STSM REPORT

STSM Application number: COST-STSM-BM1205-29171

STSM Grantee: Prof. Jelena Radovanović

Early Stage Researcher? No

STSM title: Advanced modelling of electronic structure of Quantum Cascade Lasers

Home Institution: School of Electrical Engineering, University of Belgrade, Serbia

Host Institution: School of Electronic and Electrical Engineering, University of Leeds, UK

STSM period: 10/07/2015 to 18/08/2015

STSM purpose: To develop and test a model for QCL electronic structure calculations based on the perturbation theory. The goal was first to investigate the impact of correction of energy levels, obtained by using 2nd order perturbation theory, with the Hamiltonian which includes band nonparabolicity. Then, we assessed the effects of external magnetic field on the intersubband transition matrix element which directly influences the optical gain of the structure. As an outcome of this STSM, specific program codes were developed.

Working Group: WG2

Description of the work carried out during the STSM and the main results obtained:

During the STSM, we addressed the problem of detailed modelling of the electronic structure of quantum cascade laser, in particular taking into account nonparabolicity effects (NPE) in quantum nanostructures in the presence of external electric and magnetic field, by using second order perturbation theory. A suitable model was formed which includes 1st order correction for envelope wavefunction and 2nd order corrections for energy due to both bound and continuum states (in structures without the presence of external electric field). When applied to QCL structure, this model gives us new insights into effects of magnetic field on the matrix element which are usually neglected. We showed that the dipole matrix element can undergo a pronounced change for certain values of magnetic field and Landau level index, which implies change of the gain of the structure in case of lasing optical transition.

Nonparabolicity effects in the conduction band of a semiconductor quantum well material can have an essential role in modelling of electronic structure of multiple QW structure such as quantum cascade laser. Several approaches exist in the literature, e.g., the inclusion of energy-dependent electron effective mass. Ekenberg[1] determined the coefficients in the expansion of the dispersion relation up to the fourth order in wavevector, by using 14-band k•p calculation. This results in a forth order differential equation with boundary conditions obtained by double integration, which fulfill the requirement for probability current conservation. Modeling of NPE mathematically represents a nonlinear eigenvalue problem, thus it is preferable to develop an approximate solution, the details of which will be presented in our manuscript which is under preparation.

We assume that moderate electric field is applied in the QCL structure and that we can approximate the potential at the structure's ends as constant. The transfer matrix method (TMM) is used to determine the energies and wavefunctions of the unperturbed Hamiltonian $\widehat{H}_0 = \hat{k}_z^2 \alpha_0(z) \hat{k}_z^2 + \frac{\hbar^2}{2} \hat{k}_z \frac{1}{m^*(z)} \hat{k}_z + V(z)$. These quasi-bound states are then used in the perturbation theory. The gain of QCL depends on the squared modulus of dipole matrix element. We consider 3 states in QCL structure $E_1 < E_2 < E_3$ where two transitions are of interest: $E_3 \rightarrow E_2$ (lasing transition) and $E_2 \rightarrow E_1$ (transition for depopulation of the second state). Most models of QCL structures calculate the dipole matrix element $d_{if} = \int_{-\infty}^{\infty} \eta_i^* \, z \, \eta_f dz$ with unperturbed wavefunctions, thus the effect of external magnetic field cannot be seen. We have explored this effect and illustrated the dependence of dipole matrix element on B for different Landau levels by using wavefunctions with first order correction.

The model was applied to the mid- infrared (MIR) QCL proposed by Kruck et al[2] who realized this structure experimentally and reported lasing at wavelength of λ≈11.3 µm. Since this QCL has GaAs/Al0.33Ga0.67 active region, and nonparabolicity parameters from [1] are given for molar fraction of x=0.3, we use linear interpolation to determine the corresponding values of these parameters. First we apply TMM method to find unperturbed energies and wavefunction and the results of our simulations are presented in figure 1.

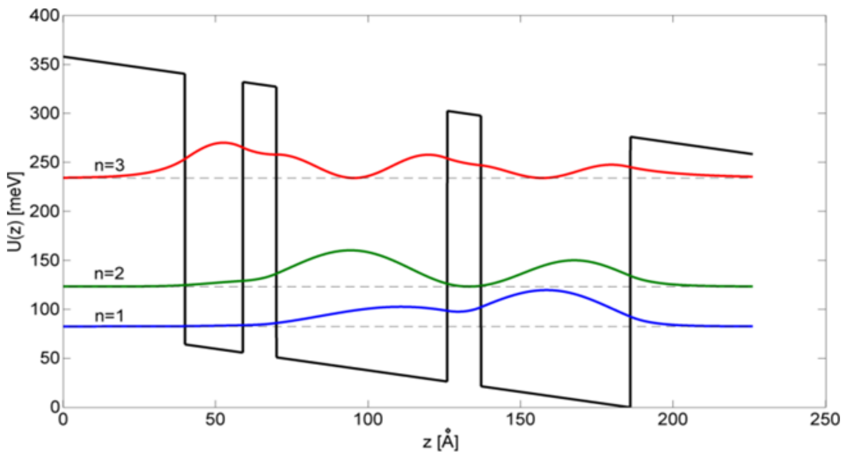

Fig. 1. *The active region of QCL [2] under an electric field of $K = 44 \; kVcm^{-1}$. The layer thikness starting from the left well are 19, 11, 56, 11, 49 Å, respectively. Relevant energies and the moduli squared of unperturbed wavefunctions are also displayed.*

Numerically obtained lasing wavelength for this structure reads λ≈11.2 µm. Then, we consider the application of an external magnetic field and calculate corrections for energy and wavelength by

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[1] Ekenberg U 1989 Nonparabolicity effects in a quantum well: Sublevel shift, parallel mass, and Landau levels Phys. Rev. B 40 7714

[2] P. Kruck, H. Page, C. Sirtori, M. Stellmacher, J. Nagle: Improved temperature performance of $Al_{0.33}Ga_{0.67}As/GaAs$ quantum-cascade lasers with emission wavelength at $\lambda \approx 11\mu m$, Appl. Phys. Lett.76, 2000, pp. 3340-3342.

using our model. The results are presented in figure 2 and figure 3, and depend on the value of magnetic field and Landau level index (for lasing optical transition, these levels are matched).

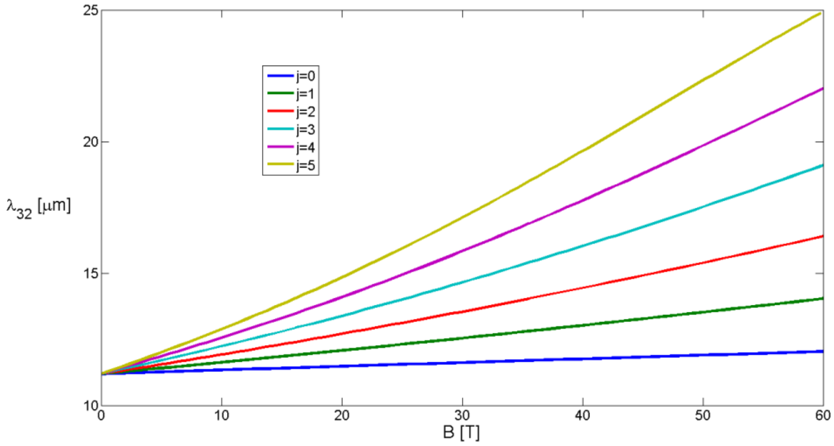

Fig. 2. *Lasing wavelength of the structure from [2] as it depends on the magnetic field for different Landau levels.*

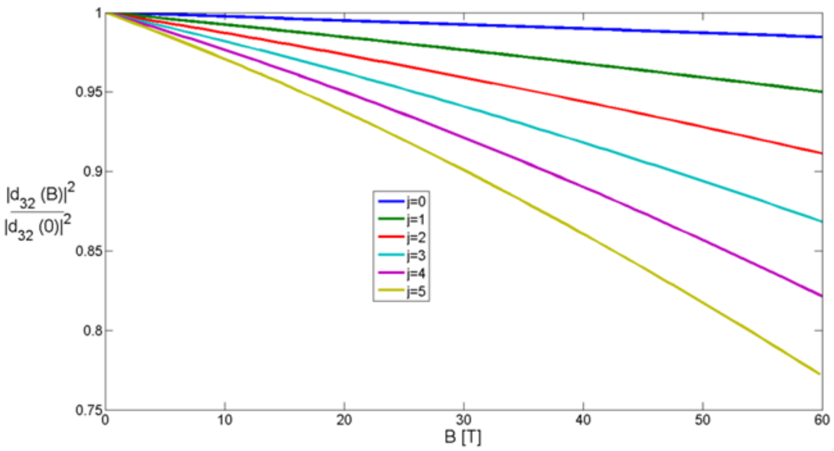

Fig. 3. *The Dipole matrix element* $|d_{32}|^2$ *for the structure from [2] as it depends on the magnetic field for different Landau levels,* $|d_{32}(0)| = 26.02\ \dot{A}$.

Figure 2 shows the dependence of the lasing wavelength (transition energy) on magnetic field, and the change is evidently more rapid when higher Landau levels are considered. Figure 3 illustrates the dependence of the modulus squared of the dipole matrix element on magnetic field, in comparison to the case when there is no magnetic field (unperturbed value). It is interesting to note that for higher Landau levels we have rapid decrease of $|d_{32}|^2$ which is also reflected in the decrease of the gain of the QCL structure.

We have also evaluated the value of the transition matrix element $|d_{21}|$ which describes the process of depopulation of the second laser state. Note that for $|d_{21}|$ the Landau levels of both states can be arbitrary (since non-radiative scattering processes are considered) thus we will present the cases $j_1 = j_2 = j$ (figure 4) and $j_1 \neq j_2$ (figure 5) separately.

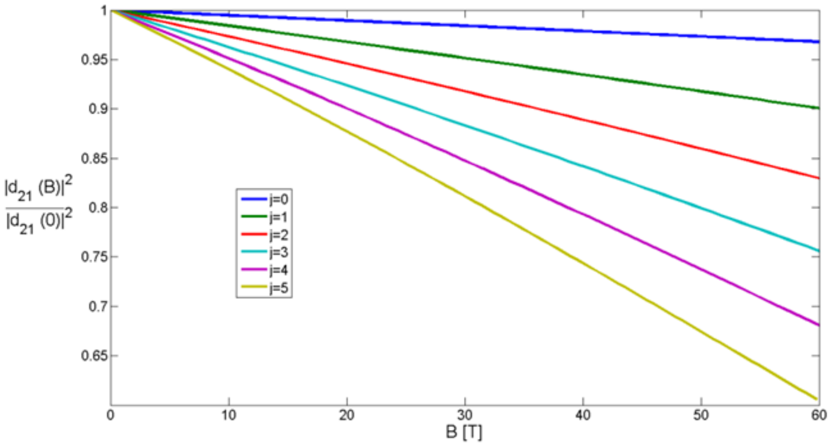

Fig. 4. *Dipole matrix element* $|d_{21}|^2$ *for structure from [2], as it depends on magnetic field for different Landau level (and* $j_1 = j_2 = j$*),* $|d_{21}(B)| = 31.64\ \dot{A}$.

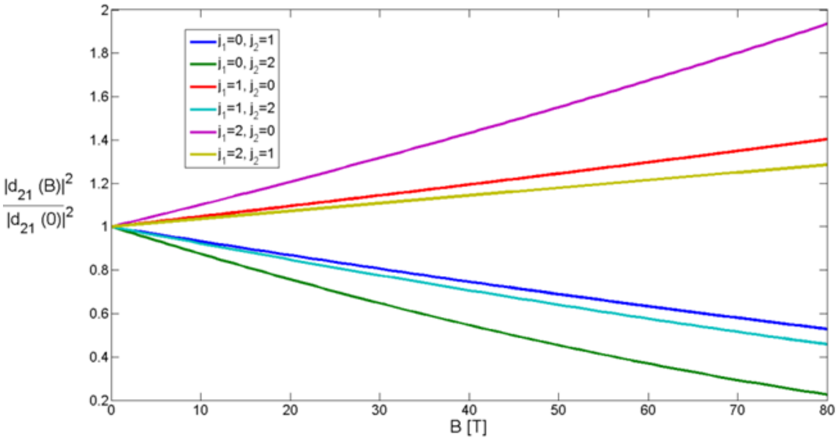

Fig. 5 *Dipole matrix element* $|d_{21}|^2$ *for structure from [2] as it depends on magnetic field, for different Landau level (and* $j_1 = j_2 = j_n$*).*

Figure 4 depicts the dependence of the modulus square of the dipole matrix element on magnetic field for transition 2→1 when both states have same value of the Landau level index. The effect is also decreasing as in transition 3→2 (figure 3), but it is also more pronounced. On the other hand, figure 5 shows $|d_{21}|^2$ for the case when Landau levels inices for particular states do not match. We can see that for $j_1 < j_2$ we have a decrease and that the effect is similar as in the previous case, but for $j_1 > j_2$ the situation is different.

The gain of QCL is proportional to $|d_{32}|^2$ hence for low values of $|d_{32}|^2$ we might generally expect lower gain (if all other relevant factors are constant). These effects will be further explored on a variety of different structures during our future work.

Mutual benefits for the Home and Host institutions:

This research visit has strengthened the collaboration between the Quantum Electronics group at the School of Electronic and Electrical Engineering, University of Leeds, UK and the Semiconductor Quantum Nanostructures group at the School of Electrical Engineering, University of Belgrade. Joint work has provided the opportunity to access experimental data and expertise not available at the University of Belgrade, as well as the possibility to use advance computing facilities in Leeds.

Future collaboration with the Host institution (if applicable):

Future collaboration will involve the continuation of the model and code improvement, and application to the design, modelling and testing of new quantum cascade laser based structures for the THz region. In addition, strong emphasis will be placed on planning and preparing joint grant application (Including Horizon 2020 calls).

STSM outcome form

STSM application number	Home institution & country	Host institution & country	BM1205 WG	Objective of the collaboration	Results of the collaboration
COST-STSM-BM1205-29171	School of Electrical Engineering, University of Belgrade, Serbia	School of Electronic and Electrical Engineering, University of Leeds, UK	WG2	Advanced modelling of electronic structure of Quantum Cascade Lasers	-improved model of electronic structure of quantum cascade lasers in external magnetic field, based on the application of perturbation theory

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Confirmation of successful execution of the STSM

To the Grant Holder of the COST Action BM1205

Leeds, 01 September 2015

STSM Participant: Jelena Radovanovic

Home Institution: School of Electrical Engineering, University of Belgrade, Serbia

Host Institution: School of Electronic and electrical Engineering, University of Leeds, UK

I hereby confirm the successful completion of the STSM entitled "Advanced modelling of electronic structure of Quantum Cascade Lasers" carried out by Dr. Jelena Radovanović, at the Institute of Microwaves and Photonics, School of Electronic and Electrical Engineering, University of Leeds in the period 10/07/2015 to 18/08/2015.

The STSM was completed according to the work plan described by Dr Jelena Radovanovic in the STSM Application and the most important results are presented in her report. The STSM had a mutual benefit for the applicant and the host group, in consideration of both the particular research activities that were performed and the expected strengthening of cooperation between the applicant's and the Host institution.

Yours sincerely,

First name and last name: Dragan Indjin,

Signature: Dragan Indjin