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Quantum transport in quantum dot cascade structures

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Introduction

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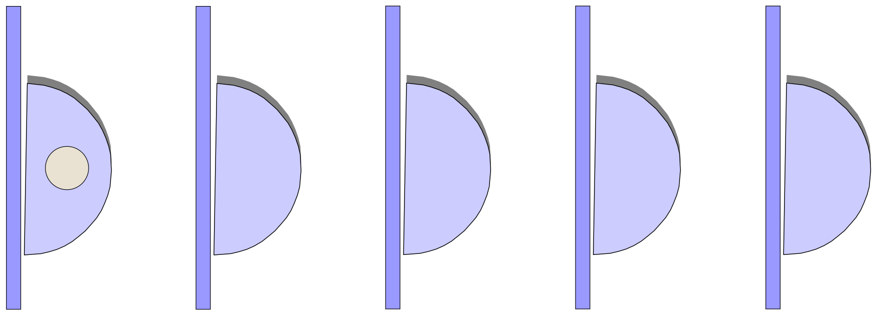
♦Electron transport through arrays of closely stacked quantum dots.



♦The interest comes from several anticipated device applications:

- Solar cells
- Thermoelectric devices
- **Quantum cascade lasers**

Outline of the talk

♦Theoretical approach – the formalism of nonequilibrium Green's functions.

♦Transport through a superlattice consisting of one QD per period

- Electron-phonon resonances

♦Simulation of a simple QD quantum cascade structure designed to exhibit gain in the terahertz range.

Theoretical approach – the formalism of nonequilibrium Green’s functions

The choice of the theoretical approach

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♦Semiclassical models often work relatively well in nanostructures with continuous spectra and are used in simulations of QW based QCLs.

♦Quantum dots

- Discrete electronic spectrum – the phase space for relaxation and dephasing processes is significantly reduced.
- Electronic coupling between neighbouring dots – the effect of electron tunnelling in closely stacked quantum dots.

♦An approach taking fully into account coherent effects is therefore necessary.

♦Two such formalisms exist in the literature

- The density matrix formalism.
- **The formalism of nonequilibrium Green's functions**.

A bit of theory (1)

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♦Steady-state transport

♦The Green's functions (in energy domain) satisfy the following equations

- The Dyson equation: $\sum_{\gamma}\left[E\delta_{\alpha\gamma}-\left(H_{\alpha\gamma}+\Sigma^{R}_{\alpha\gamma}(E)\right)\right]G^{R}_{\gamma\beta}(E)=\delta_{\alpha\beta}$
- The Keldysh relation: $G^{<}_{\alpha\beta}(E)=\sum_{\gamma\delta}G^{R}_{\alpha\gamma}(E)\Sigma^{<}_{\gamma\delta}(E)G^{A}_{\delta\beta}(E)$

♦Rough analogy with semiclassical equations: Dyson ~ Schrödinger, Keldysh ~ Boltzmann, $G^R(E)$ ~ density of states, $G^<(E)$ ~ populations (and coherences), $\Sigma^<(E)$ ~ scattering.

♦Electronic miniband structure was solved using the 8-band **k·p** model with the effects of strain taken into account

♦The basis of maximally localised Wannier states, well localised to one period of the structure, was then constructed – gives an insight into the carrier transport in real space.

A bit of theory (2)

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♦Electron – LO phonon interaction modelled with the Frölich Hamiltonian and taken into account within the self consistent Born approximation

$$\Sigma^{<}_{\alpha\beta}(E) = i\sum_{\gamma\delta,q} M_{\beta\delta}(q)^{*} M_{\alpha\gamma}(q)\frac{1}{2\pi}\int dE' G^{<}_{\gamma\delta}(E-E')D^{<}(E')$$

(and a similar expression for $\Sigma^R(E)$)

♦Finite LO phonon lifetime Γ also considered

$$D^R(E) = \frac{1}{E - E_{LO} + i\Gamma} - \frac{1}{E + E_{LO} + i\Gamma}$$ (and a similar expression for $D^<(E)$)

♦Electron - acoustic phonon interaction also modelled within the SCBA.

♦Low carrier and doping limit – no e-e interactions, no interactions with impurities, no formation of domains (constant electric field).

♦Shift-invariance property of a periodic system in a constant el. field used to close the system of equations which was then solved self-consistently.

♦Current calculated from $I = -\frac{|e|}{L_z\hbar}\sum_{\beta}{}'\sum_{\alpha}[H_0, z]_{\alpha\beta}\frac{1}{2\pi}\int \mathrm{d}E G^{<}_{\beta\alpha}(E)$

Transport through a superlattice consisting of one QD per period

Current-field characteristics

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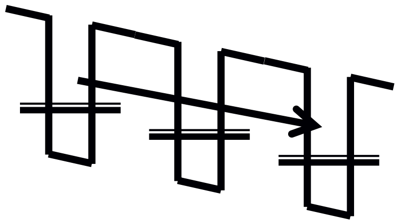
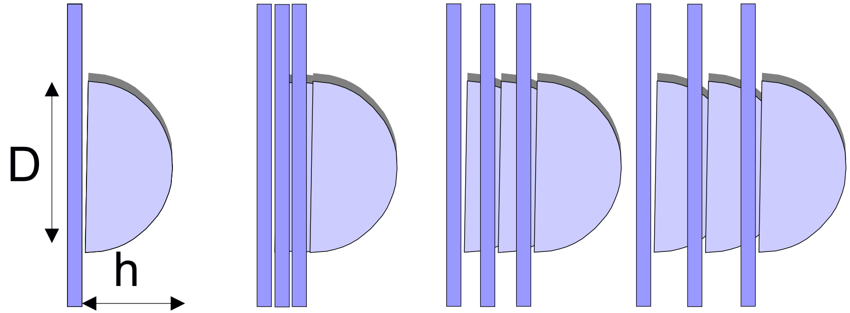
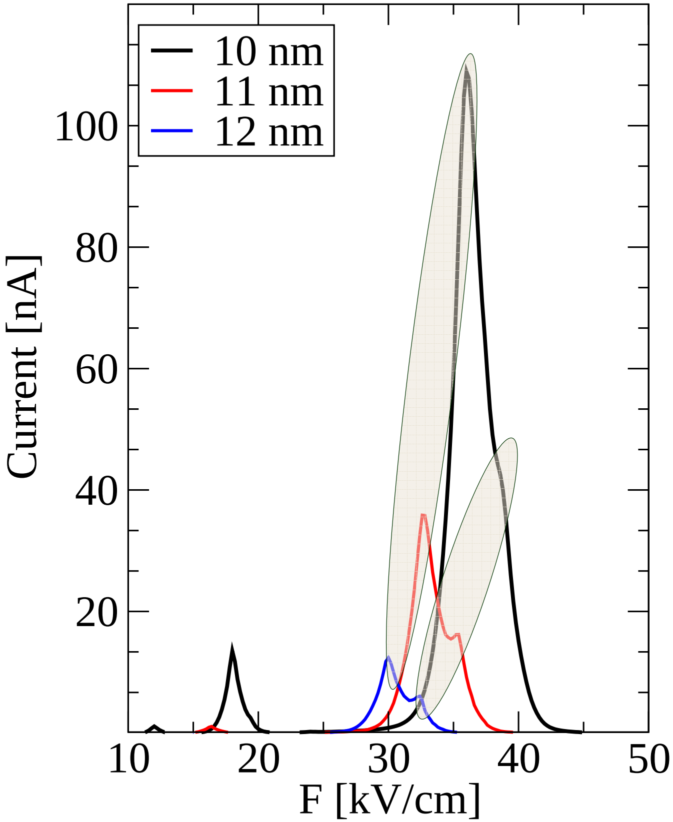
♦InAs/GaAs lens-shaped QDs,
D=20nm, h=5nm, T=77K.
♦Transport takes place through QD ground states.



♦Calculation for different values of the period of the structure.





The main peak and its doublet structure

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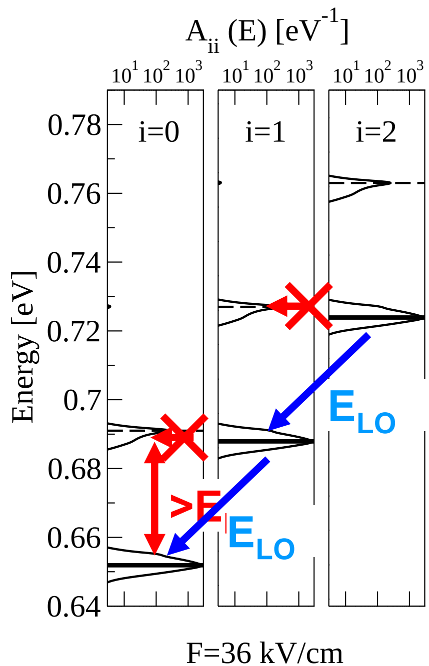
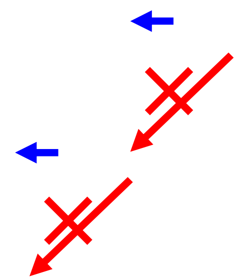
♦The density of states has a maximum at the energy of the ground state, as well as at the energy of phonon replica separated by energy larger than E_{LO} (by polaron shift).

♦The stronger peak of the doublet originates from LO phonon scattering between ground states of neighbouring periods.

♦The weaker peak of the doublet comes from tunneling to phonon replica.

♦The doublet structure is a transpor signature of polaron effects.



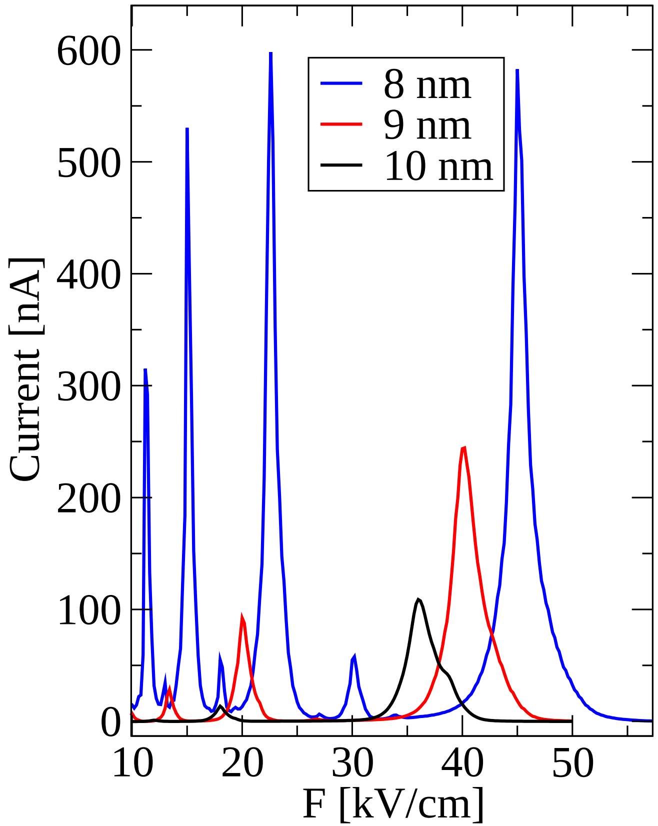


Other peaks

♦For smaller values of the period, the nature of transport at the main peak is the same, however due to broadening the components of the doublet are indistinguishable.

♦Additional peaks appear

- When potential drop per period V_F is half the LO phonon energy.
- In principle the peaks are present whenever $nV_F=mE_{LO}$.



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Transport through a QD cascade structure

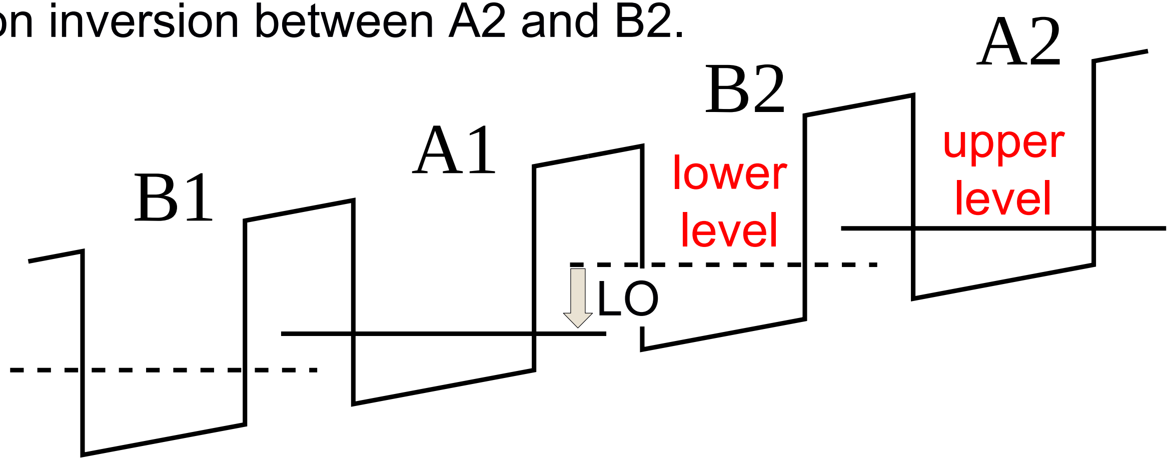
Design of the structure

♦Discrete states in QDs – reduced transition rates – reduced current (compared to QW structures).

♦QD QCLs are therefore expected to have significantly lower operating currents.

♦The design consisting of two QDs per period (A and B, h_A=5nm, h_B=4.5nm, D=20nm, separating barrier 3nm).

♦Fast LO phonon depopulation B2 to A1 at the design field, enables population inversion between A2 and B2.



Simulation

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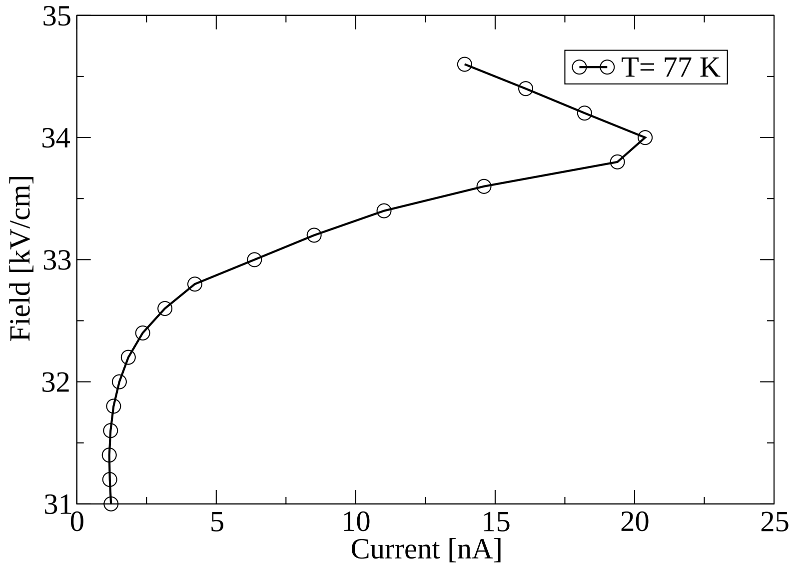
♦Field-current characteristic simulated around the design field.

♦Population inversion present in the whole range of fields in the figure.

♦At F=32kV/cm and T=77K population inversion is 56%, transition energy 19meV (4.6 THz).



♦Assuming carrier density of 10^{10}cm^{-2}

- The current at F=32kV/cm is J=15A/cm^2.
- The estimated peak gain is 470cm^{-1} (assuming FWHM 12%).

♦The region of positive differential resistivity and significant values of gain – stable device operation in this region should be feasible.

Summary

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♦Theoretical approach – the formalism of nonequilibrium Green's functions.

♦Transport through a superlattice consisting of one QD per period

- Doublet structure of the main peak as a signature of polaron effects

♦Simulation of a simple QD quantum cascade structure designed to emit in the terahertz range.

- Region of positive differential resistivity and significant values of gain, with low operating current.