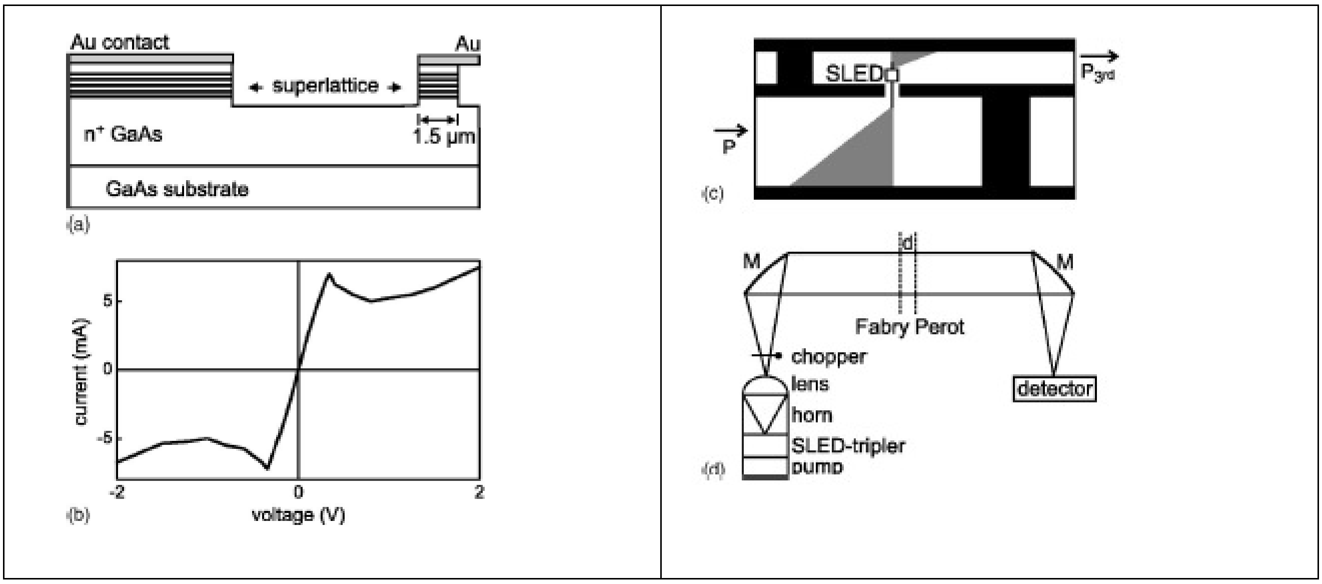

Fig.1. The superlattice multiplier from Ref. (2). (a) SLED in a quasiplanar design. (b) Current-Voltage (I-V) curve of the SLED. (c) Two-waveguide schematics of the SLED. P is the pump input radiation and P_{3rd} is the third harmonic radiation output. (c) Optics setup.

From Fig. 1 we see that the contact area is 2.25×10^{-8} cm^2, which is used as scaling factor in our calculations which deliver a current density in A/cm^2. Furthermore we have voltage per period as input and since there are 18 periods, the scaling for comparison is a factor 18 for the x-axis. Figure 2 shows our calculated voltage current.

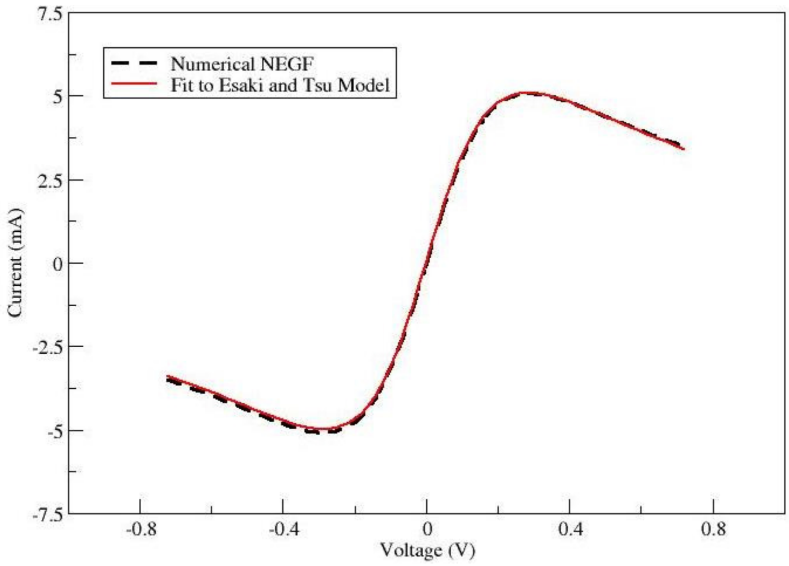

Fig.2. Comparison between the NEGF current calculated for the superlattice of Ref. 2 and the fit to the Esaki and Tsu Model of Eq.2.

The following features are striking in Fig.2. First the excellent agreement of peak current value and position compared to experiments and the fact that we can use the exact numerical results to find values for the Vc and J0 for the Esaki and Tsu Model [3] in Eq. 2

$$J(V) = 2J_0 \frac{V/V_c}{1+\left(V/V_c\right)^2} \tag{2}$$

This means that we can start from a relatively fast and easily converging calculation of the static current, determine the values of Vc and J0 and use them for systematic and fast approximations to obtain qualitative insight into the desired design before engaging in fully dynamical calculations, which are time consuming and require very large matrices.

Note that even though the actual structure of the nonlinear response is more complex than the static, we can in a zeroth order approximation assume that the main characteristics of the response will follow the qualitative shape of the static response. In other words, the static I-V curve clearly defines the nonlinear range (around and below -Vc and around and above Vc) and some qualitative information can be extracted from it. Thus, now that we obtained values for Vc and J0, let's investigate some general characteristics of the model.

If we assume that light from a monochromatic source with frequency ω is applied to the nonlinear, superlattice, E = A sin(ωt), the nonlinear response can be calculated and expanded in a Fourier series (harmonics). and the amplitudes determining the the strength of the nonlinear response for the harmonics (3rd, 5th, 7th etc ..). Equivalently we can investigate the current response to input voltage $V=V_0$ sin(ωt) and expand the current in a Fourier series as in Eq. (3).

$$J(V)=\sum_{n=1}^{\infty} b_n \sin(n\omega t), \qquad b_n=\frac{4J_0}{\pi}\int_0^{\pi}\frac{V/V_c \sin(x)}{1+(\sin(x)V/V_c)^2}dx \tag{3}$$

Results for the Klappenberg superlattice of Ref. [2] are given in Fig. 3

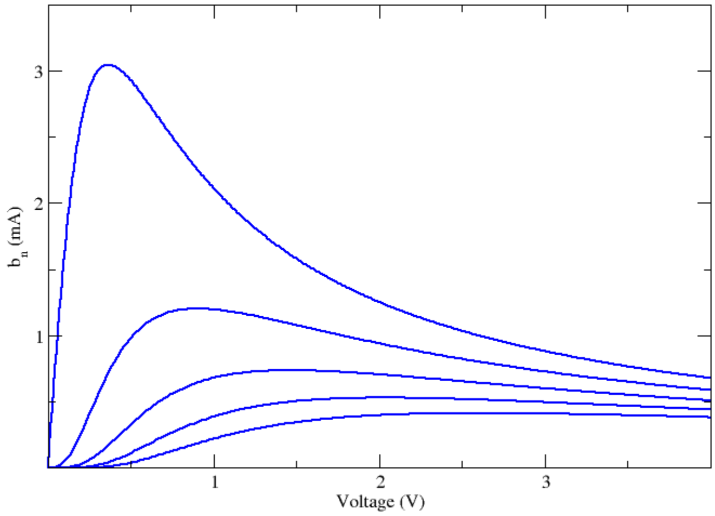

Fig.3. Nonlinear terms on the general structure of the static response underlying the qualitative ratio of, from top to bottom b_1, b_3, b_5,b_7 and b_9 for the superlattice in Ref. [2].

It is extremely interesting to see that the maximum output occurs for higher input amplitudes for higher order as seen experimentally and that the values of V_c and J_0 can be engineered to be maximized for a given harmonic.

However, that does not include the dynamics.

The selfenergy module has been adapted to the ULUND version of simulator that gave recently rise to a Microscopic approach to second harmonic generation in quantum cascade lasers [3]. In this approach, if a periodic signal $E=E_0\sin(\omega t)$ is injected in the system, the current response (for the case of an asymmetric current-voltage curve such as a superlattice) can be written as a Fourier series.

Following the injection of a periodic input in the system, $F = F_{ac}\sin(\omega t)$, the current response is once more written as a Fourier series, $J(t) = \sum_{n=-n_{max}}^{n_{max}} J^{(n)} \sin(n\omega t)$.

where J_0 is the stationary response and the $J^{(n)}$ terms are induced by the oscillating field. For numerical reasons the value of n_{max} should be kept as low as possible as computational time increases by the square of the system size, which is linear in n_{max}. In practice this amounts to converging the calculations of the desired parameters with respect to n_{max} for a given ac field strength. Naturally convergence is more easily reached for observables involving terms related to n = 1 than those relying on terms with n = 3, and so on …

A very serious numerical difficulty arises from the fact that, in order for the assymptoptic expressions used in the dynamic case to be valid, we must have

$$\frac{eF_{ac}d}{\hbar\omega} < \left[\frac{(n_h+1)!}{10}\right]^{\frac{1}{n_h+1}} \tag{4}$$

where d is superlattice period, ω is the input frequency and n_h is the number of harmonics. Since we are interested in multiplying small frequencies in the THz range with input fields as strong as possible to achieve a high power THz output, the number of harmonics requires is large. Figures 4 and 5 have results with 8 harmonics with an input field of 330 GHz that is then multiplied to the 1 THz range.

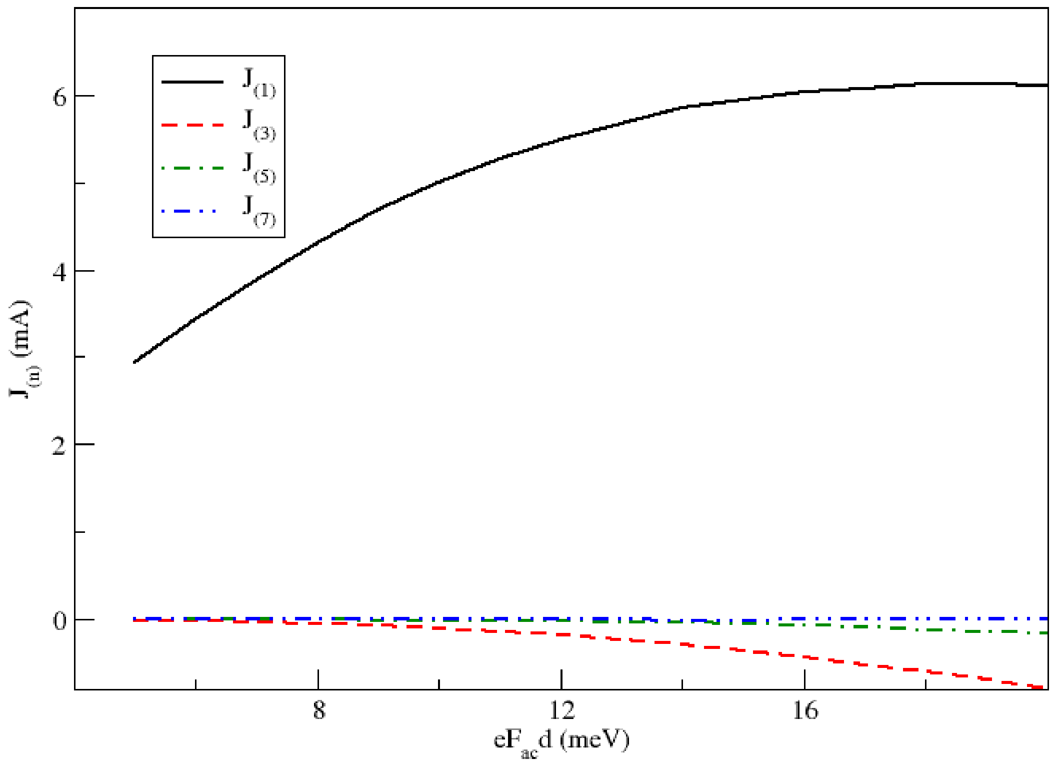

Fig. 4. Amplitudes of the harmonic components for the structure in Ref. [2].

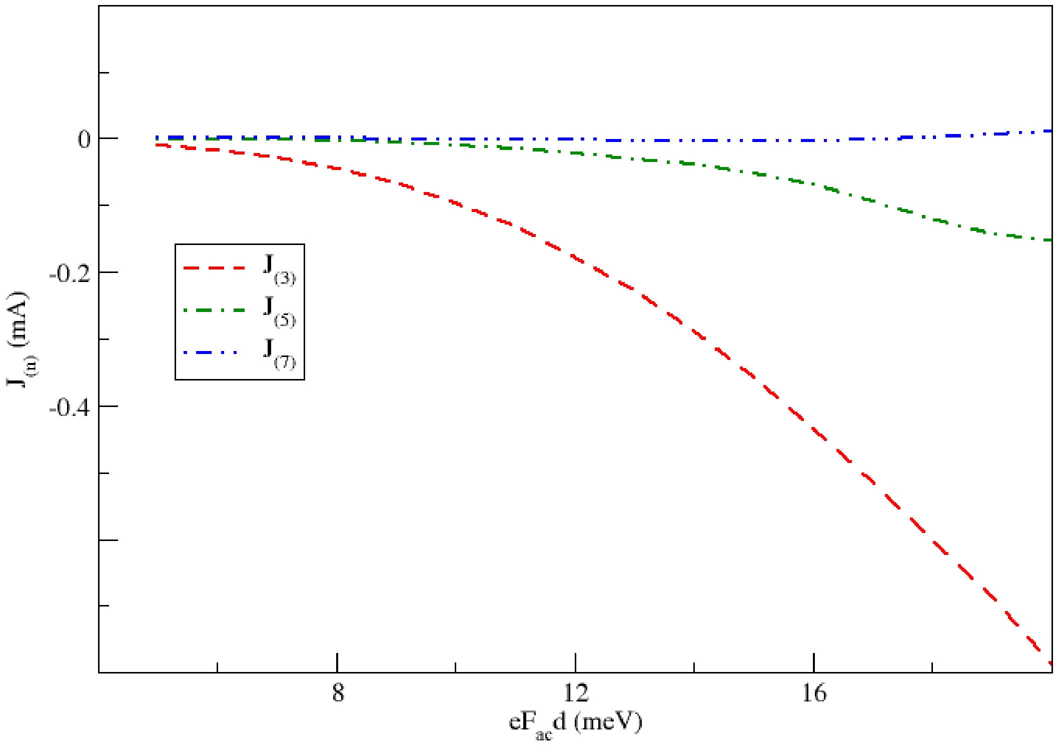

Fig. 5. Amplitudes of the harmonic components for the structure in Ref. [2].

Many numerical complications from non convergence to loss of hermiticity arise. What we show is $J_n = Re[J^{-n} + J^n]$. Any As expected from the analysis of the general structure of the static response, the amplitude decreases with increasing harmonic.

In summary our approach leads to predictive calculations of the high order harmonic currents generated in a superlattice and will become a powerful design tool after we manage to optimize the algorithms for smaller matrices and faster calculations. We plan to combine further analytical approximations based on first steps of the simulation process with more efficient versions of the full algorithms in forthcoming joint research.

References:

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2. F. Klappenberger et al., Appl. Phys. Lett. 84, 3924 (2004).
3. R. Tsu and L. Esaki, Appl.Phys.Lett. 22, 562 (1973).
4. D.O. Winge, M. Lindskog and A. Wacker, Optics Express 22, 18389 (2014).

LUND UNIVERSITY
Faculty of Science

30 Jun 2015

To the Grant Holder of the COST Action BM1205

Mathematical Physics
Prof. Andreas Wacker

Visit of Prof. Mauro Pereira in Lund May 2015

Hereby I confirm that Mauro Pereira visited our group at Lund University from May 19 to May 25. We had a very successful cooperation on frequency multiplication in superlattices, which showed promising resuls and are likely to lead to a joint publication.

Yours sincerely

Andreas Wacker

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