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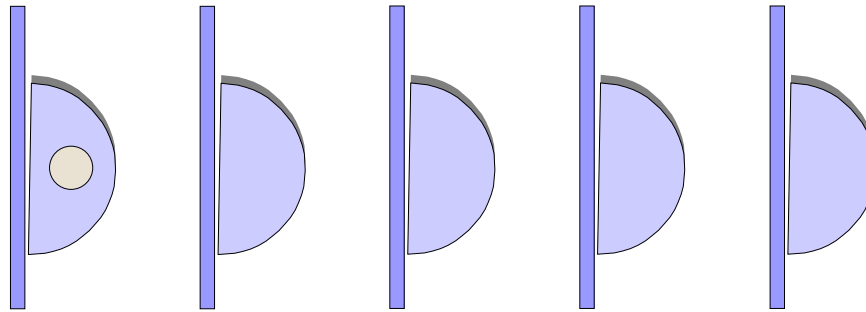
Quantum transport in quantum dot cascade structures

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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**



- ◆ 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:
$$\sum_{\gamma} [E\delta_{\alpha\gamma} - (H_{\alpha\gamma} + \Sigma_{\alpha\gamma}^R(E))] G_{\gamma\beta}^R(E) = \delta_{\alpha\beta}$$

- The Keldysh relation:
$$G_{\alpha\beta}^<(E) = \sum_{\gamma\delta} G_{\alpha\gamma}^R(E) \Sigma_{\gamma\delta}^<(E) G_{\delta\beta}^A(E)$$

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

◆ Electronic miniband structure was solved using the 8-band $\mathbf{k}\cdot\mathbf{p}$ 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

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

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

- ◆ Finite LO phonon lifetime Γ also considered

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

- ◆ 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 $I = -\frac{|e|}{L_z \hbar} \sum_{\beta} \sum_{\alpha} [H_0, z]_{\alpha\beta} \frac{1}{2\pi} \int dE G_{\beta\alpha}^{\leftarrow}(E)$



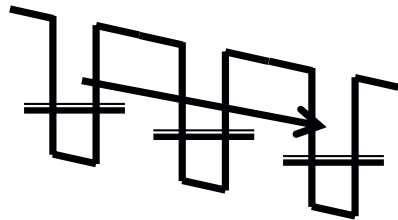
Transport through a superlattice
consisting of one QD per period

Current-field characteristics

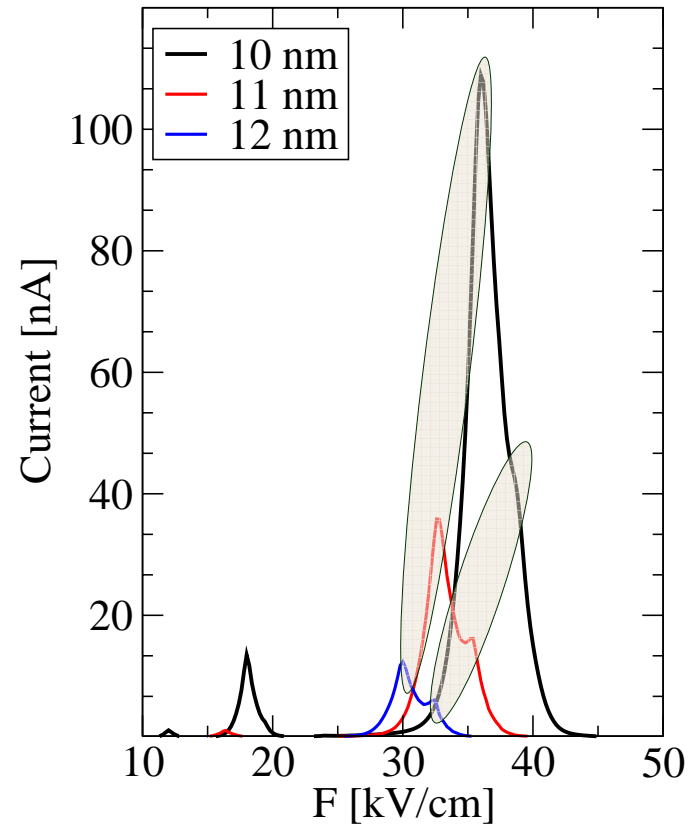
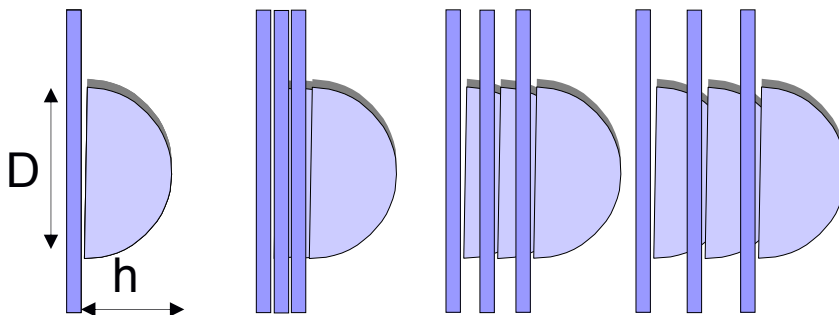


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- ◆ InAs/GaAs lens-shaped QDs, $D=20\text{nm}$, $h=5\text{nm}$, $T=77\text{K}$.
- ◆ Transport takes place through QD ground states.



- ◆ Calculation for different values of the period of the structure.

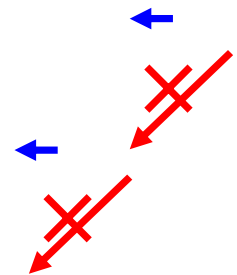
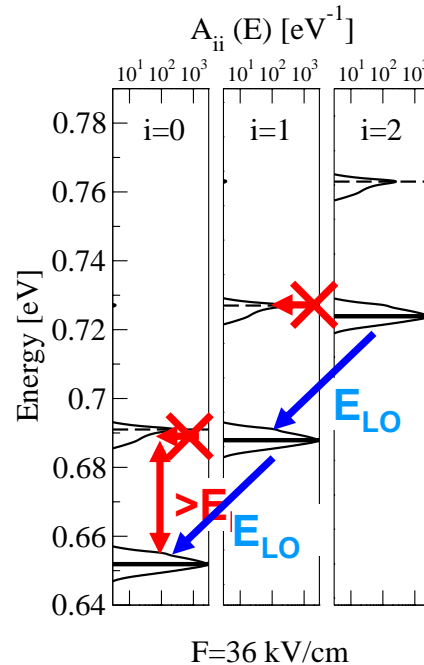


The main peak and its doublet structure



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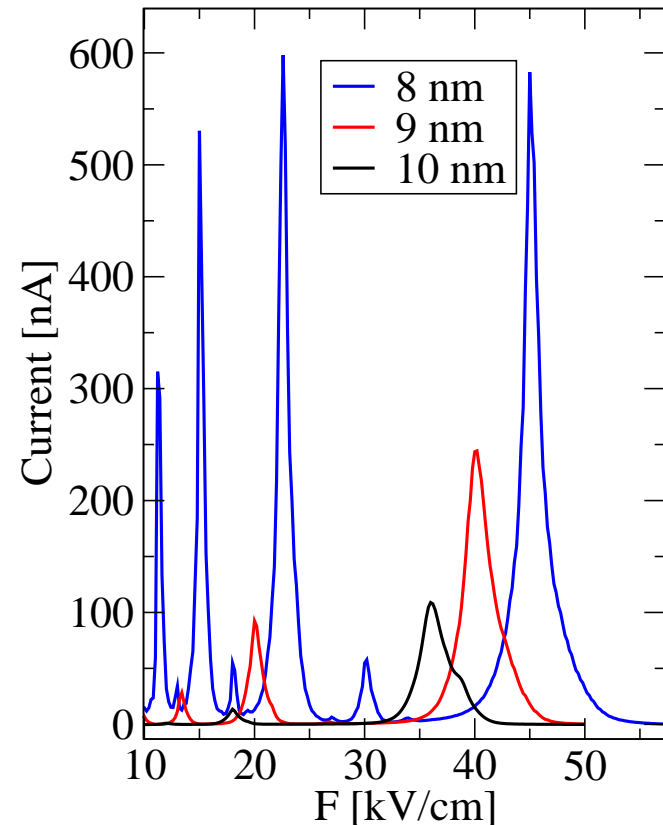
- ◆ The density of states has a maximum at the energy of the ground state, as well as at the energy of phonon replica separated by energy larger than E_{LO} (by polaron shift).
- ◆ The stronger peak of the doublet originates from LO phonon scattering between ground states of neighbouring periods.
- ◆ The weaker peak of the doublet comes from tunneling to phonon replica.
- ◆ The doublet structure is a transport signature of polaron effects.



Other peaks



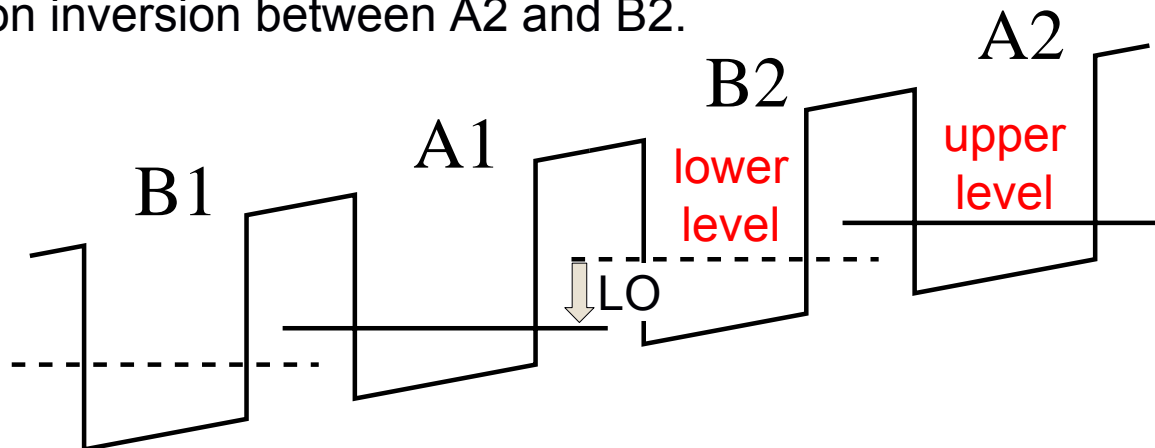
- ◆ For smaller values of the period, the nature of transport at the main peak is the same, however due to broadening the components of the doublet are indistinguishable.
- ◆ Additional peaks appear
 - When potential drop per period V_F is half the LO phonon energy.
 - In principle the peaks are present whenever $nV_F = mE_{LO}$.



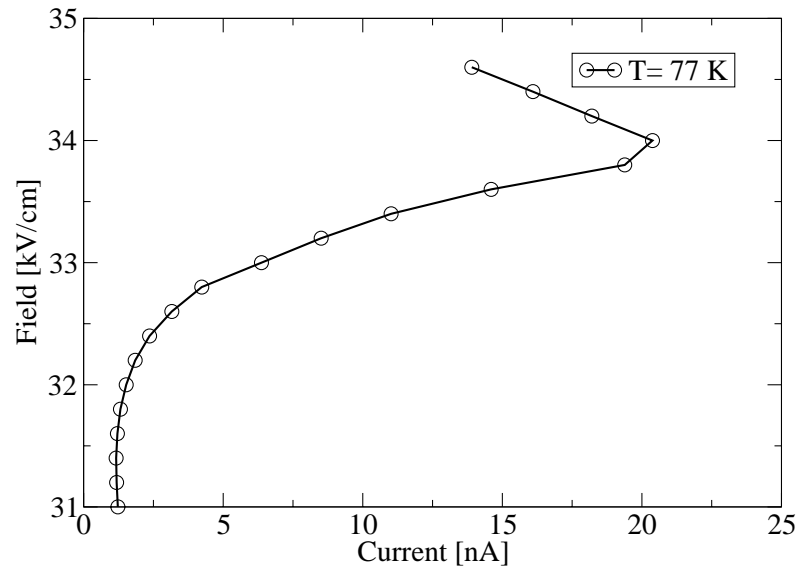


Transport through a QD cascade structure

- ◆ 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, $h_A=5\text{nm}$, $h_B=4.5\text{nm}$, $D=20\text{nm}$, separating barrier 3nm).
- ◆ Fast LO phonon depopulation B2 to A1 at the design field, enables population inversion between A2 and B2.



- ◆ Field-current characteristic simulated around the design field.
- ◆ Population inversion present in the whole range of fields in the figure.
- ◆ At $F=32\text{kV/cm}$ and $T=77\text{K}$ population inversion is 56%, transition energy 19meV (4.6 THz).



- ◆ Assuming carrier density of 10^{10}cm^{-2}
 - The current at $F=32\text{kV/cm}$ is $J=15\text{A/cm}^2$.
 - 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.



- ◆ 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.