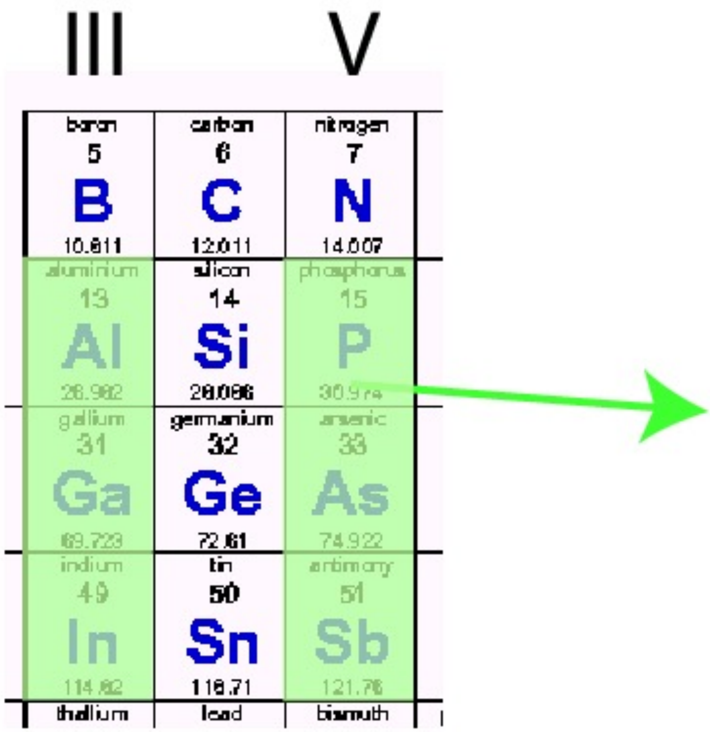
(THz) Quantum cascade lasers: Basics

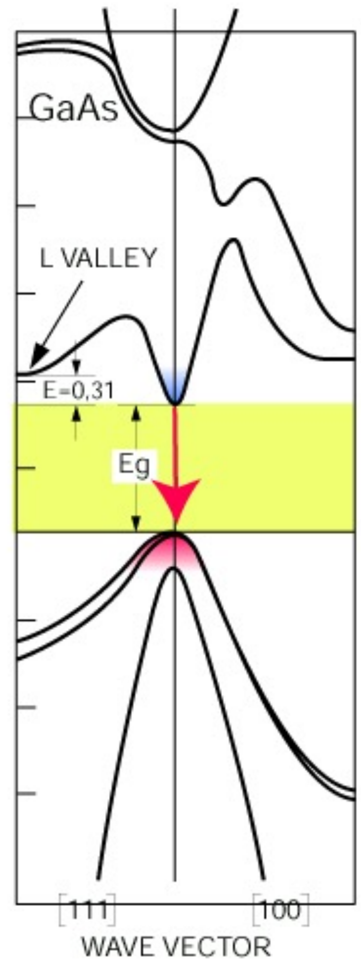
G. Scalari
J. Faist

Bibliography:

- G. Bastard , “*Wave mechanics applied to semiconductor heterostructures¨, Ed.* Les Editions de Physique
- J. Faist *”Quantum Cascade Lasers” , Oxford Univ. Press.*

Building block: semiconductor

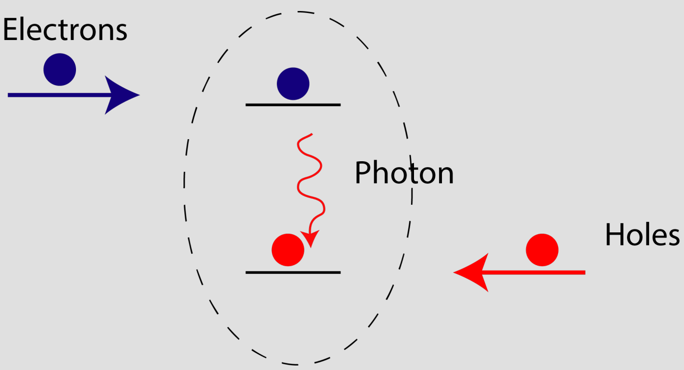




Direct semiconductor band structure

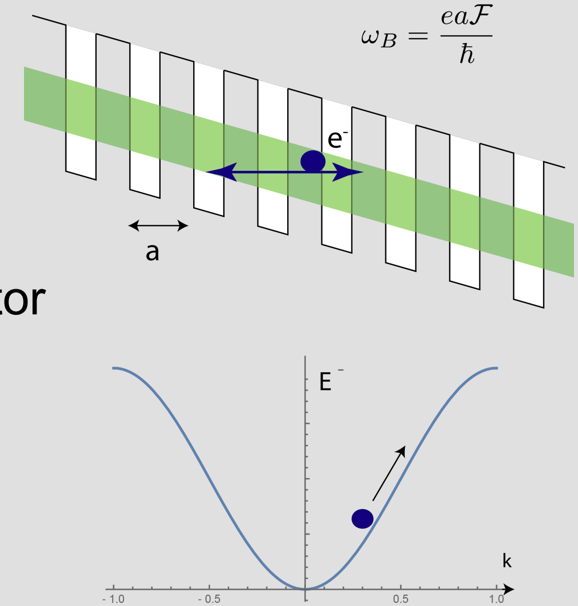
The journey from materials to quantum structures

Interband transition in a crystal



Photon energy determined by chemistry

Bloch oscillator

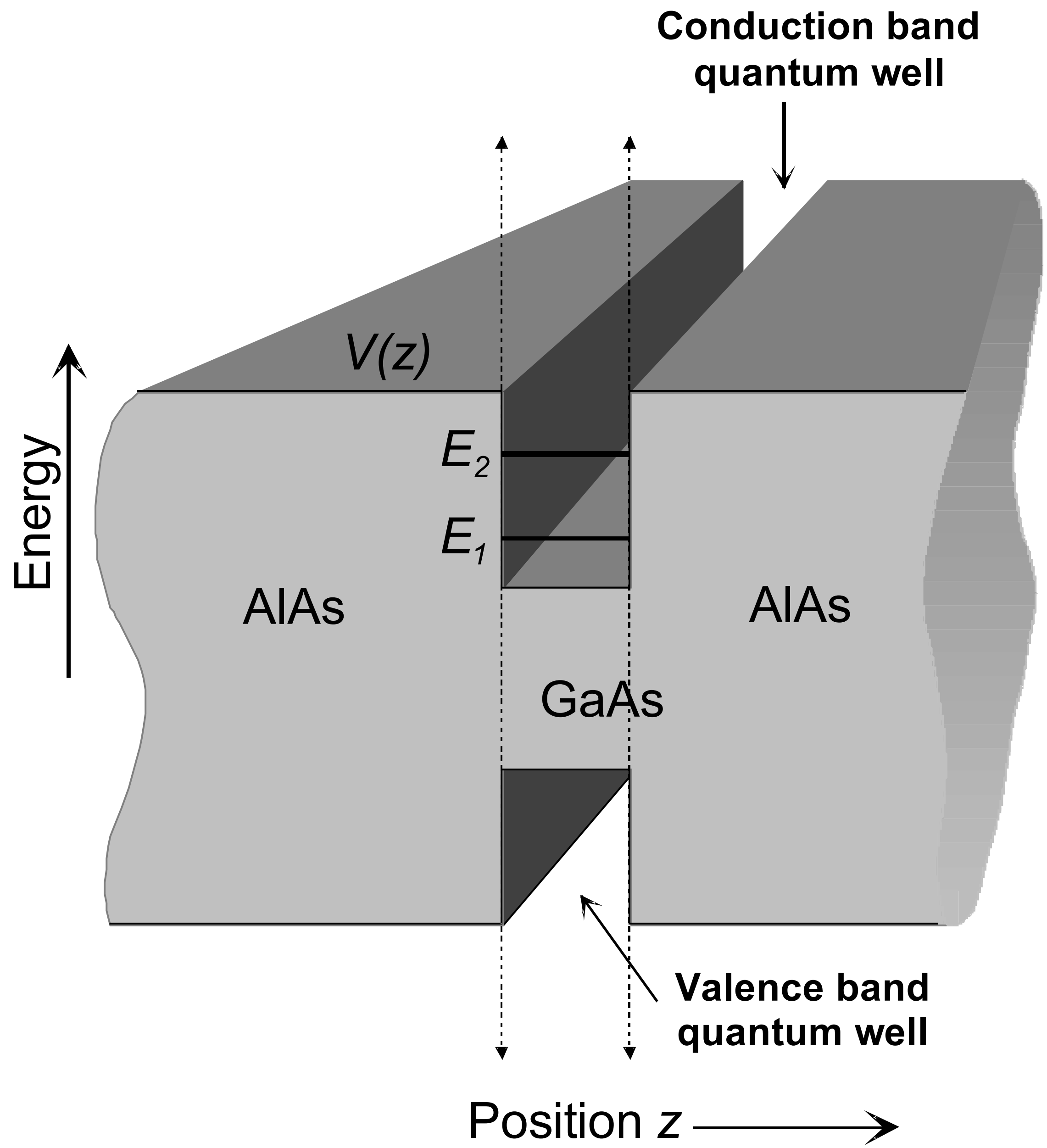


Photon energy determined by design and applied field

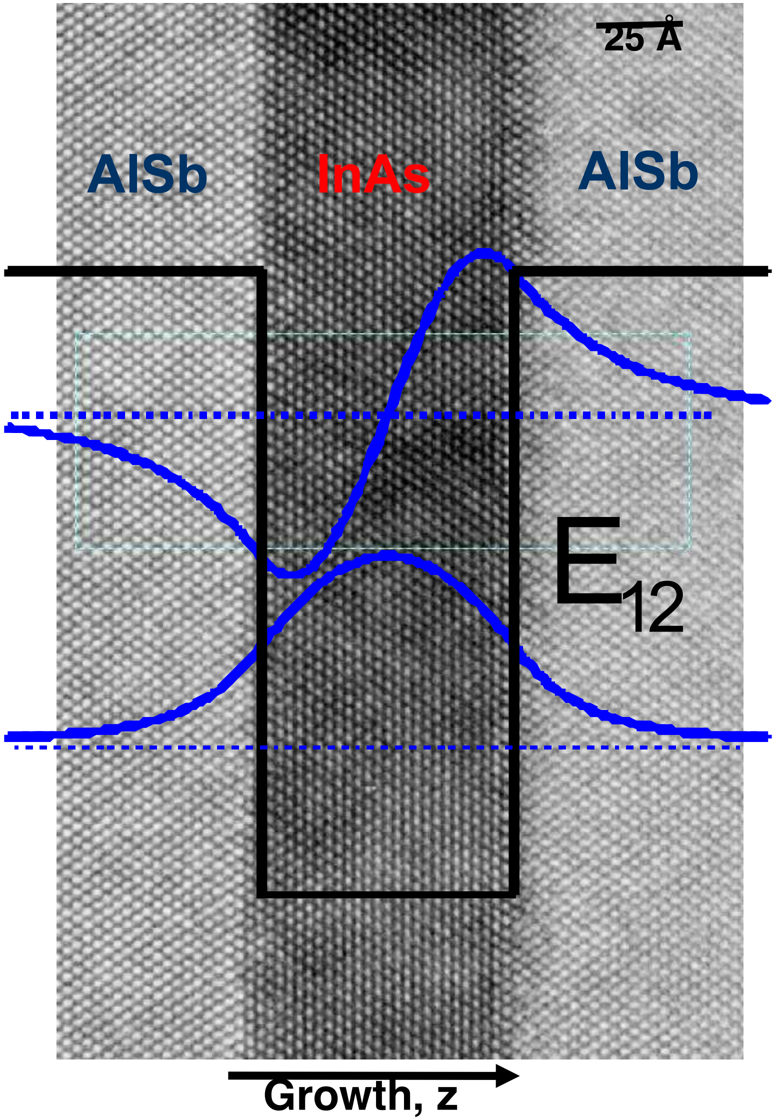
Building block: the quantum well

The confinement potential is effective only in the direction of growth (*z*).

Electrons are free particles in the plane



Epitaxial quantum wells: monolayer control

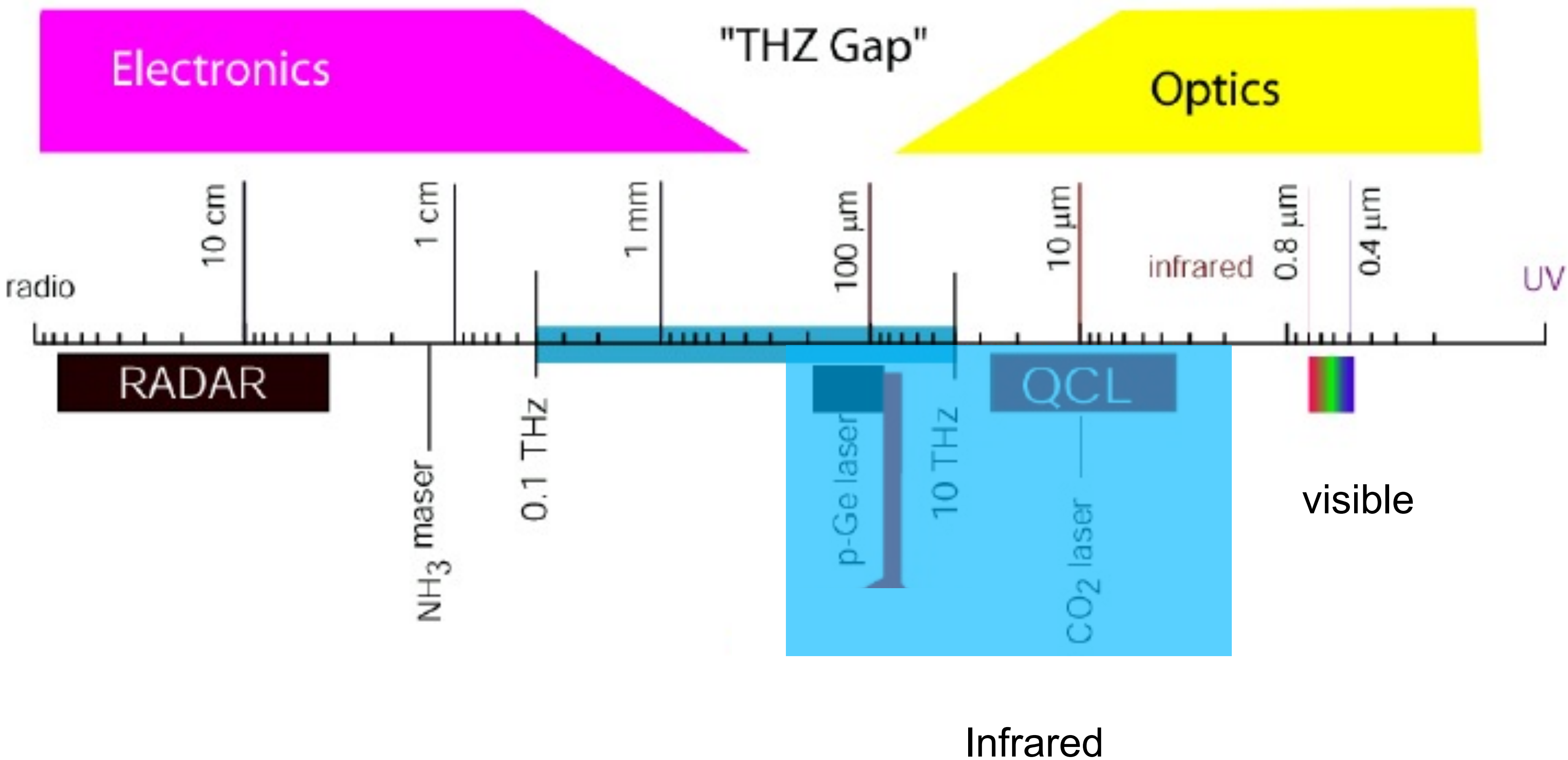


Epitaxial growth

Molecular Beam Epitaxy (MBE),

Metal-Organic Chemical Vapour Deposition (MOCVD)

Quantum Cascade Lasers: unlocking the IR!

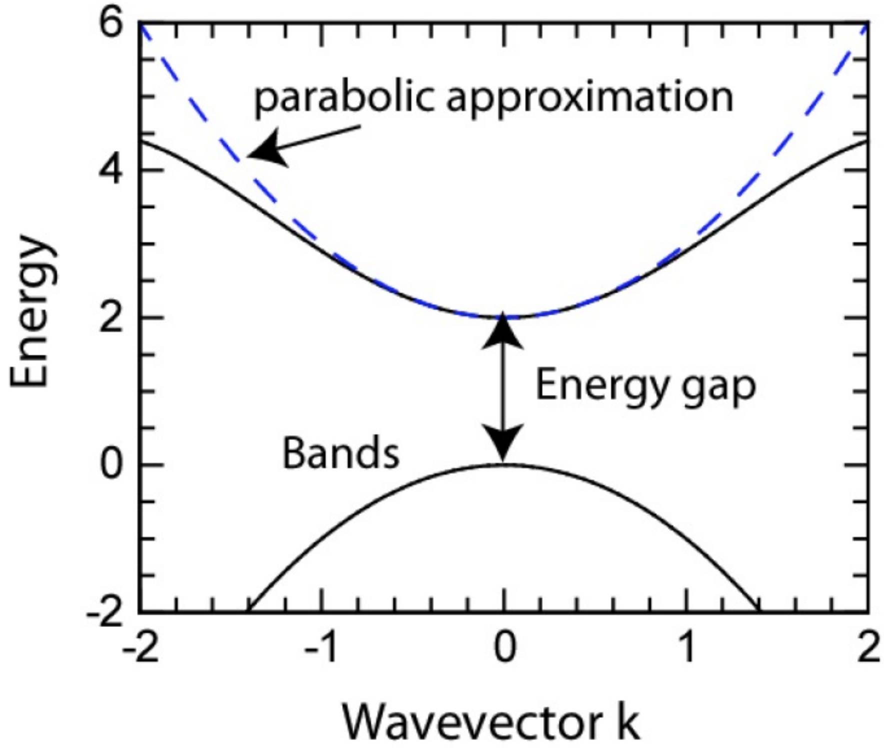


Interesting for many applications in sensing, medical applications, and so on..

Effective mass approximation

In the vicinity of a band extremum, the dispersion relation may be expanded in a quadratic form:

$$\epsilon(k) = \epsilon_0 + \sum_{i=1..3} \frac{\partial^2 \epsilon}{\partial k_i^2} \cdot (k_i - k_0)^2$$



Effective mass approximation

The dispersion obtained is the same as the one of a free electron with a mass m* given by:

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 \epsilon}{\partial k^2}$$

Quick summary on **kp**

- Perturbative expansion around k=0: Bloch states
- Key element: the Kane energy is accessible via optical measurements

$$E_P = \frac{2}{m_0} |\langle u_{c,0}|p|u_{v,0}\rangle|^2$$

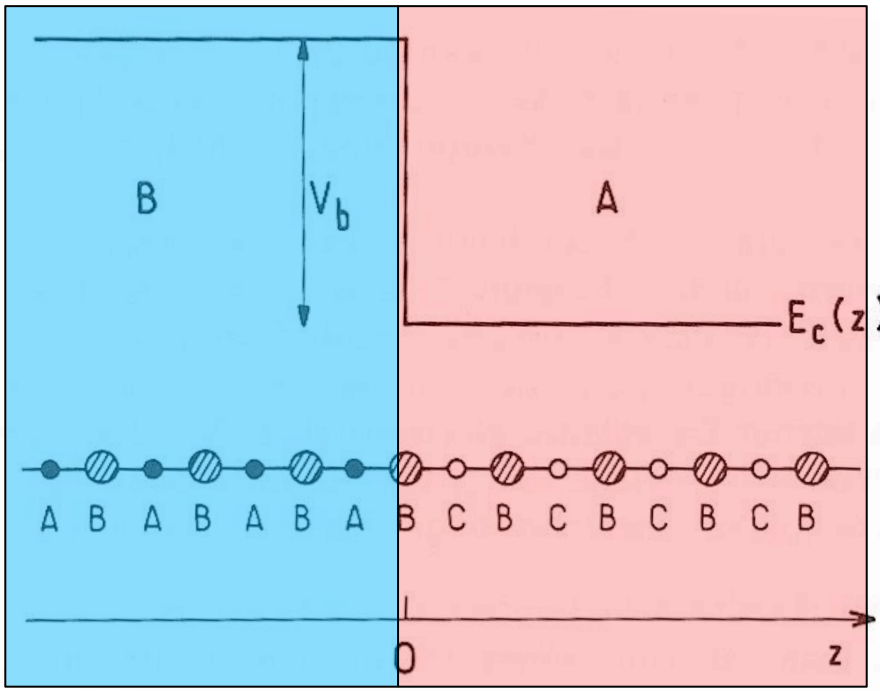
- Effective mass directly proportional to band gap

$$(m^*)^{-1} = (m_0)^{-1}\left(1 + \frac{E_P}{E_G}\right)$$

- Kane model: non-parabolicity as effect of other bands

$$E(k) = \frac{\hbar^2 k^2}{2m^*(0)}(1 - \gamma k^2) \qquad \gamma = \frac{\hbar^2}{2m^*(0)E_G}$$

Heterojunction



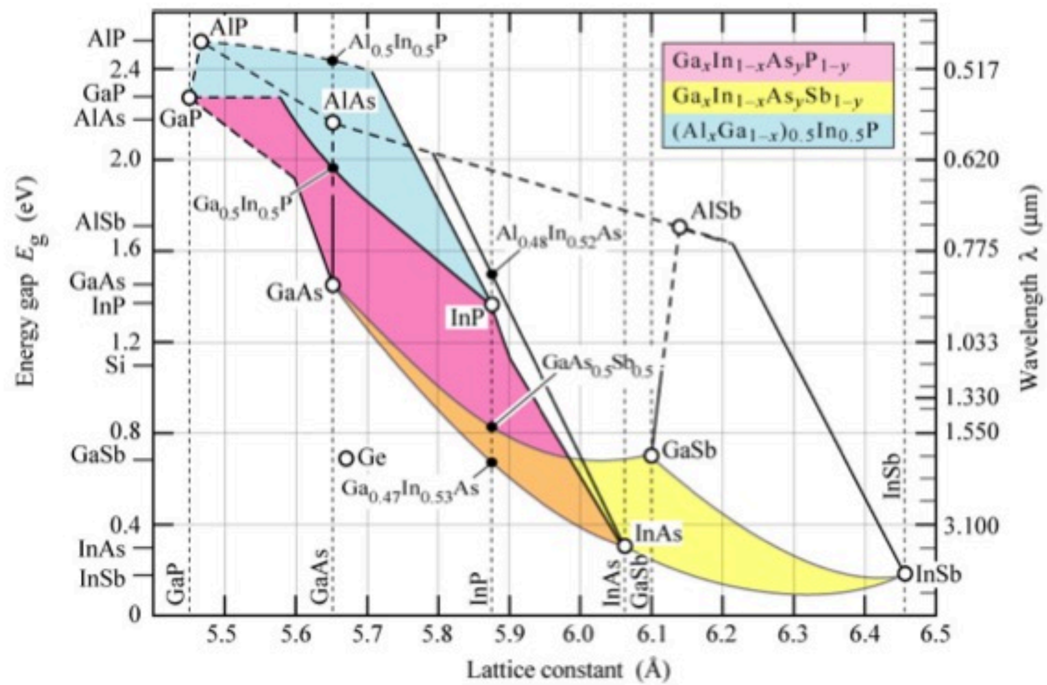


Fig. 17.9 Lattice constant versus energy gap at room temperature for various III–V semiconductors and their alloys (after Tien, 1985).

At the interface there is a transfer of electrical charge (over a few atomic layers): it creates an interface charge dipole : ABRUPT change in the electrostatic potential

-> Band discontinuity

Band aligning

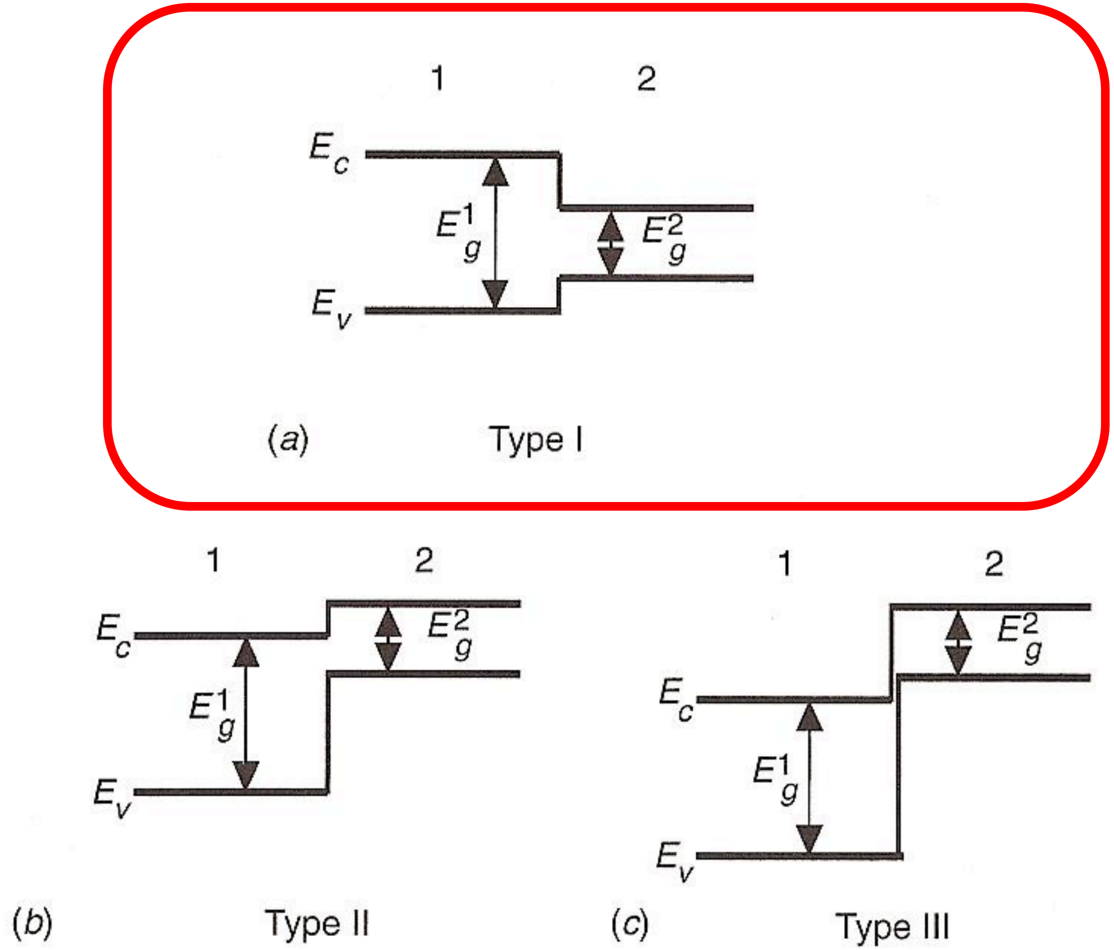
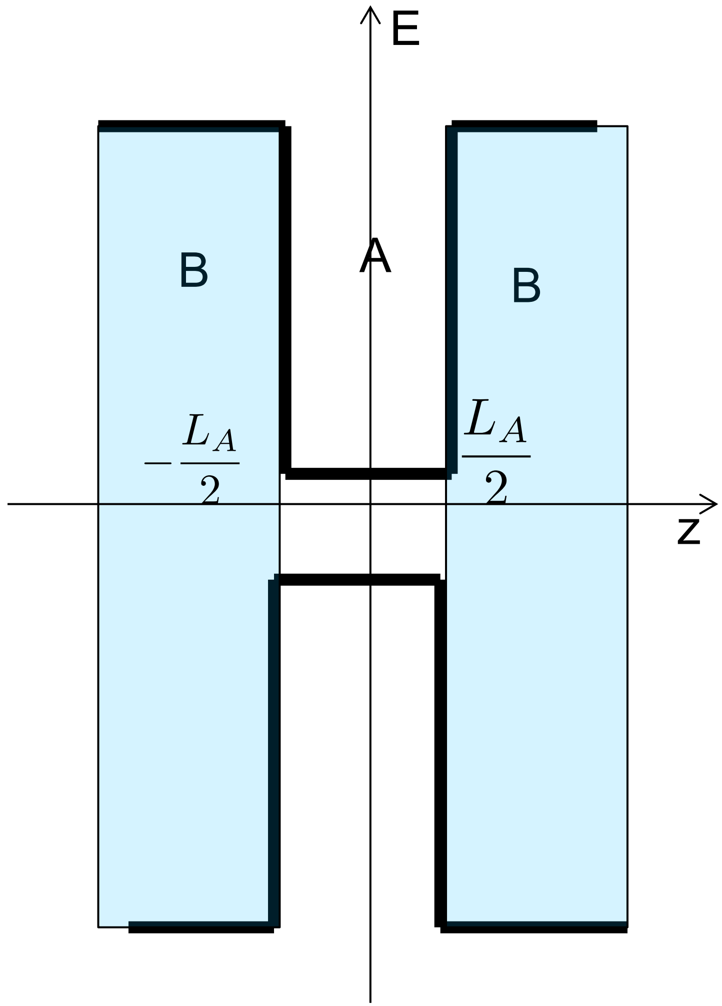


Fig. 8.1. (*a*)–(*c*) The three heterojunction types which may exist between two semiconductors possessing bandgaps E_g^1 and E_g^2. E_c and E_v denote the conduction and valence bands, respectively.

System : quantum well with envelope functions



$$H = \frac{p^2}{2m_0} + V_A Y_A + V_B Y_B$$

$$Y_A = \theta(z + \frac{L_A}{2}) - \theta(z - \frac{L_A}{2})$$

$$Y_B = 2 \cdot \theta(z - \frac{L_A}{2}) + \theta(\frac{L_A}{2} - z) - \theta(\frac{L_A}{2} + z)$$

Basic assumptions for envelope functions

The wavefunction may be separated into the product of a Bloch part and an envelope part:

material

$$\Psi_l(r) = f_l^{A,B} u_{l,k_0}^{A,B}(r)$$

band wavevector

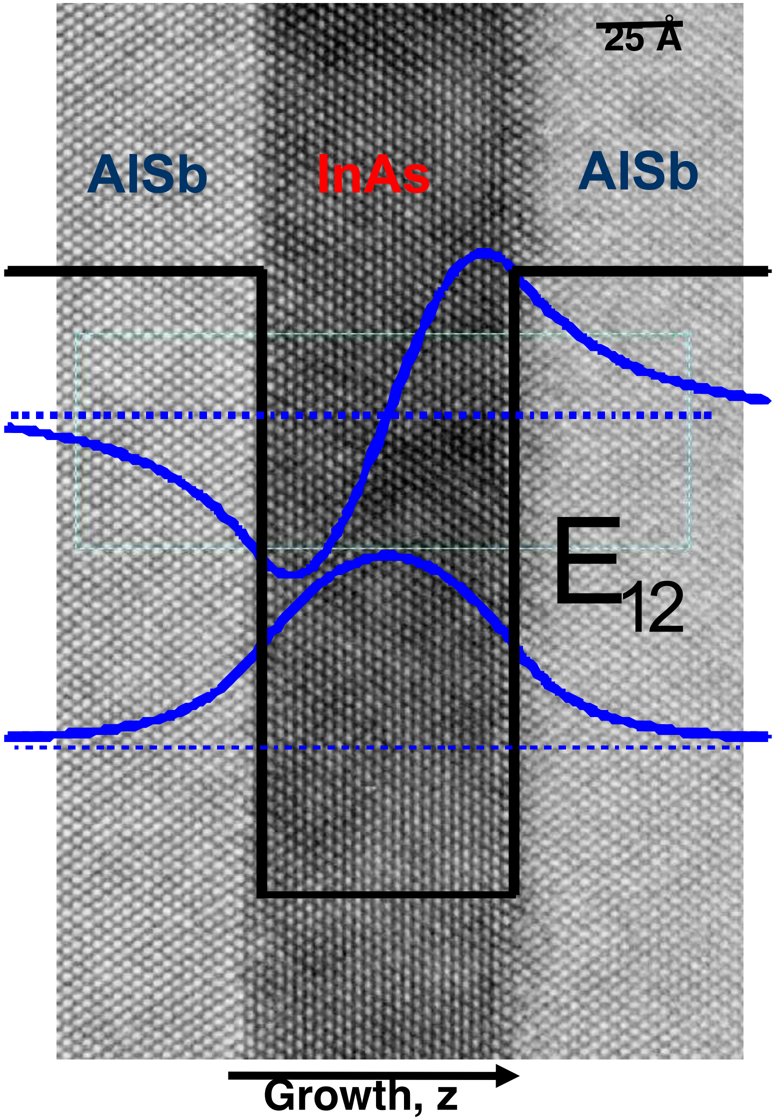
The envelope part is slowly varying

$$|\partial_z f_l^{A,B}(z)| << |\partial_z u_{l,k_0}^{A,B}(z)|$$

The Bloch part is the same in both materials (after all, same chemical properties..)

$$u_{l,k_0}^{A}(r) = u_{l,k_0}^{B}(r)$$

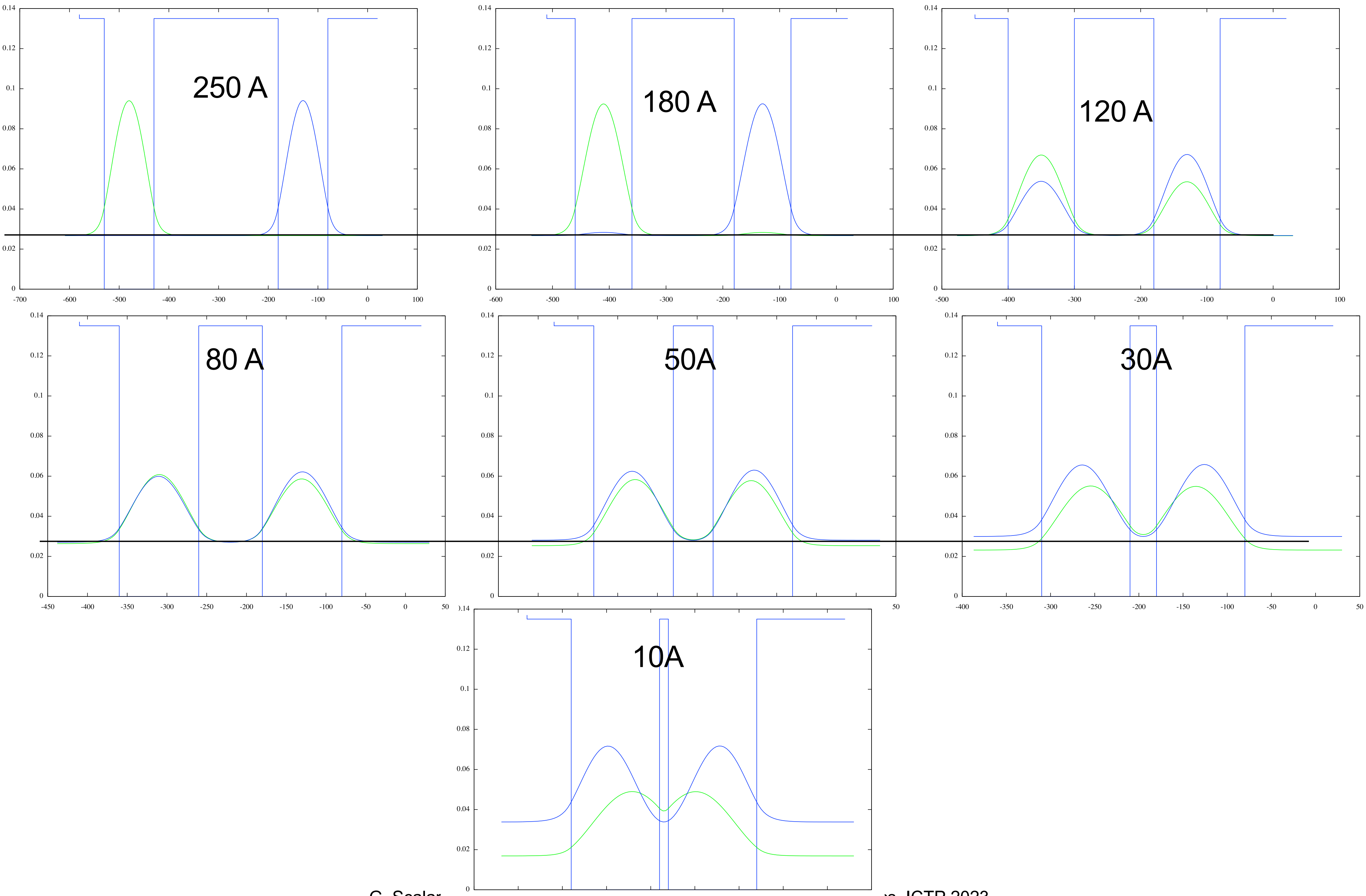
ETH zürich Envelope Function: spanning several atomic lattice sites



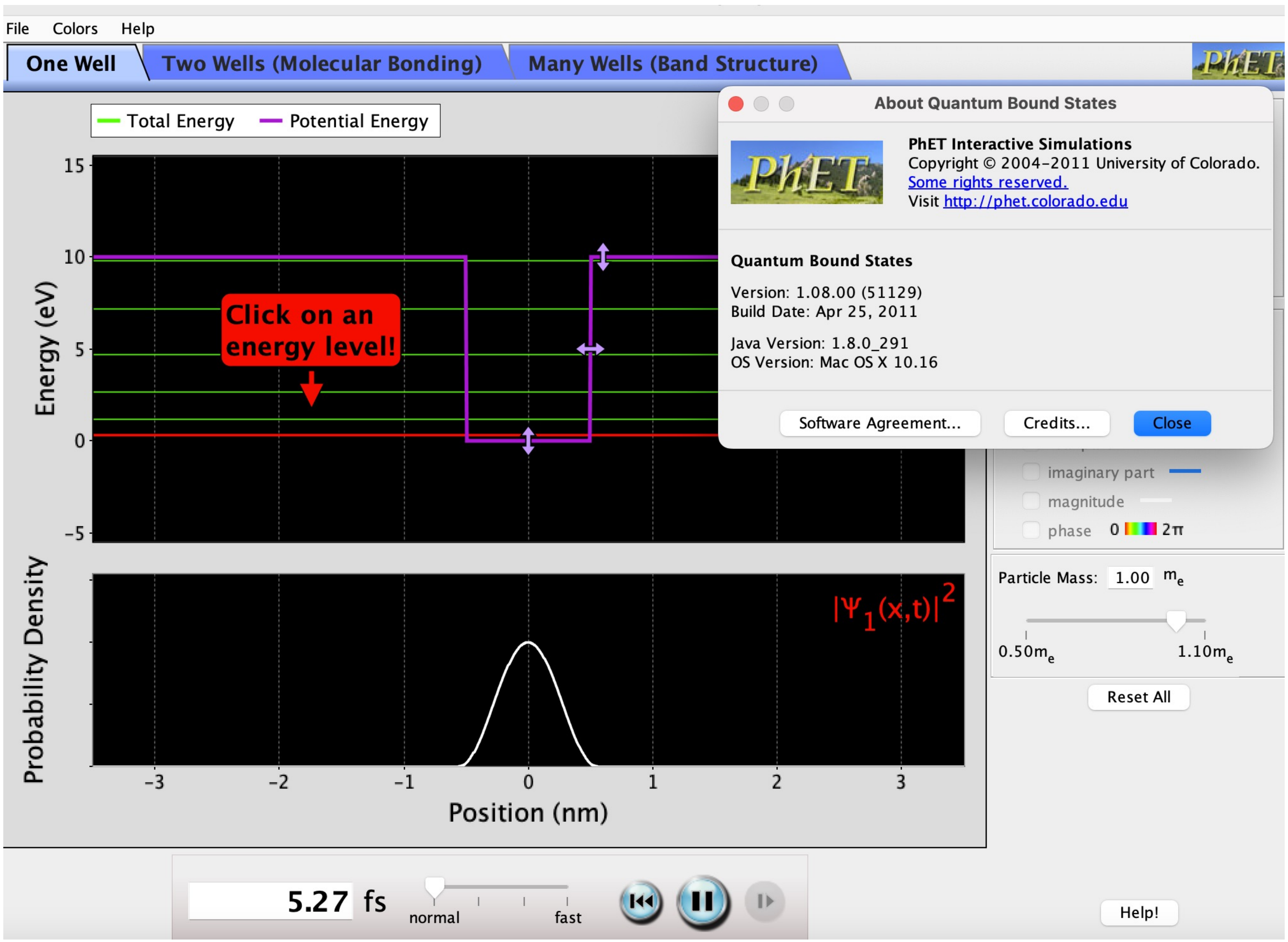
Blue lines: envelope functions

Remember: in-plane still parabolic dispersion!!

Numerical example

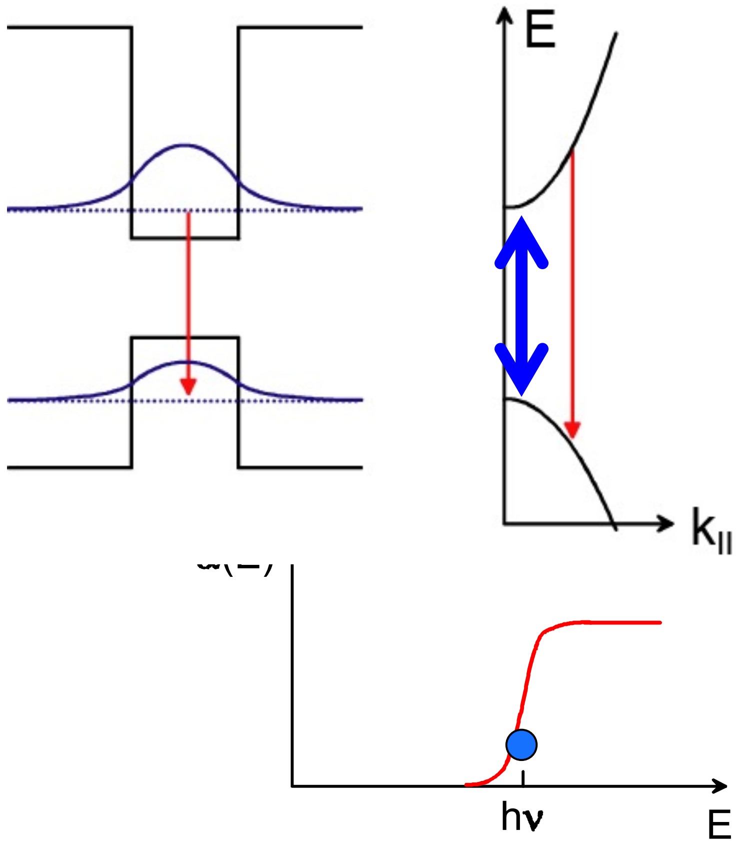


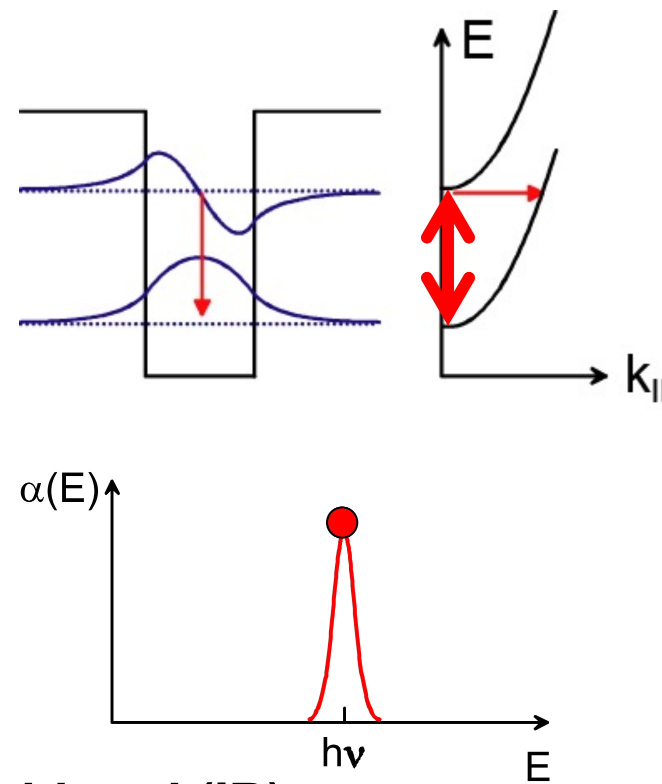
- Let's play a bit with the applet from Colorado https://phet.colorado.edu/en/simulations/browse



ETH zürich

Interband Vs intersubband



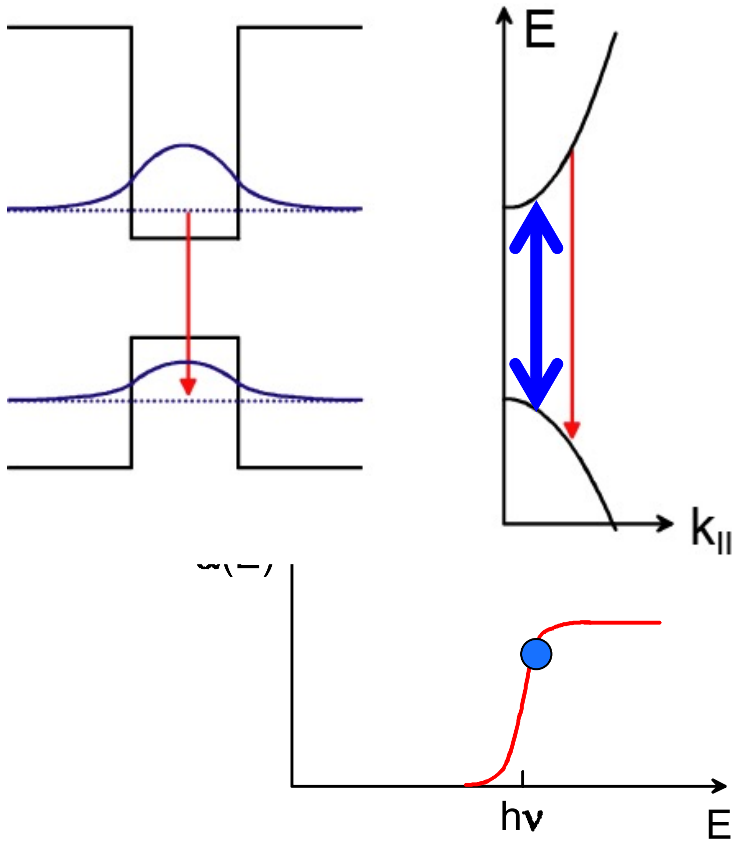


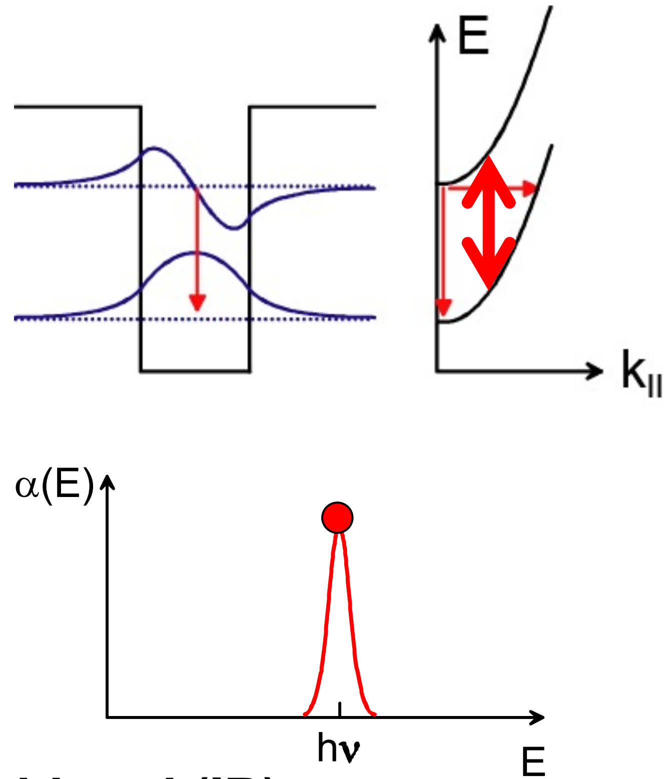
- **Interband (IB)**
  - Absorption above E=hν
  - Broad absorption features
  - Long lifetime (>1 ns)
  - Transition energy <->gap

- **Intersubband (IB)**
  - Absorption at E = hν
  - Narrow absorption features
  - Short lifetime (1 ps)

  -Transition energy <->QW thickness

Interband Vs intersubband





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ETH zürich

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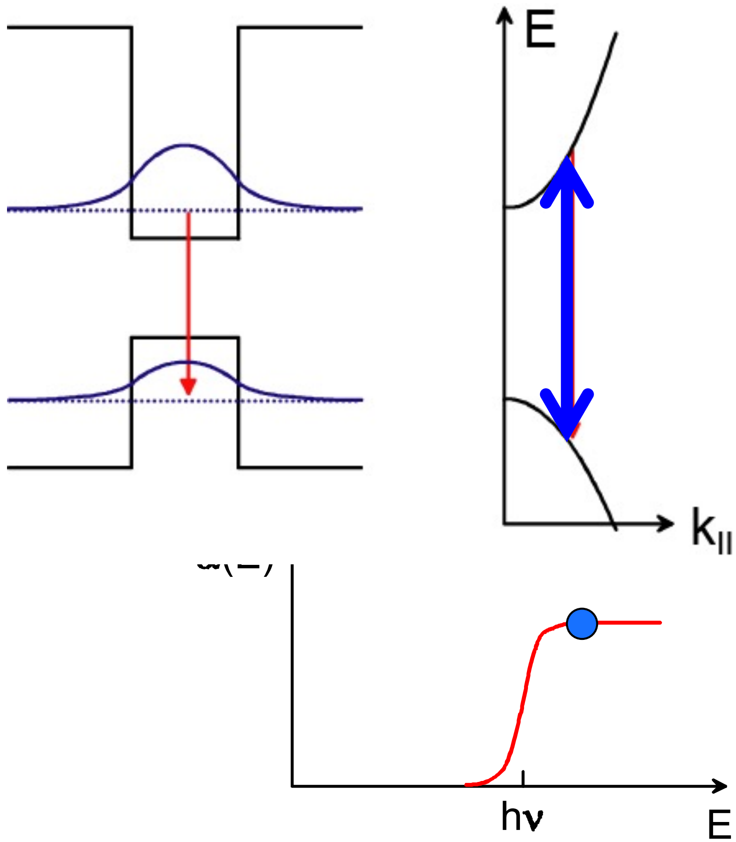

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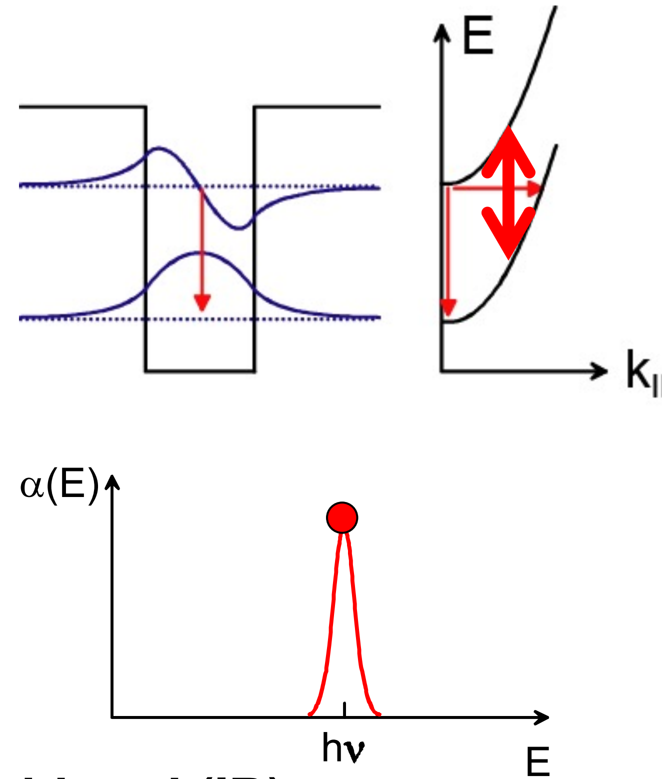

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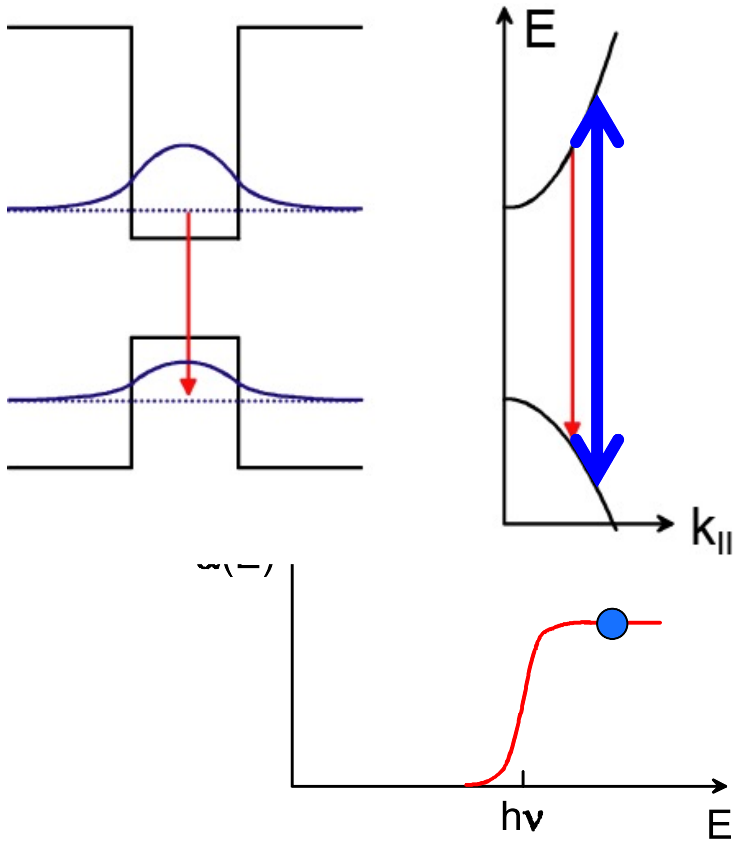

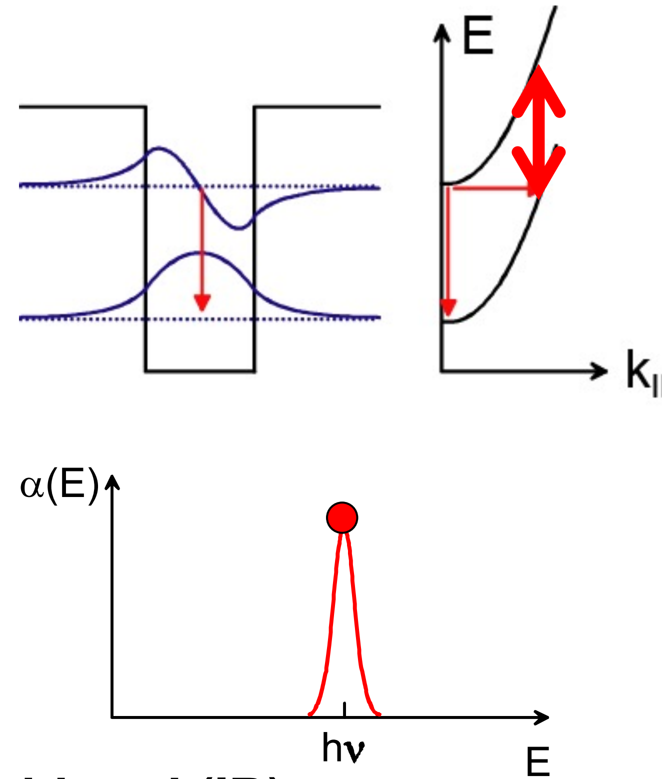

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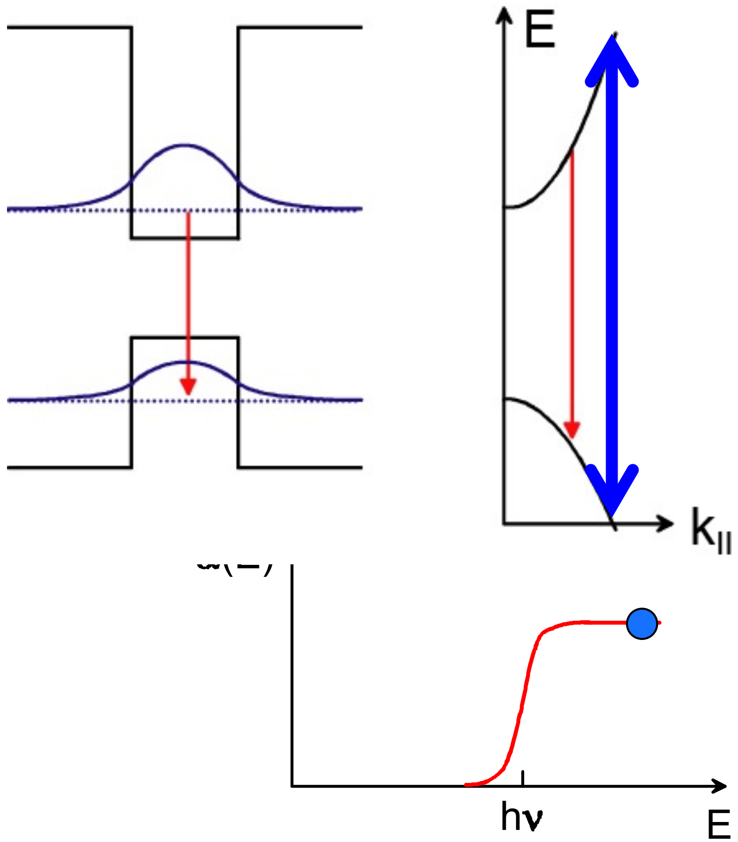

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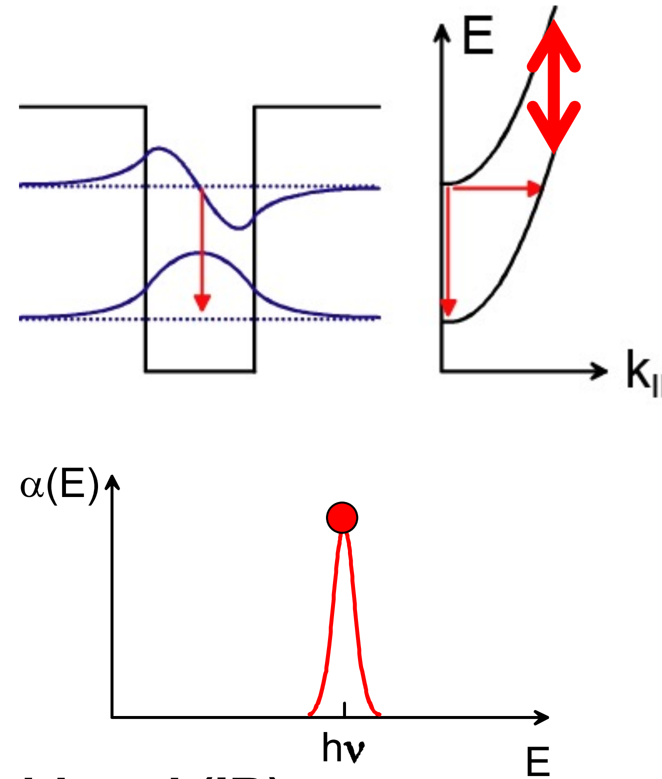

- **Intersubband (IB)**
  - Absorption at E = hν
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  - Short lifetime (1 ps)

-Transition energy <->QW thickness

Selection rules

$$\langle f_{\mathrm{i}} | \boldsymbol{\varepsilon}.\boldsymbol{p} | f_{\mathrm{f}} \rangle = \frac{1}{S} \int \mathrm{d}^3 r \, \chi_{n_{\mathrm{i}}}^{*}(z) \exp(-i \boldsymbol{k}_{\perp}.\boldsymbol{r}_{\perp})[\varepsilon_x p_x + \varepsilon_y p_y + \varepsilon_z p_z] \times$$

$$\chi_{n_{\mathrm{f}}}(z) \exp(i \boldsymbol{k}'_{\perp}.\boldsymbol{r}_{\perp})$$

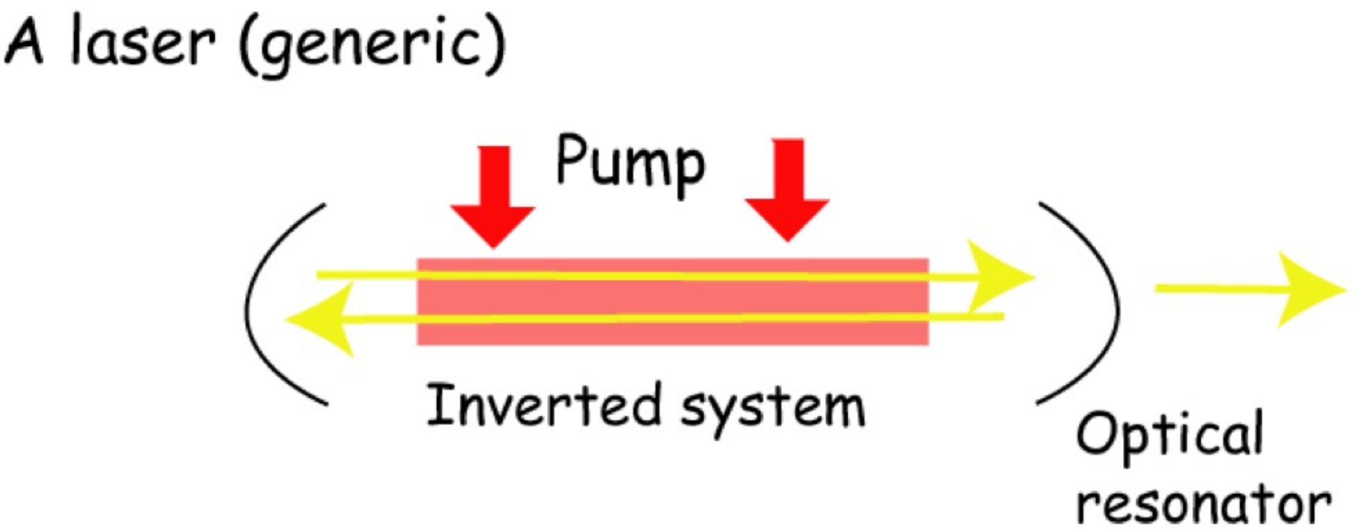
$$\langle f_{\mathrm{i}} | \boldsymbol{\varepsilon}.\boldsymbol{p} | f_{\mathrm{f}} \rangle = (\varepsilon_x \hbar k_x + \varepsilon_y \hbar k_y) \, \delta_{n_{\mathrm{i}}, n_{\mathrm{f}}} \, \delta_{\boldsymbol{k}'_{\perp}, \boldsymbol{k}_{\perp}} + \varepsilon_z \, \delta_{\boldsymbol{k}'_{\perp}, \boldsymbol{k}_{\perp}} \times$$

$$\int \mathrm{d}z \, \chi_{n_{\mathrm{i}}}^{*}(z) \, p_z \, \chi_{n_{\mathrm{f}}}(z)$$

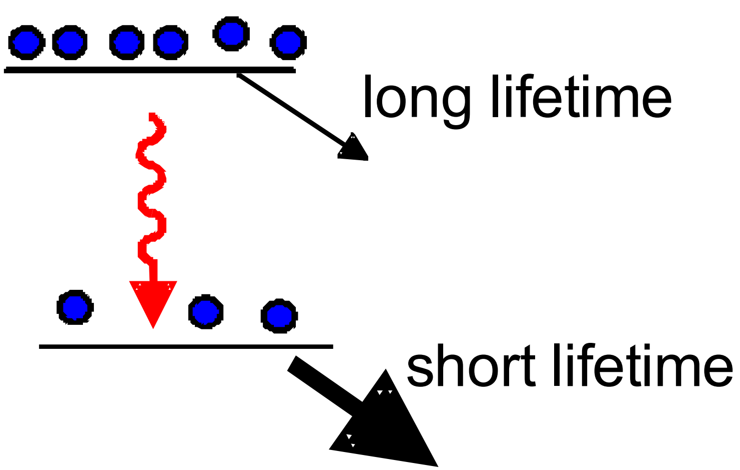
ISB is TM polarized (in the conduction band)

From Bastard's book

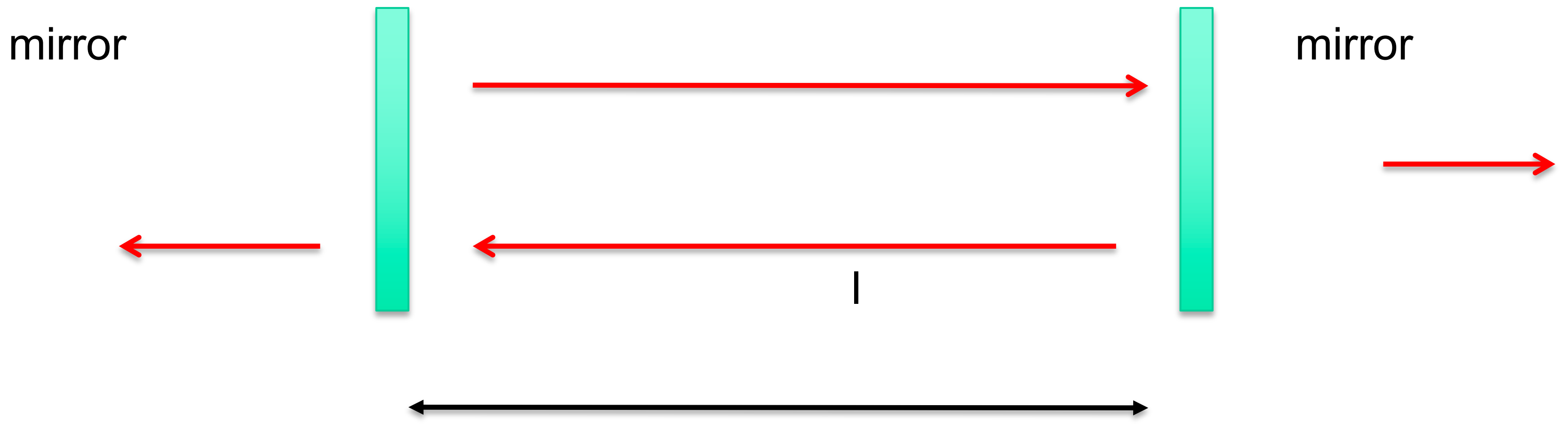
Needed for a laser:



- An optical transition
- Population inversion:
  - need to engineer lifetimes $\tau_{up} > \tau_{dn}$
- Low loss optical resonator



Fabry Pérot cavity



$$\delta = \frac{4\pi n l}{\lambda} = 2m\pi$$

m integer

$$\nu_m = m\frac{c}{2nl}$$

The distance between two successive resonances of the FP resonator is then:

$$\nu_{m+1} - \nu_m = \frac{c}{2nl}$$

And is called *free spectral range*

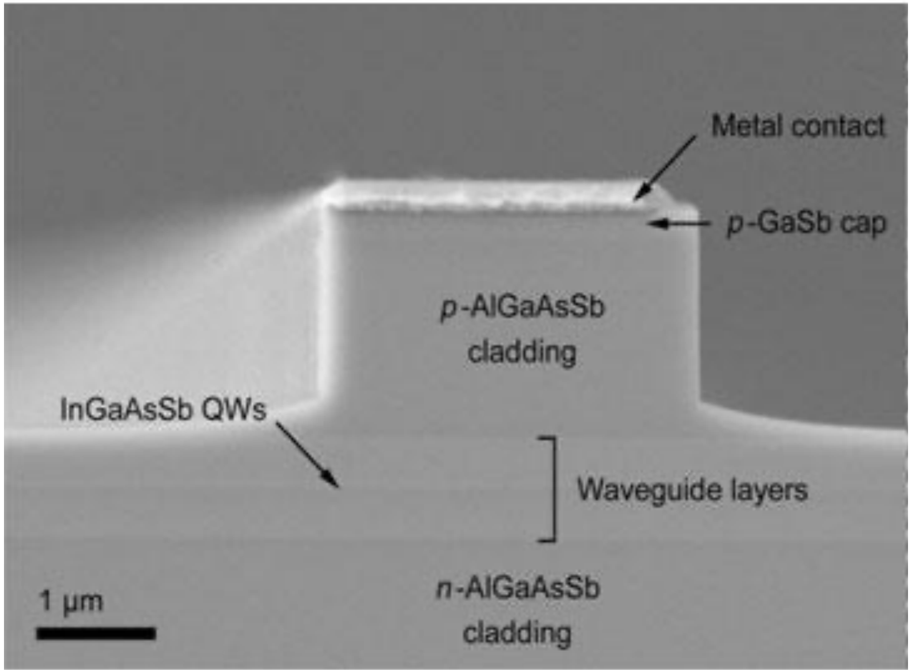
Fabry-Pérot natural with semiconductors: cleave a bar

From Fresnel normal incidence reflection we have

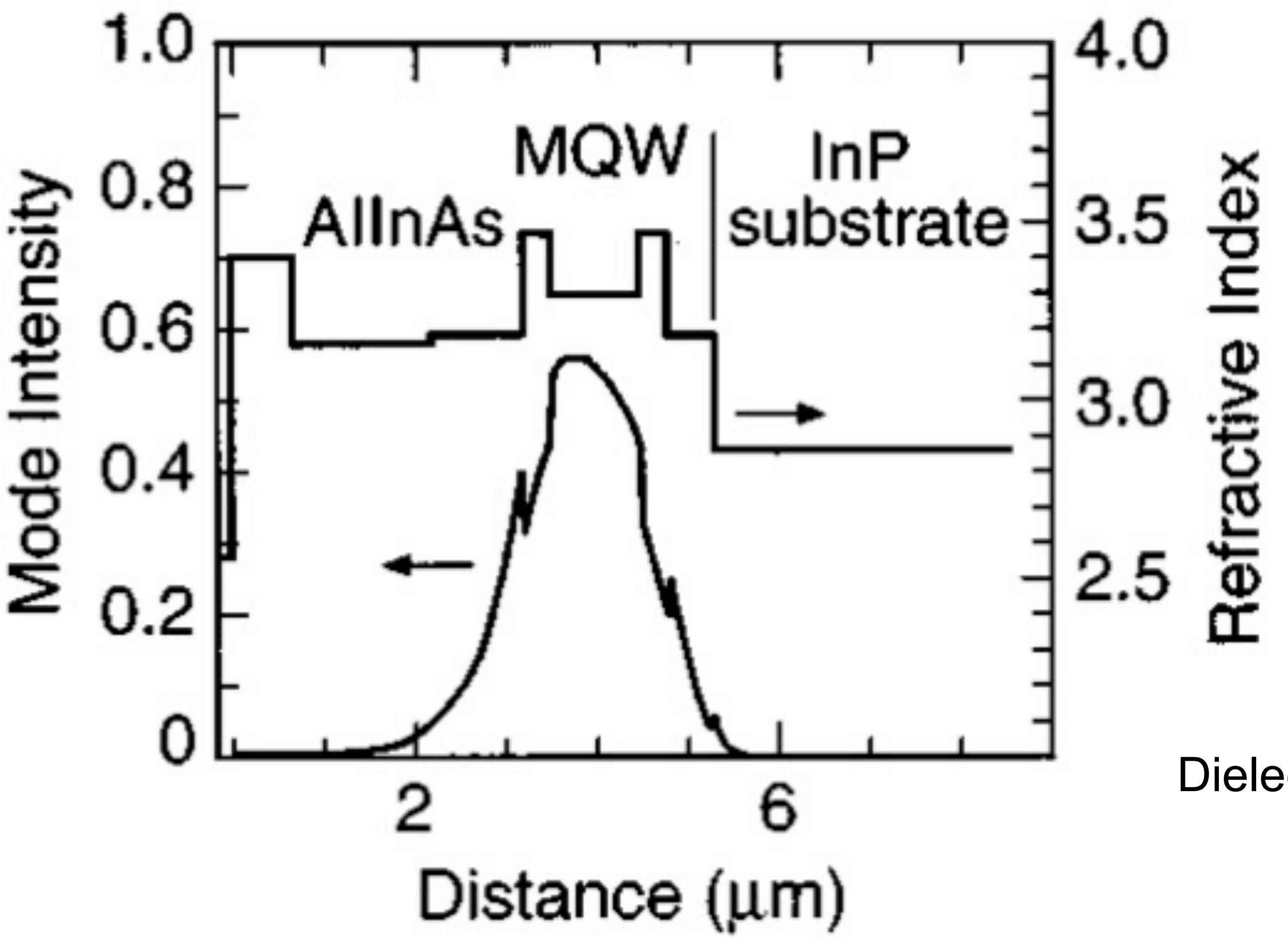
$$\mathcal{R} = \left| \frac{(\tilde{n} - 1)}{\tilde{n} + 1} \right|^2$$

Typical refractive indexes of commonly used semiconductors : 3.2-3.7

Cleave the facet along semiconductor's crystalline planes : built-in mirror of reflectivity 0.28-0.32.



Mid-IR : dielectric waveguides



InP has a pronounced index contrast to InGaAs/InAlAs

Dielectric waveguide at 4.2 µm

J. Faist et al., Appl. Phys. Lett. **65** (23), 5 December 1994

ETH zürich

B. Lax's review (1960)

CYCLOTRON RESONANCE AND IMPURITY LEVELS IN SEMICONDUCTORS*

B. LAX
Lincoln Laboratory, Massachusetts Institute of Technology

FOR SOME time, semiconductors have been seriously considered as a possible medium for generating infrared and millimeter radiation. Some success has already been attained in generating incoherent radiation in the infrared. Consequently, it is a logical step to consider semiconductors as likely candidates for use as quantum amplifiers and oscillators. A number of proposals have been made in the literature and elsewhere. I would like to review these, comment on them, and also add one or two suggestions of my own. The basic phenomena that are involved in most of these proposals concern cyclotron resonance and impurity levels.

B. Lax, in Proceedings of the International Symposium on Quantum Electronics. C.H. Townes, Ed. (Columbia Univ. Press, New York 1960), p. 428

Intersubband gain: first theoretical proposal

- Beyond the Bloch oscillator: use intersubband transitions in quantum wells

SOVIET PHYSICS – SEMICONDUCTORS VOL. 5, NO. 4 OCTOBER, 1971

POSSIBILITY OF THE AMPLIFICATION OF ELECTROMAGNETIC WAVES IN A SEMICONDUCTOR WITH A SUPERLATTICE

R. F. Kazarinov and R. A. Suris

A. F. Ioffe Physicotechnical Institute, Academy of Sciences of the USSR, Leningrad

Translated from Fizika i Tekhnika Poluprovodnikov, Vol. 5, No. 4, pp. 797–800, April, 1971
Original article submitted January 5, 1971

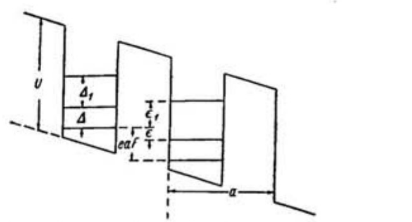


Fig. 1. Schematic representation of the superlattice potential and of the electron levels.

R. Kazarinov

R. Suris

R. F. Kazarinov, R.A. Suris, Sov. Phys. Semicond. **5**, 707 (1971)

1986-93: Proposals for QC's using resonant tunneling in superlattices:
F. Capasso et al, JQE (1986)
H. C. Liu et al, JAP (1988)

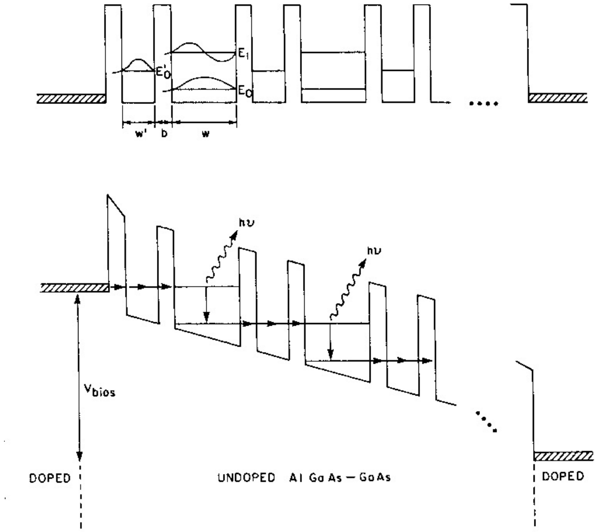
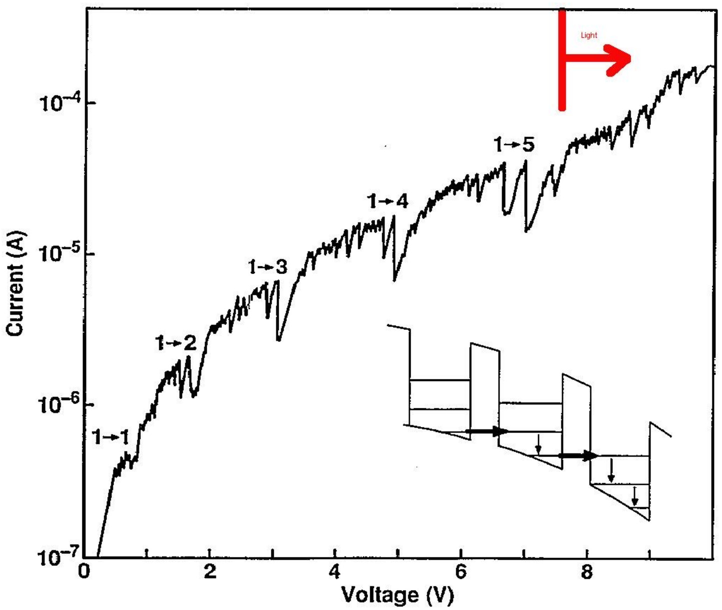
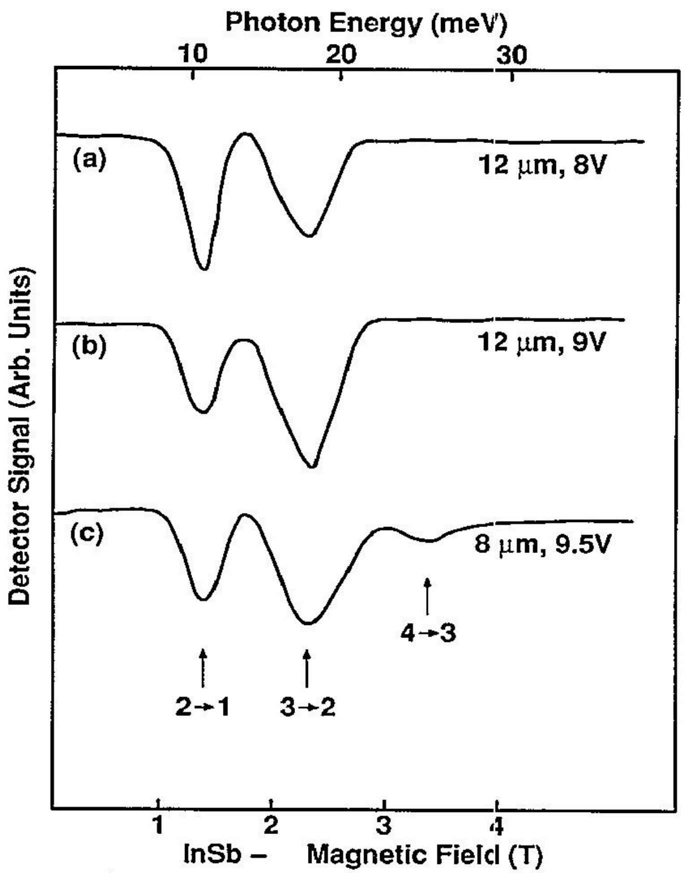


FIG. 1. Upper part: conduction-band edge profile of the proposed device under no bias. Lower part: biased device in operation. Heavily doped contact layers at either ends of the structure are hatched to show the Fermi seas. Photon ($h\nu$) emission processes occur in the wide wells.

First intersubband luminescence

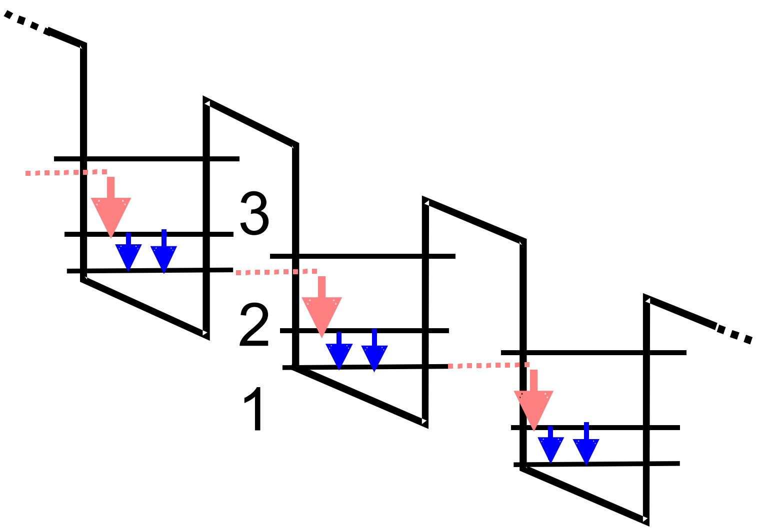




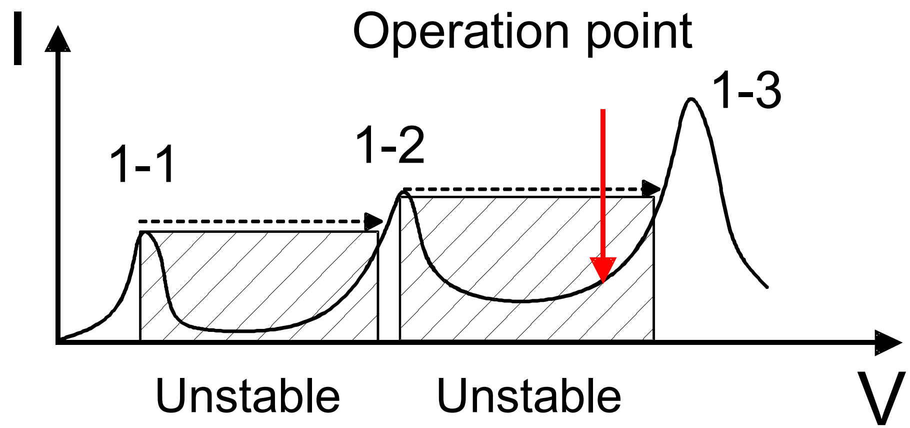
- Resonant tunneling in a periodic superlattice
- Emission observed in the Far-Infrared

M. Helm et al, PRL **63**, 74 (1989)

Electrical stability



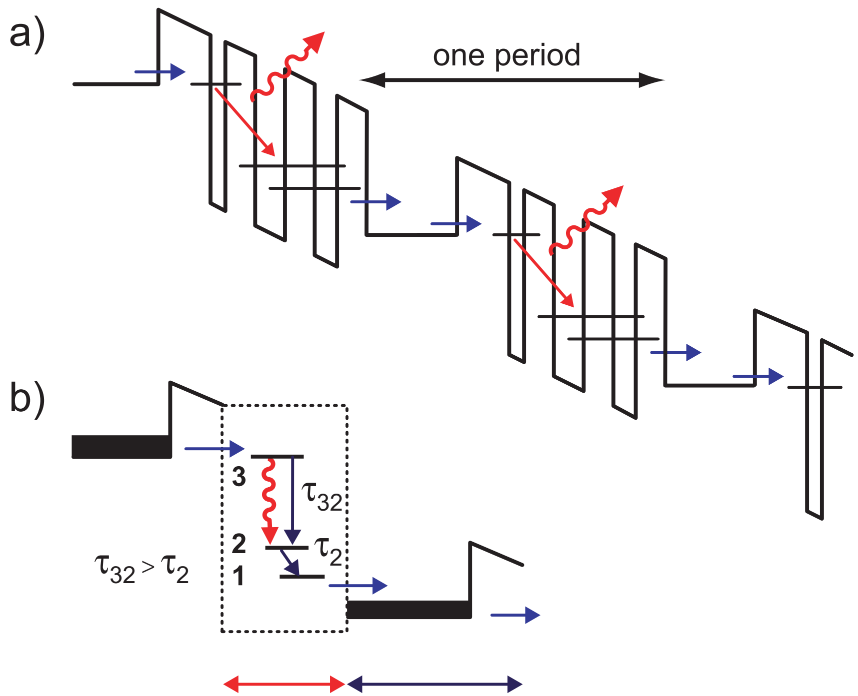
Schematic I-V curve:



Population inversion is obtained at an unstable point of the I-V curve !

R.F. Kasarinov and R. A. Suris, Soviet Physics (1971)

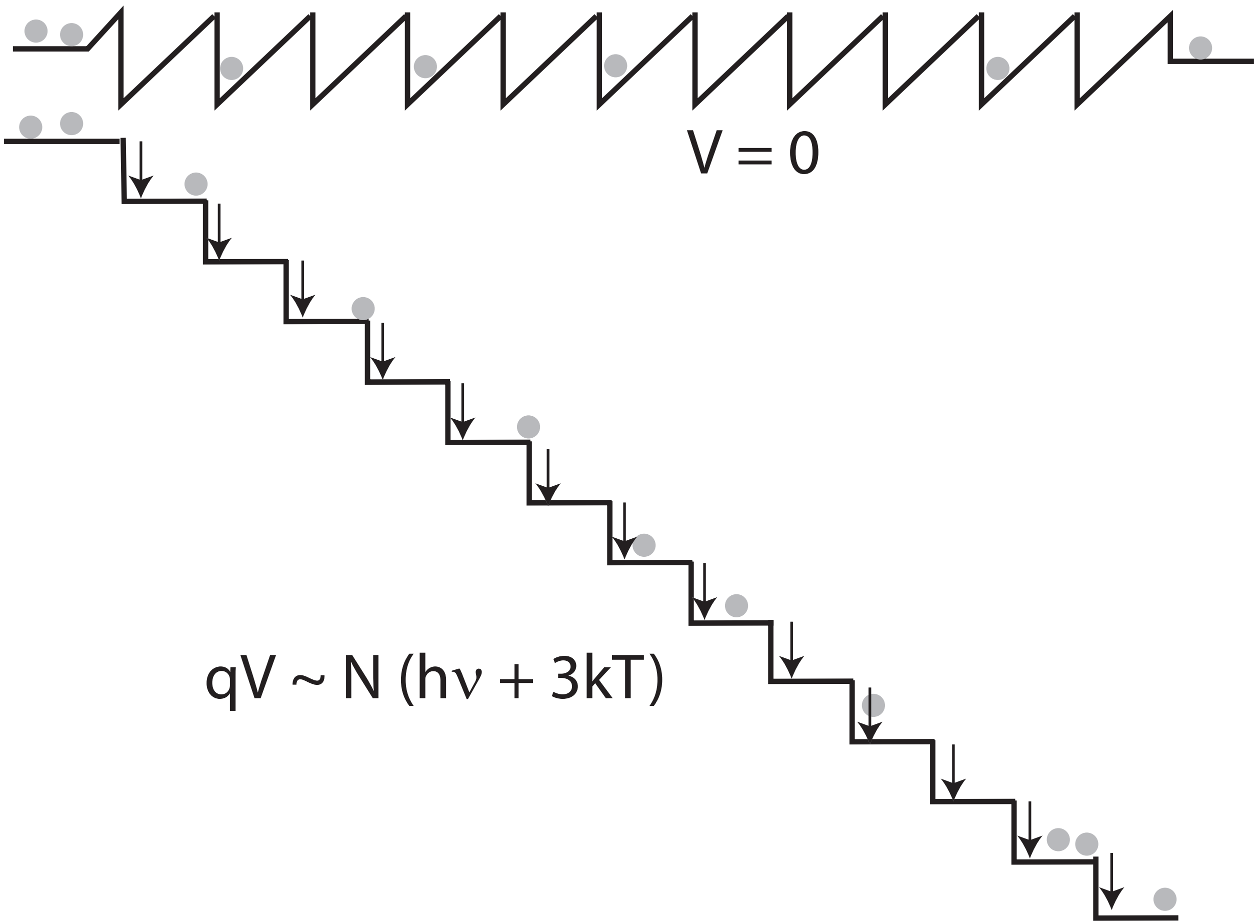
Basic design concept



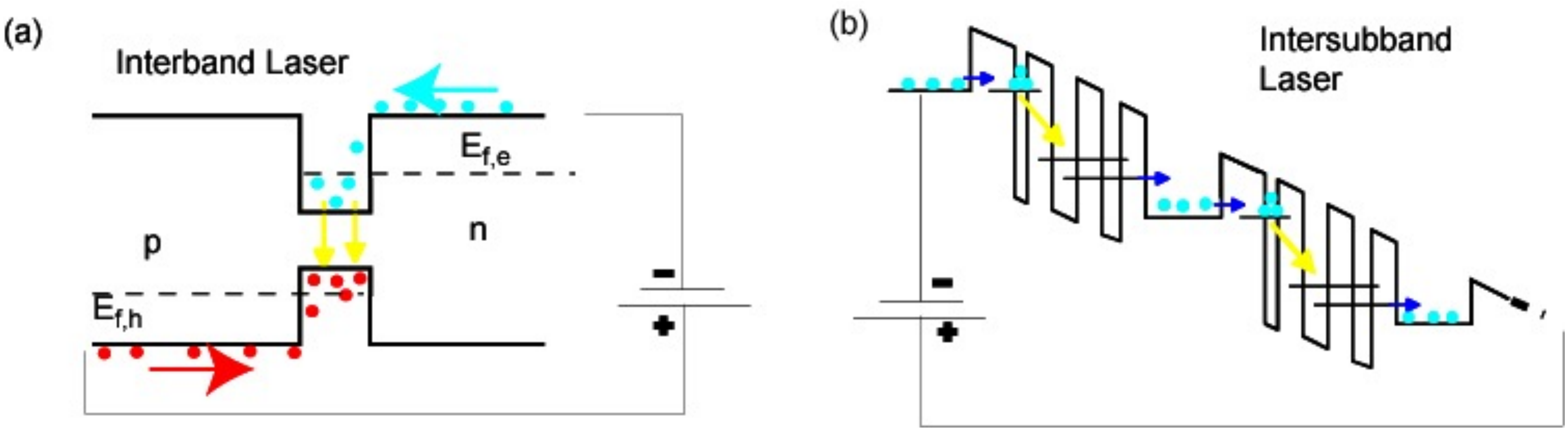
Requirements:
- establish population inversion → Active region
- prevent domain formation
- cool electron distribution → **Injection region**

J. Faist, F. Capasso, C. Sirtori, D. L. Sivco, A.L. Hutchinson, A.Y. Cho, Science **264**, 477 (1994)

Sawtooth to staircase transition



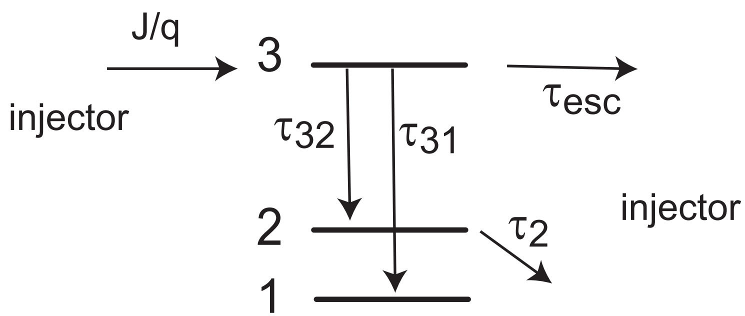
Interband versus intersubband laser



Similarities:
- Optical beam
- LIV curve

Differences:
- cascading
- electron dynamics

Rate equation analysis



$$
\begin{aligned}
\frac{\mathrm{d}n_3}{\mathrm{d}t} &= \frac{J}{q_0} - \frac{n_3}{\tau_3} - Sg_c(n_3 - n_2) \\
\frac{\mathrm{d}n_2}{\mathrm{d}t} &= \frac{n_3}{\tau_{32}} + Sg_c(n_3 - n_2) - \frac{n_2 - n_2^{\mathrm{therm}}}{\tau_2}
\end{aligned}
$$

Populations n_3, n_2

$$
\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{c}{n}\left[\Big(g_c(n_3 - n_2) - \alpha_{tot}\Big)S + \beta\frac{n_3}{\tau_{\mathrm{sp}}}\right]
$$

Photon flux S

Population inversion and threshold

- Setting gain = losses, we get

$$\Delta n)_{thres} = \frac{\alpha_{tot}}{g_c}$$

Simple model with
No gain saturation

- We therefore get the threshold current density:

$$J_{\text{th}} = q_0 \frac{\alpha_{\text{tot}}/g_c + n_2^{\text{therm}}}{\tau_{\text{eff}}}$$

- where

$$\tau_{\text{eff}} = \tau_3(1 - \tau_2/\tau_{32})$$

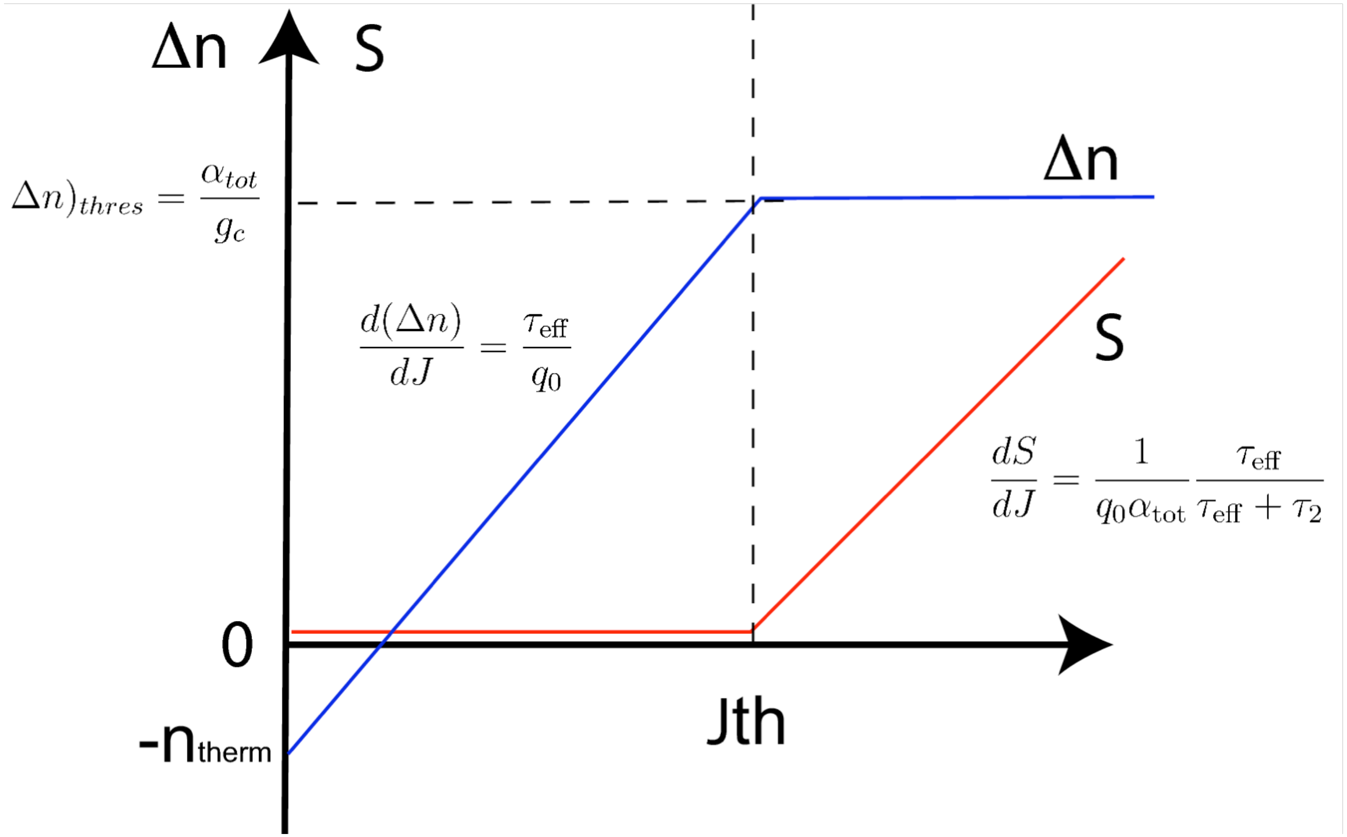
- introducing the expression for the gain cross section g_c

$$J_{th} = \frac{1}{\tau_3(1-\tau_2/\tau_{32})}\left[\frac{\epsilon_0 n L_p \lambda(2\gamma_{32})}{4\pi q_0 \Gamma_p N_p z_{32}^2}(\alpha_{tot}) + q_0 n_2^{therm}\right]$$

$$\Delta n = \frac{J\tau_{\text{eff}}}{q_0} - n_2^{\text{therm}}$$

$$\frac{d(\Delta n)}{dJ} = \frac{\tau_{\text{eff}}}{q_0}$$

Qualitative solutions below and above J_{th}



Slope efficiency

$$\frac{\mathrm{d}P}{\mathrm{d}I} = N_p h\nu \alpha_{m,1} \frac{\mathrm{d}S}{\mathrm{d}J} = \frac{N_p h\nu}{e} \frac{\alpha_{m,1}}{\alpha_{\text{tot}}} \frac{\tau_{\text{eff}}}{\tau_{\text{eff}} + \tau_2}$$

Threshold current (set S=0)

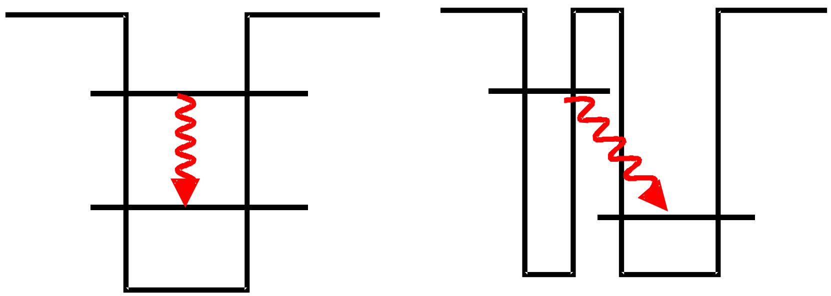
Linewidth

$$J_{th} = \frac{1}{\tau_3(1-\tau_2/\tau_{32})}\left(\frac{\varepsilon_0\,\lambda\, nL_p\gamma}{4\pi q\Gamma z^2}(\alpha_m+\alpha_w)\right)$$

Extraction

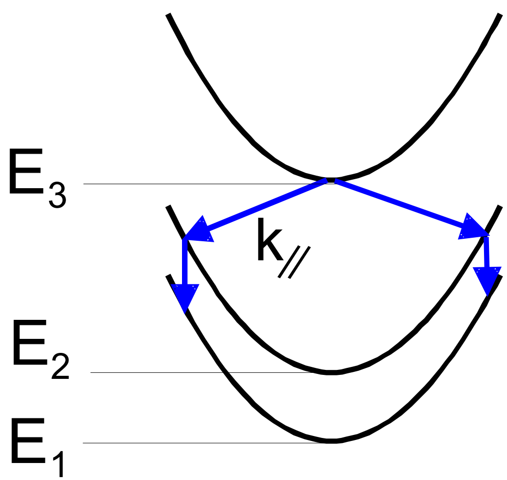
Loss

How does one engineer lifetimes?



Diagonal transitions in real space:

Reduction of matrix elements due to a decrease overlap between wavefunctions.



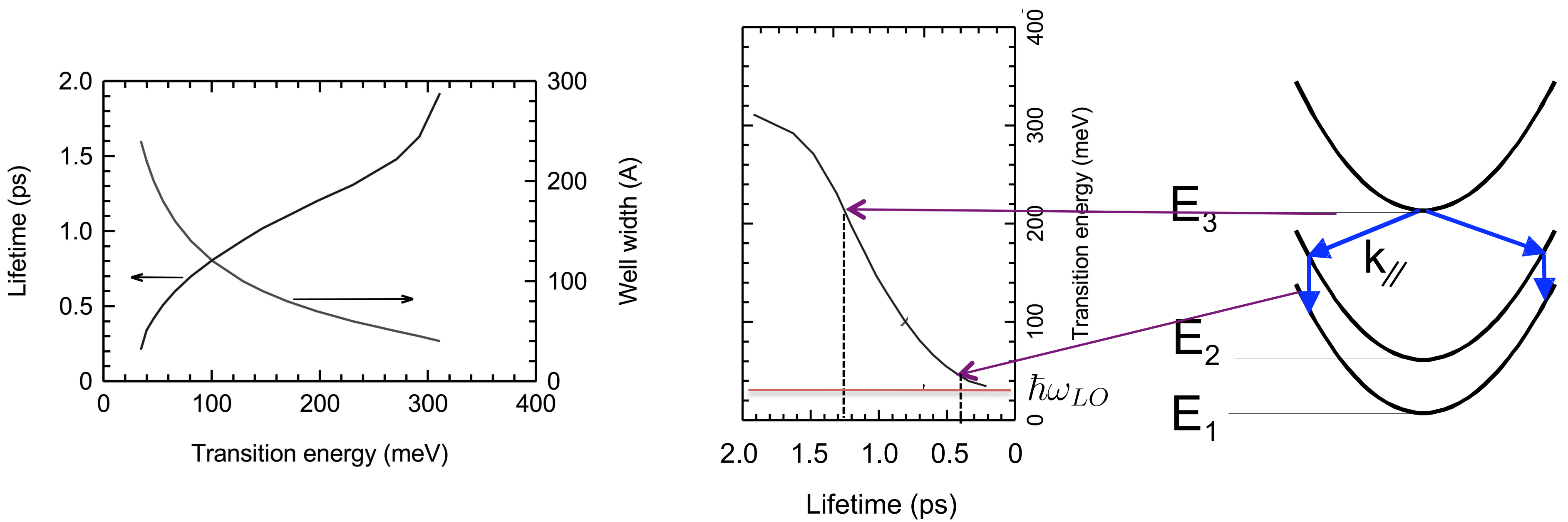
$$\tau_{ij} \div k_{//}^{2}$$

$$\boxed{\tau_{32} > \tau_{21}}$$

Phonon momentum transfer:

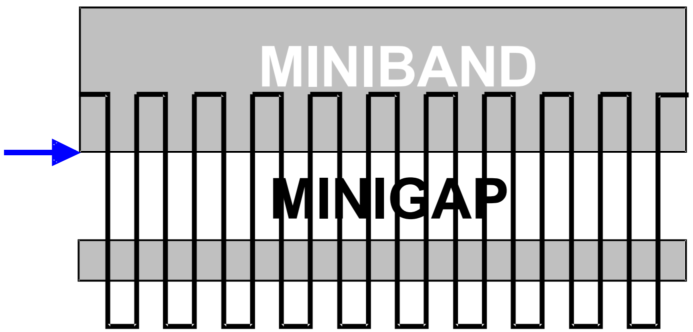
Electron lifetime on excited subbands is a function ($\sim k_{//}^{2}$) of the momentum exchanged with the lattice by the emission of an optical phonon.

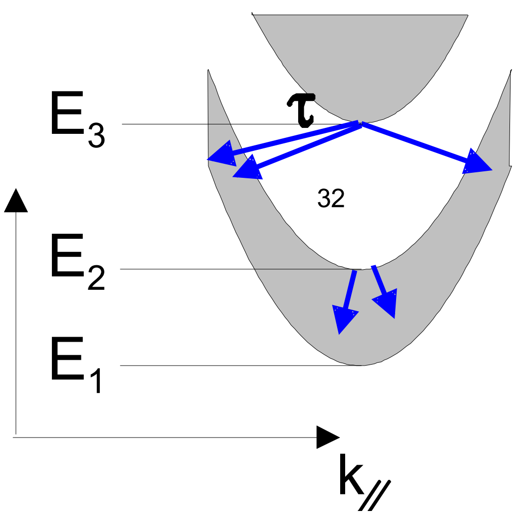
Engineering an optical phonon resonance



Get very short lifetime for the lower state at resonance!!

Engineering lifetimes (II)





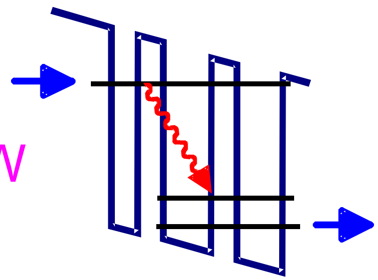
Phase space in superlattice:

The probability of injecting the electron in the upper state of the lower miniband is very small. However, once there, the electron has a large phase space to scatter out of this state.

$$\boxed{\tau_{32} >> \tau_{2}}$$

Existing architectures

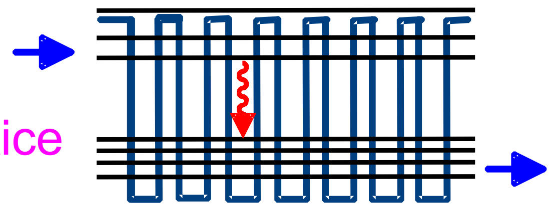
3QW



- Optical phonon resonance
- tunneling

J.Faist et al. Science 94

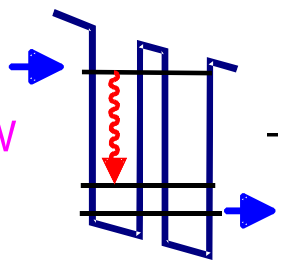
Superlattice



- Phase space

G. Scamarcio et al. Science 97

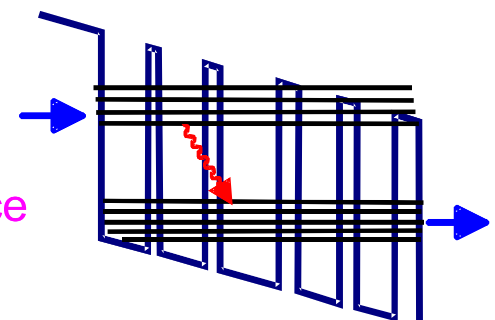
2QW



- Optical phonon resonance

C.Sirtori et al. PTL 97

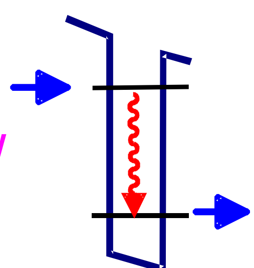
Chirped Superlattice



- Phase space

Tredicucci et al. Appl. Phys. Lett. (1998)

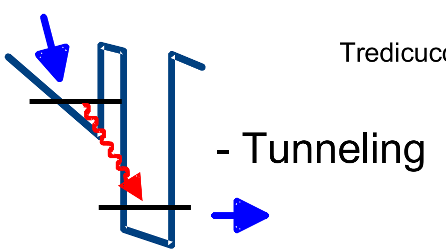
1QW



- tunneling + non-parabolicity

J.Faist et al. PRL 95

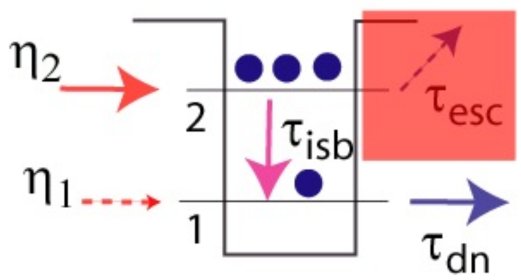
Diagonal

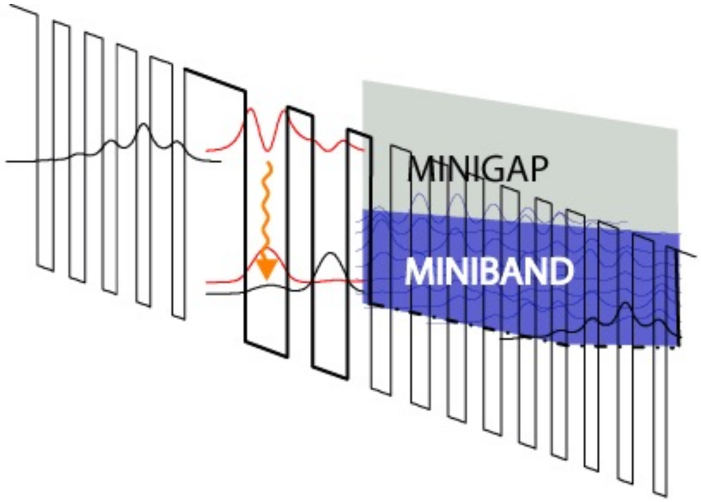


- Tunneling

J.Faist et al. Nature 97

Vertical transition (1995)



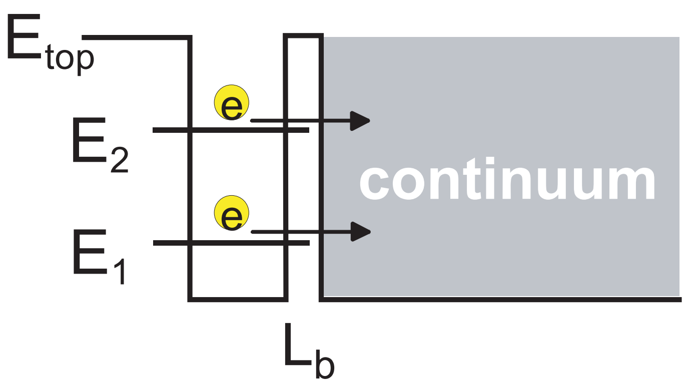


Vertical transition, two quantum well active region
Bragg reflection reduced escape

$J_{th} = 2\mathrm{kA/cm^2}$ @ 10K

(J. Faist et al., APL 1995)

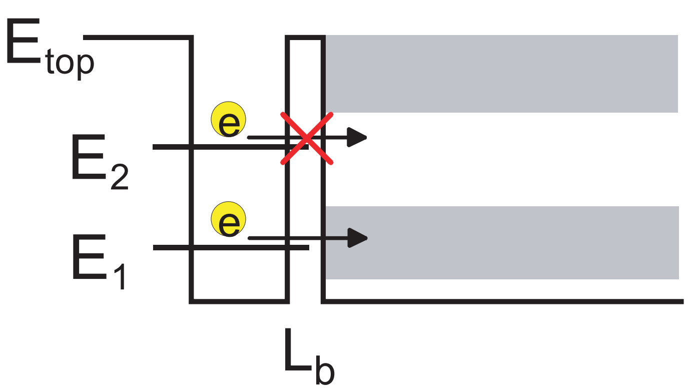
Bragg reflection in the upper state



Escape time into a continuum

$$\tau \sim \exp(-2\kappa_i L_b) \quad \kappa_i = \frac{\sqrt{2m^*(E_{top} - E_i)}}{\hbar}$$

$$\tau_2 < \tau_1$$



Escape time into a superlattice

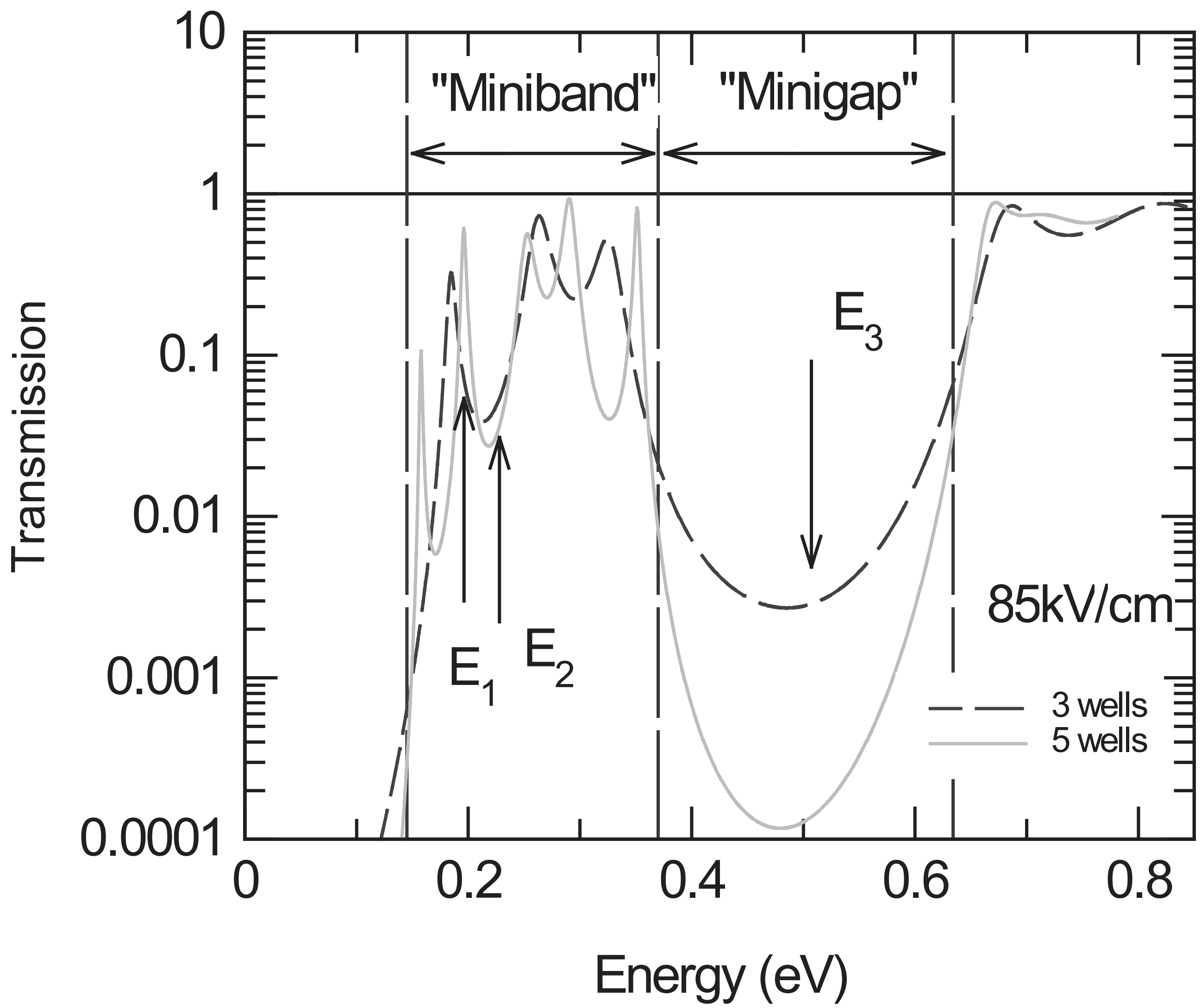
Electrons cannot tunnel into minigaps

$$\tau_2 >> \tau_1$$

$$k_w l_w + k_b l_b = \pi$$

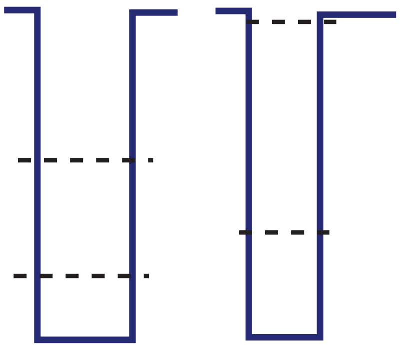
Attenuation of the wavefunction is proportional to the width of the gap

Computation of the transmission



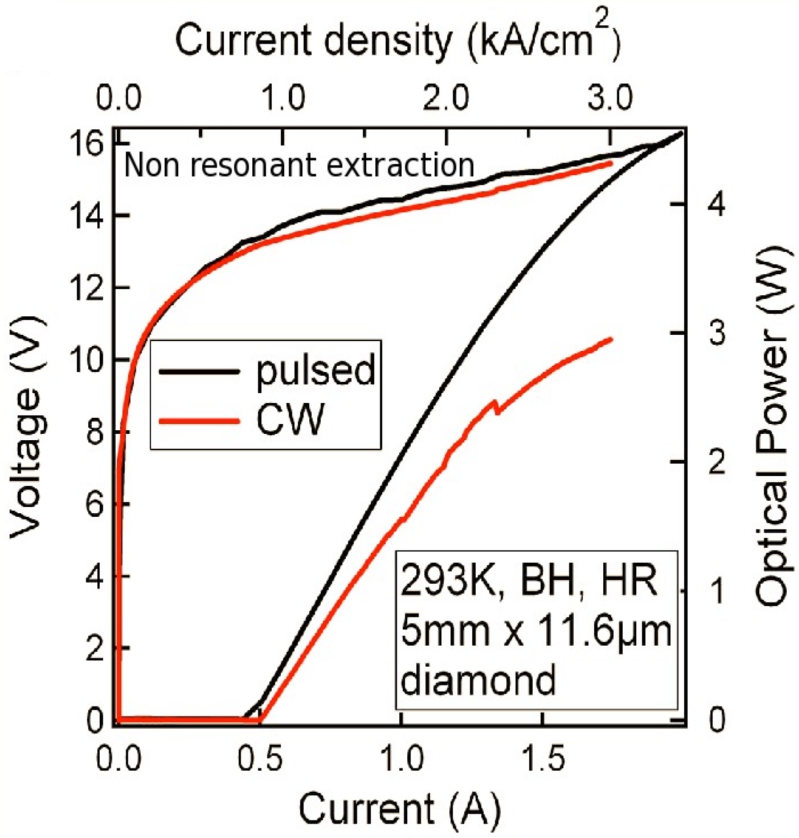
How do you construct an active region??

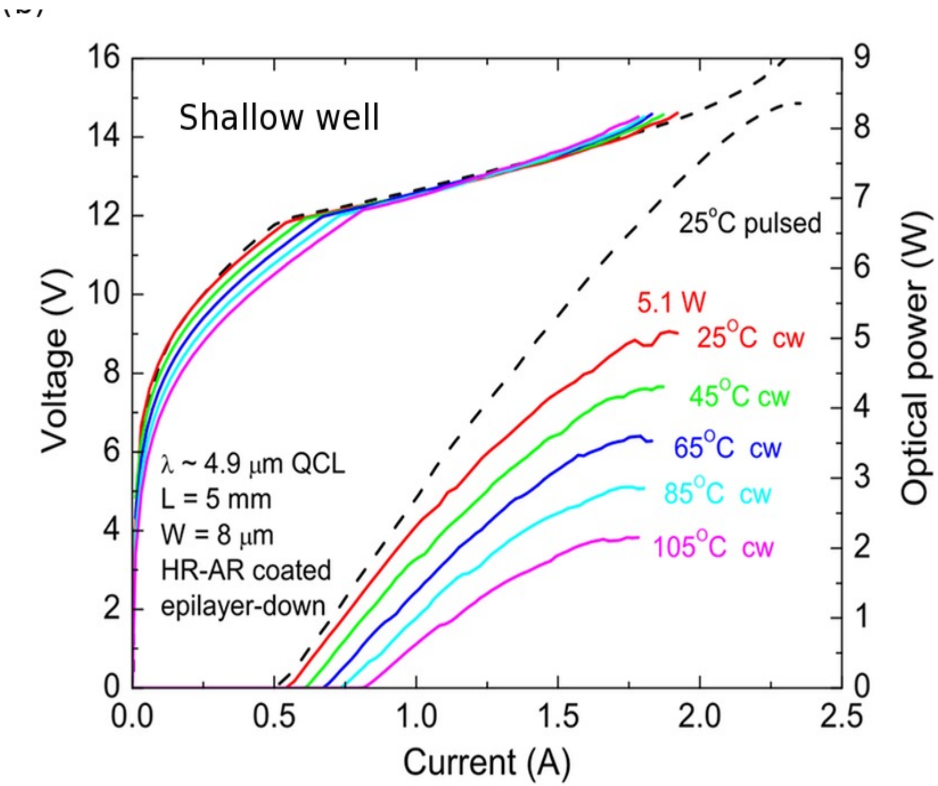
a)



State of the art Mid-IR QCLs (maybe a bit old….)

2011: High wallplug efficiency at 300K (27%) (nowadays higher than 30%)





A. Lyakh et al. *Appl Phys Lett*,. **95** 141113 (2009)

Y. Bai, et al., *Appl Phys Lett*, **98**, 181102 (2011)

Theoretical treatment: complex problem

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m_0} + \underbrace{V_{\text{crystal}}(\mathbf{r})}_{\substack{\text{ionic lattice} \\ + \\ \text{heterostructure}}}}_{\text{Exactly solvable } H_0} + \underbrace{\underbrace{V_{\text{dc}}(z)}_{\text{Wannier-Stark states}} + \underbrace{\hat{H}_{\text{ac}}(\mathbf{r}, t)}_{\hat{p} \longrightarrow \hat{p} - e\hat{A}}}_{\text{EM Field}} + \underbrace{\underbrace{V_{\text{imp.}}(\mathbf{r}) + V_{\text{alloy}}(\mathbf{r}) + V_{\text{IFR}}(\mathbf{r})}_{\substack{\text{Elastic, conserves E} \\ \text{Exact diagonalization}}} + \underbrace{\hat{H}_{\text{e-phonon}}}_{\substack{\text{In-elastic} \\ \text{TO, LO, TA, LA}}} + \hat{H}_{\text{e-e}}}_{\text{Scattering}}$$

$$\hat{H}_{\text{e-e}} \longrightarrow V_{\text{Hartree}} + \hat{H}_{\text{xc}}$$

Exactly solvable *H_0*

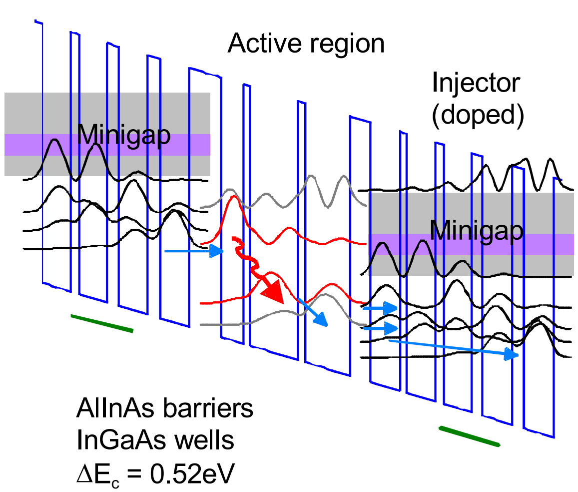
- Effective mass approx.
- Single, multi-band k.p
- Bloch + Wannier states

EM Field

- Non-equilibrium
- Time-dependence
- Classical EM field
- QM EM field: photons

Scattering

- Perturbation theory
- 1st order: Fermi Golden rule
- Infinite order: Green's function theory
- Semi-classical: Monte Carlo



Formulation of the problem (How to solve it)

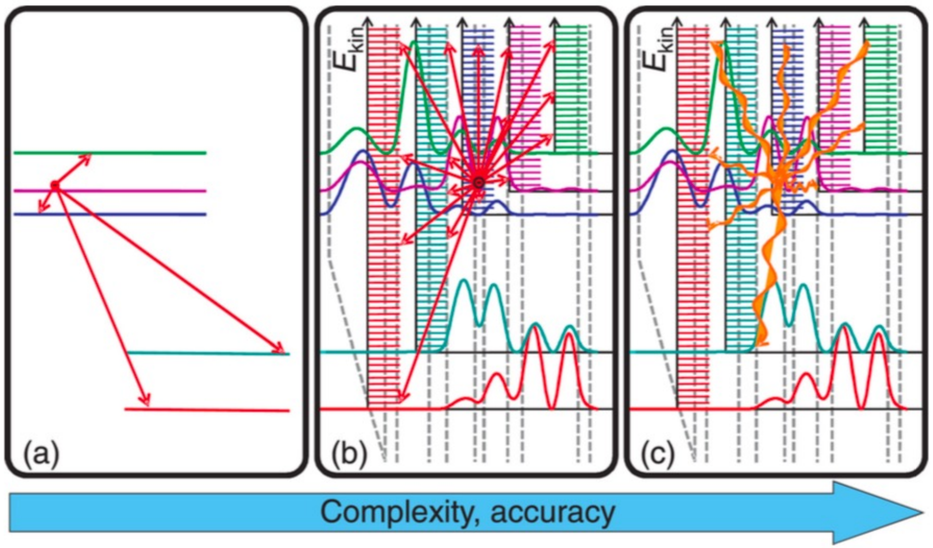
Density matrix: contains microscopic state of electronic system

$$\rho_{i,j}$$

Find observables of system: Current, Gain, etc.

$$\langle \hat{O} \rangle = \mathrm{Tr}\{\rho \hat{O}\}$$

Time evolution (von Neumann, Heisenberg's equation of motion):



Jirauschek and Kubis, APR **1** 2014

Coherent evolution

$$\dot{\rho} = \frac{1}{i\hbar}[\hat{H}, \rho] = \frac{1}{i\hbar}[\hat{H}_0, \rho] + \frac{1}{i\hbar}[\hat{H}_{\mathrm{scatt.}}, \rho]$$

$$\sum_{P,ij,i'j'} \Gamma^{P}_{ij,i'j'} \rho_{i'j'}$$

Rates from Fermi Golden Rule
(rate equations: i=j, i'=j')

$$\sum_j \Gamma_j \left(\hat{L}_j \hat{\rho} \hat{L}_j^\dagger - \frac{1}{2} \hat{\rho} \hat{L}_j^\dagger \hat{L}_j - \frac{1}{2} \hat{L}_j^\dagger \hat{L}_j \hat{\rho} \right)$$

Full density matrix (Lindblad form)

$$\mathrm{d}_t f_{i\mathbf{k}} = \sum_j \sum_{\mathbf{k}'} \left(W_{j\mathbf{k}',i\mathbf{k}} f_{j\mathbf{k}'} - W_{i\mathbf{k},j\mathbf{k}'} f_{i\mathbf{k}} \right)$$

Monte Carlo:
(Boltzmann equation)

Very successful : Non Equilibrium Green's Function (NEGF)

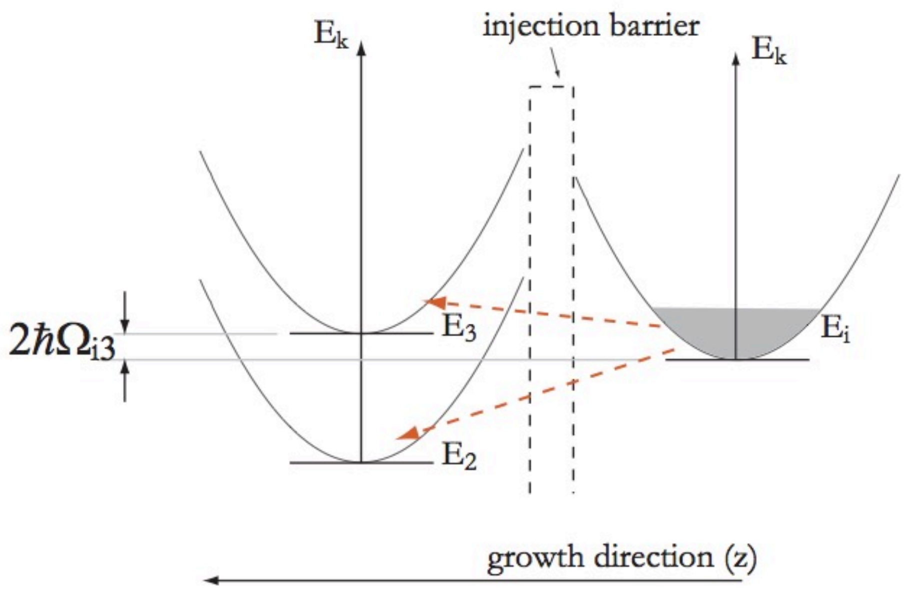
- Treat full density matrix of many-body interacting system
- Correlation function: $G(\boldsymbol{r}_1, t_1; \boldsymbol{r}_2, t_2)$
- Can obtain all observables from G (generalized DM)
- Perturbation expansion to infinite order
- Feynman diagram approach to scattering
- Basis independent (FGR needs energy eigenstates)
- Most general scheme, high flexibility
- Non-equilibrium conditions, finite temperature (statistical, thermodynamics)
- Work in interaction (Dirac) picture
- 2^{nd} quantization (many-body formalism)

- (remember Schrödinger, Heisenberg, Dirac pictures)

Transport model: density matrix

Kazarinov and Suris model (in first place neglecting in-plane disp.)

Electric and electromagnetic properties of semiconductors with a superlattice, RF Kazarinov, RA Suris, Sov. Phys. Semicond 6 (1), 120-131 (1972)



Resonant tunneling injection

Jmax: $$J_{\max} = eN_s \frac{2|\Omega|^2 \tau_\perp}{1 + 4|\Omega|^2 \tau_3 \tau_\perp}.$$

Weak coupling: $4|\Omega|^2 \tau_3 \tau_\perp \ll 1 \quad J_{\max} = (eN_s/2) 4|\Omega|^2 \tau_\perp$

Strong coupling $4|\Omega|^2 \tau_3 \tau_\perp \gg 1 \quad J = eN_s/(2\tau_3)$

How to choose Ω ? we do not want to be limited by tunneling rate -> strong coupling

The electroluminescence linewidth gives us estimate on $\tau_\perp$

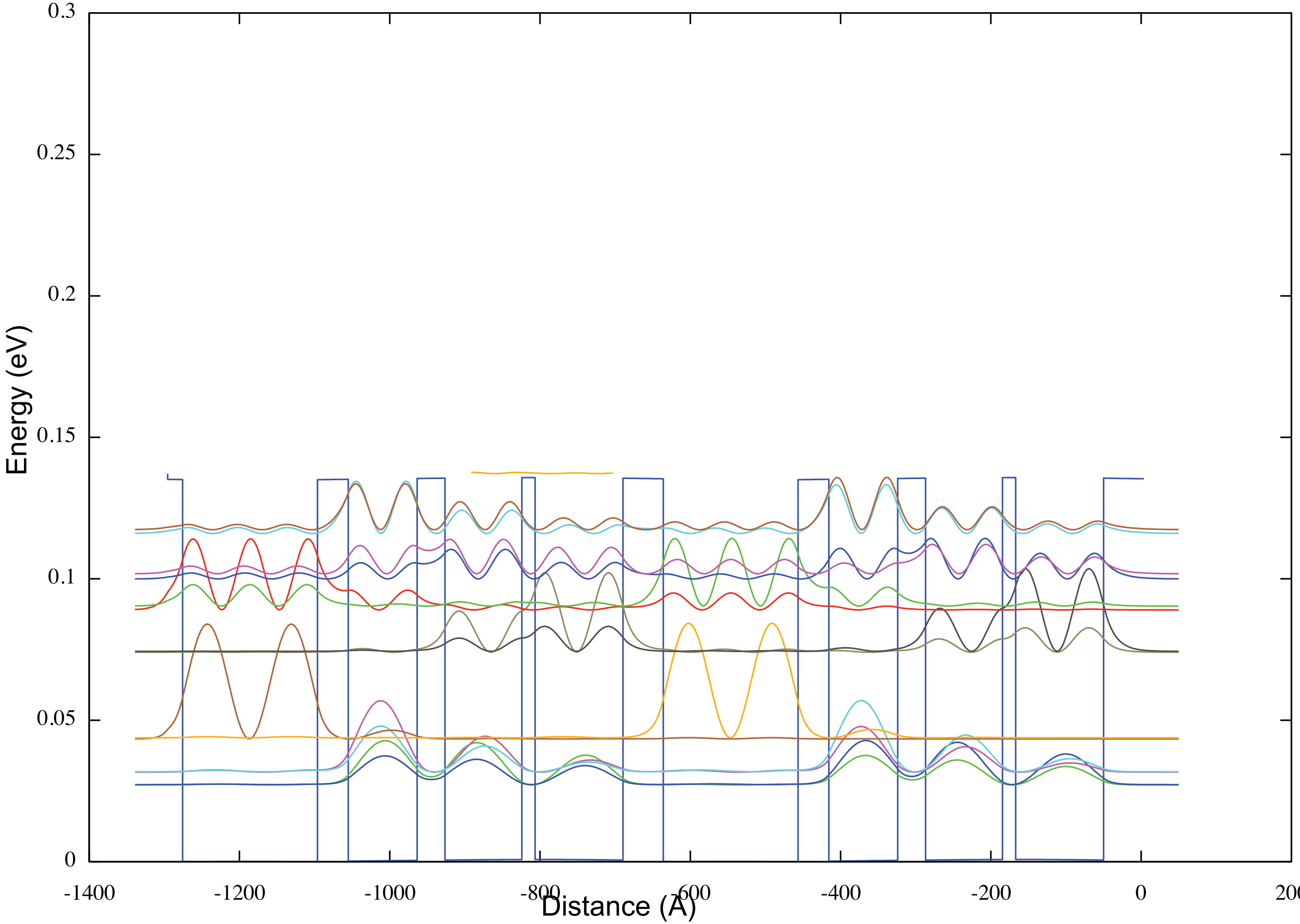
"Too strong" coupling will reduce the localization of the upper state wavefunction

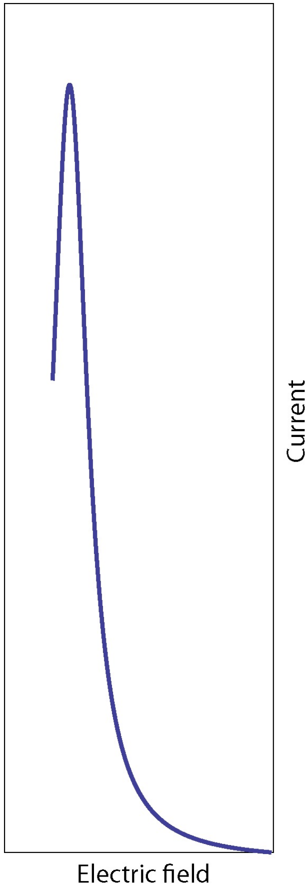
1722 IEEE JOURNAL OF QUANTUM ELECTRONICS, VOL. 34, NO. 9, SEPTEMBER 1998

Resonant Tunneling in Quantum Cascade Lasers

Carlo Sirtori, *Member, IEEE,* Federico Capasso, *Fellow, IEEE,* Jérôme Faist, *Member, IEEE,*
Albert L. Hutchinson, *Member, IEEE,* Deborah L. Sivco, and Alfred Y. Cho, *Fellow, IEEE*

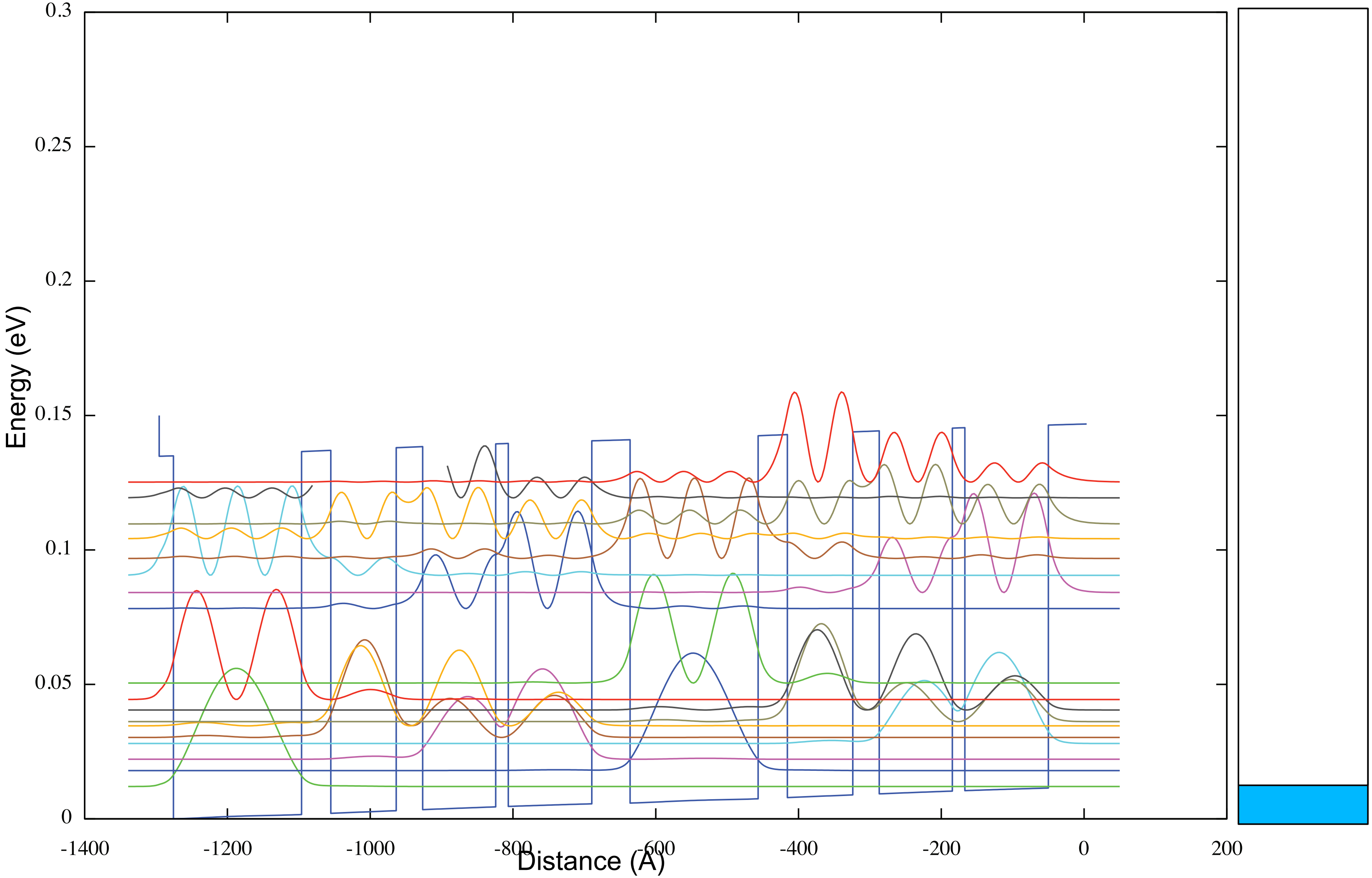
Electronic states as a function of bias

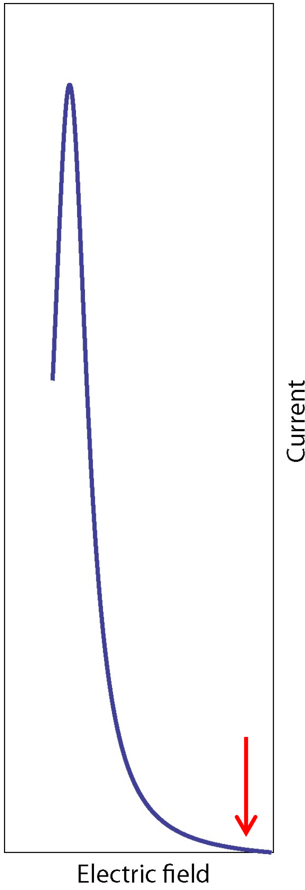




0 kV/cm

Electronic states as a function of bias

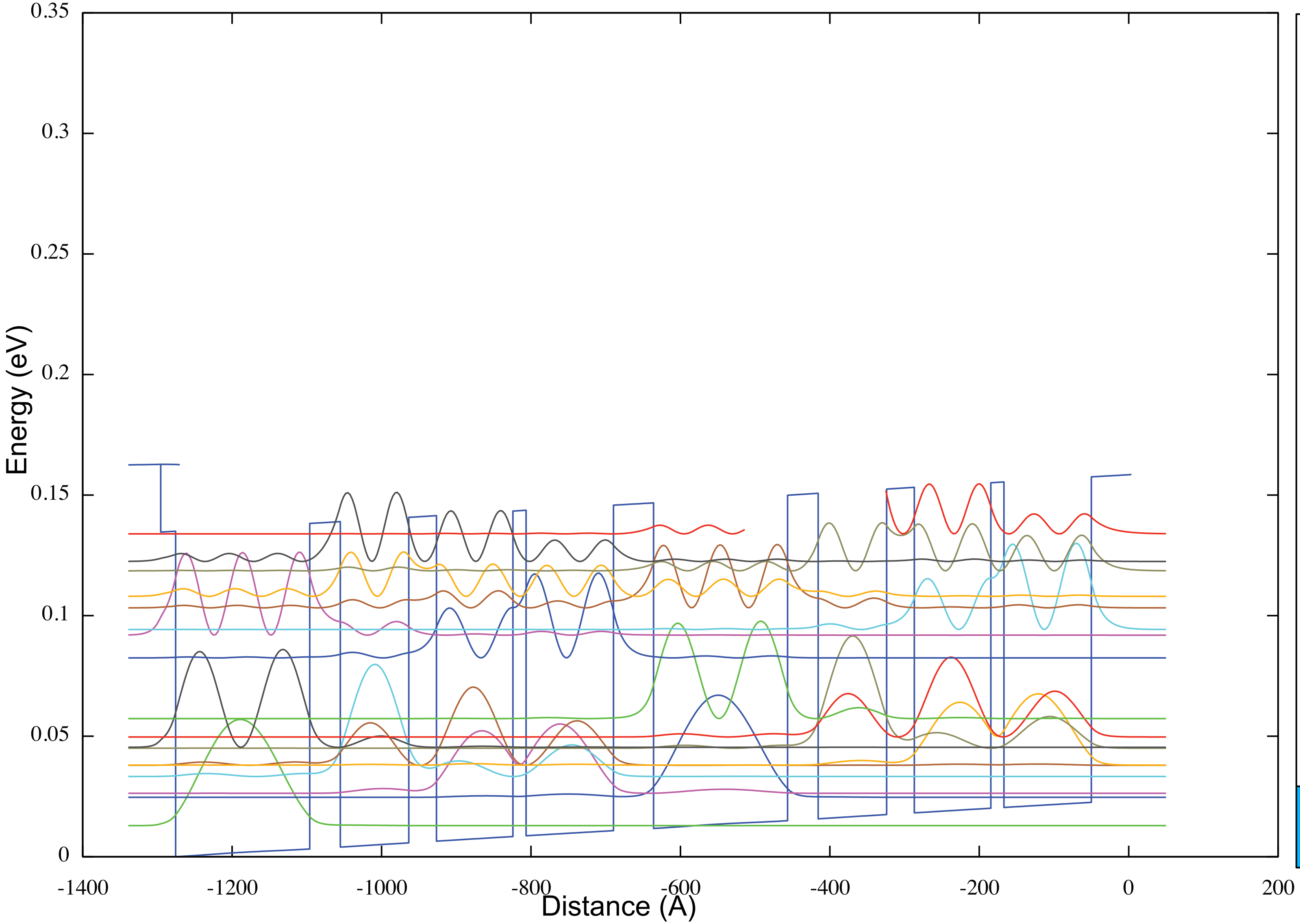


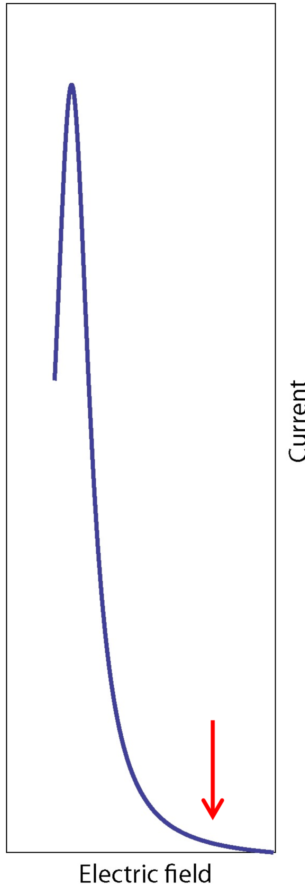


1 kV/cm

ETH zürich

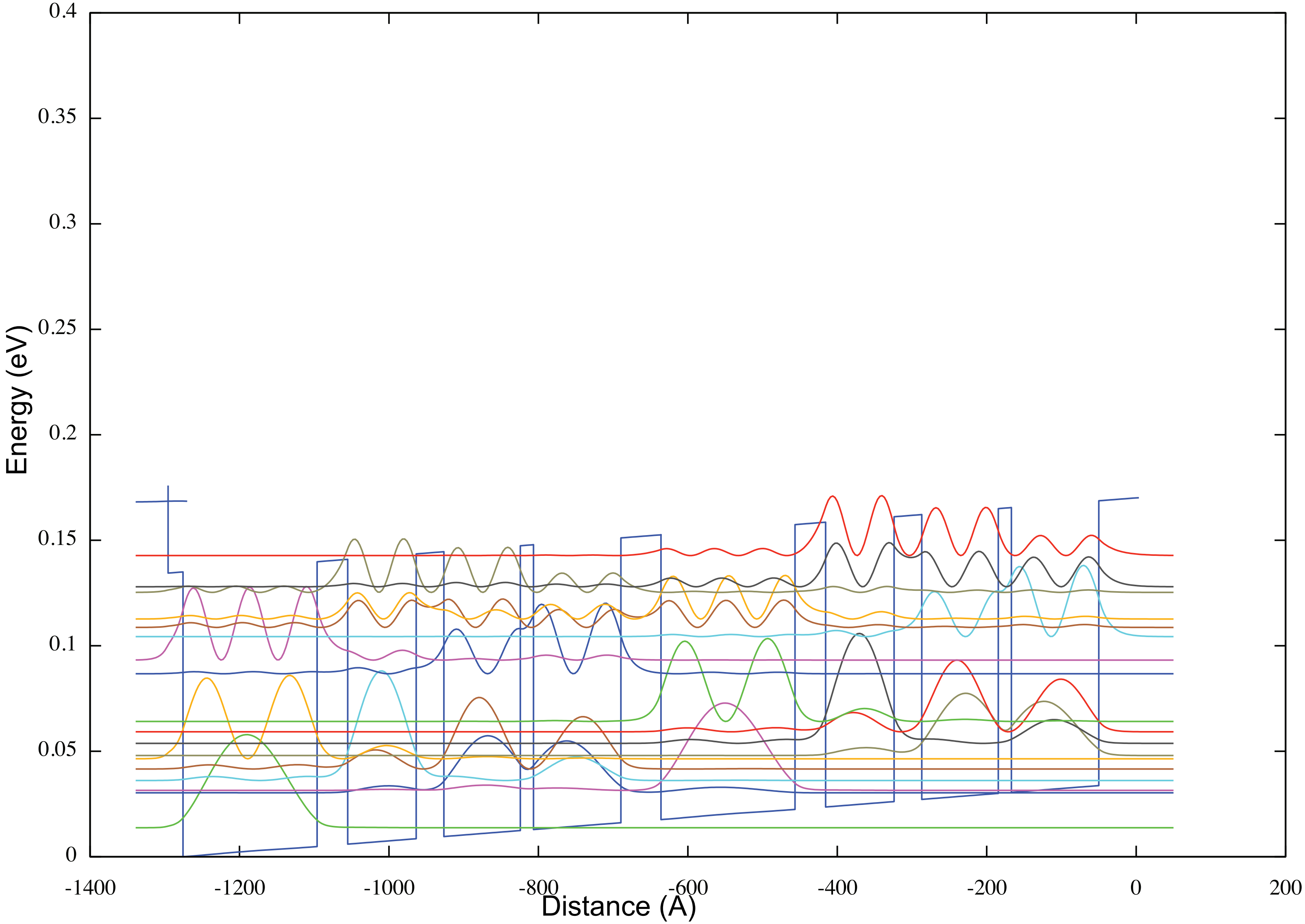
Electronic states as a function of bias

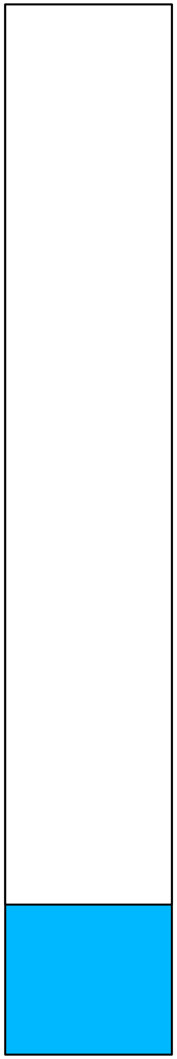


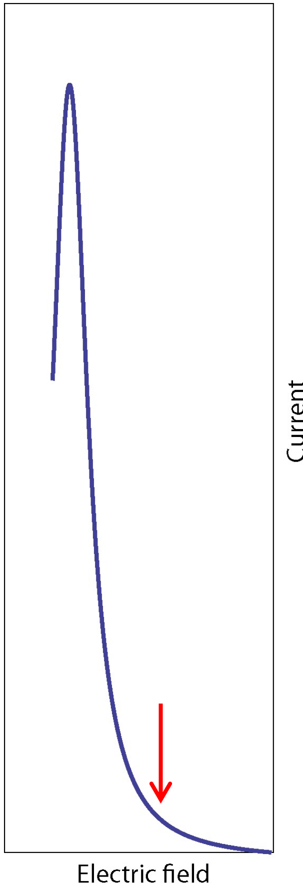


2 kV/cm

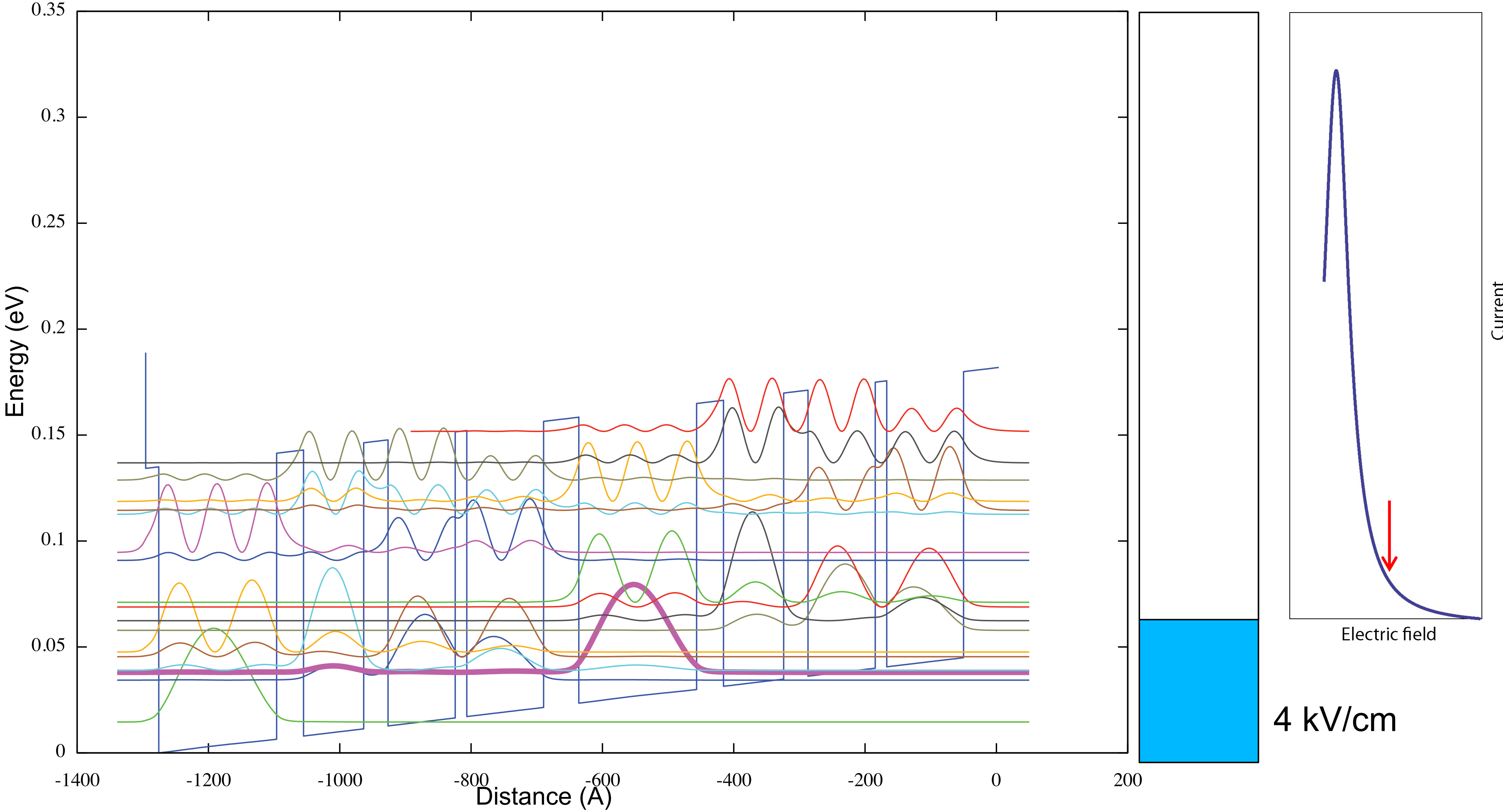
Electronic states as a function of bias



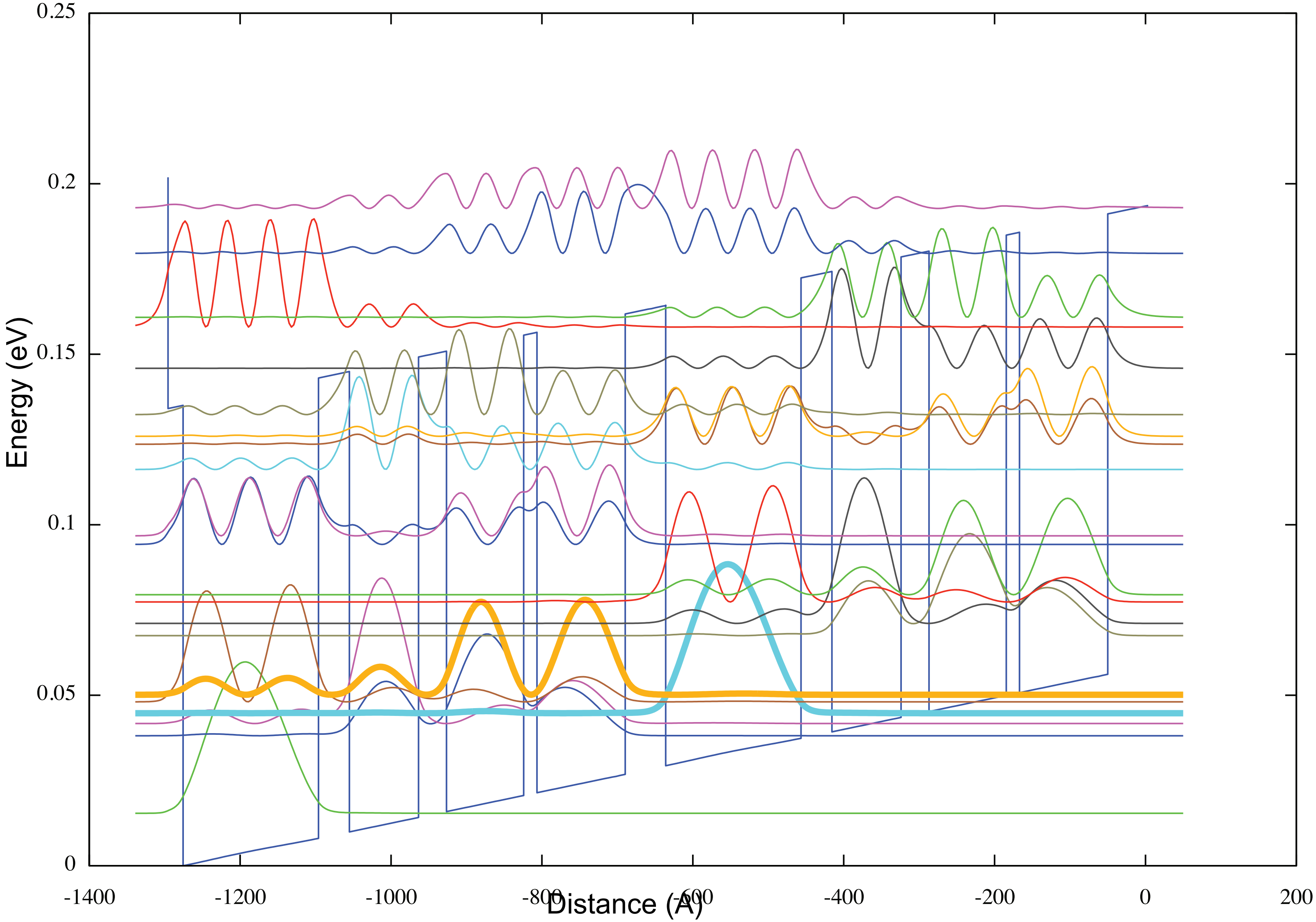


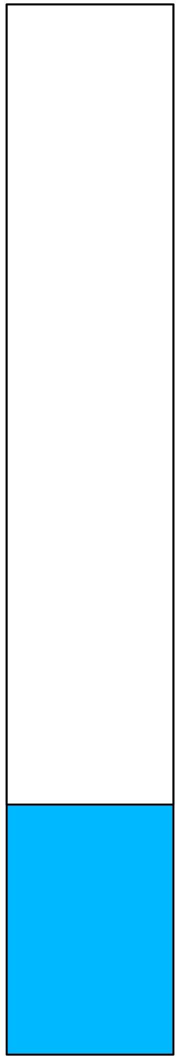


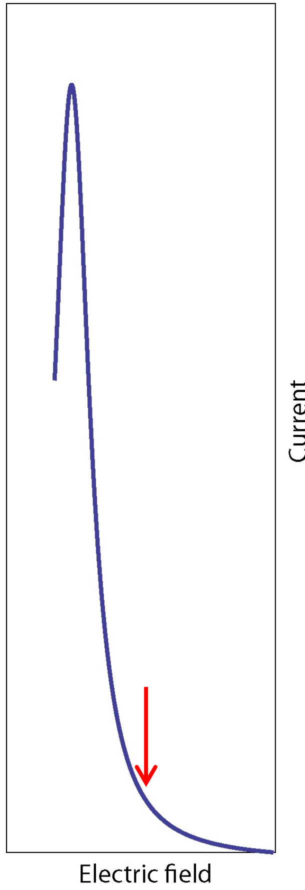
Electronic states as a function of bias



Electronic states as a function of bias

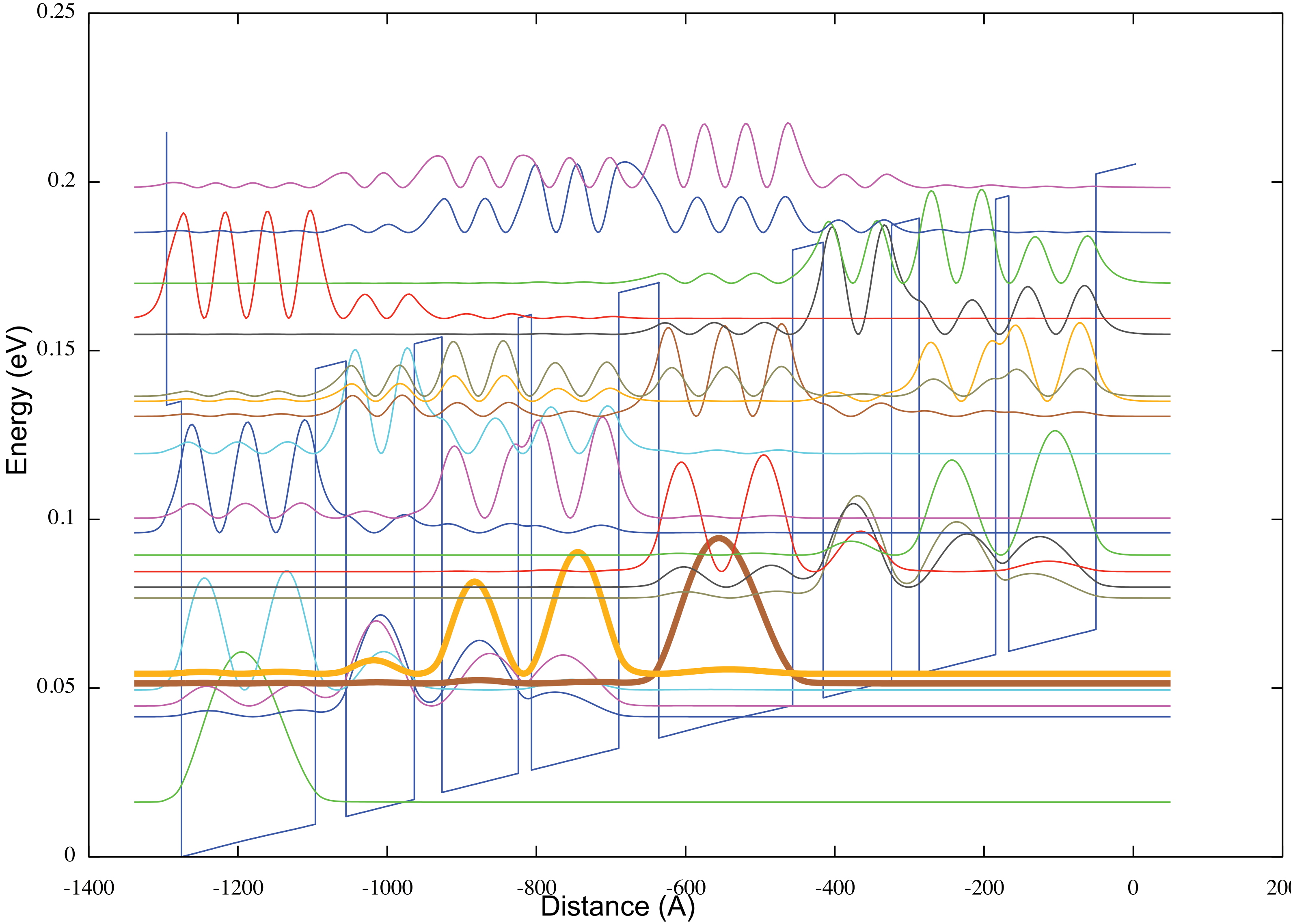


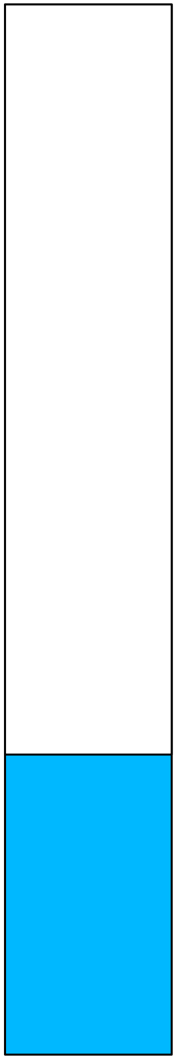


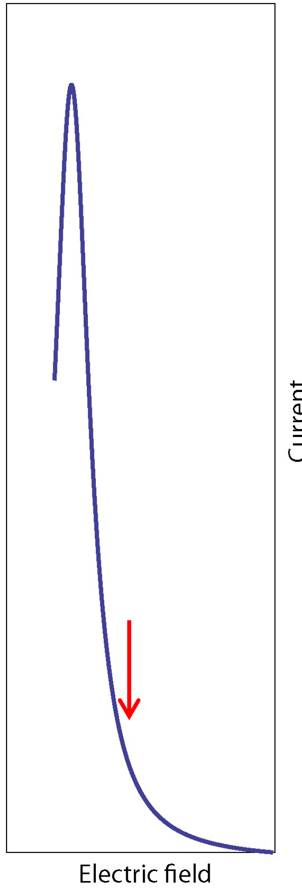


5 kV/cm

Electronic states as a function of bias

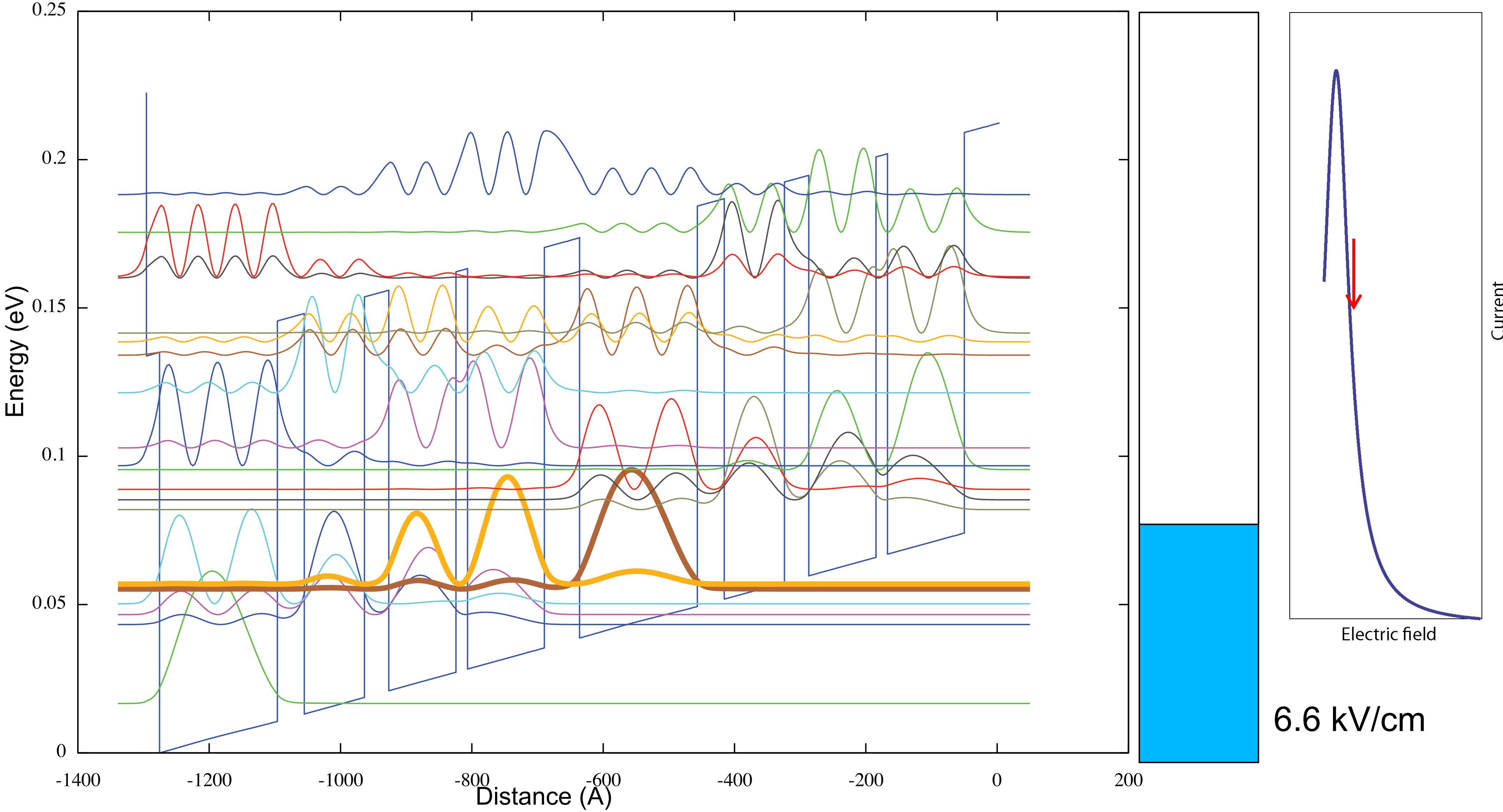




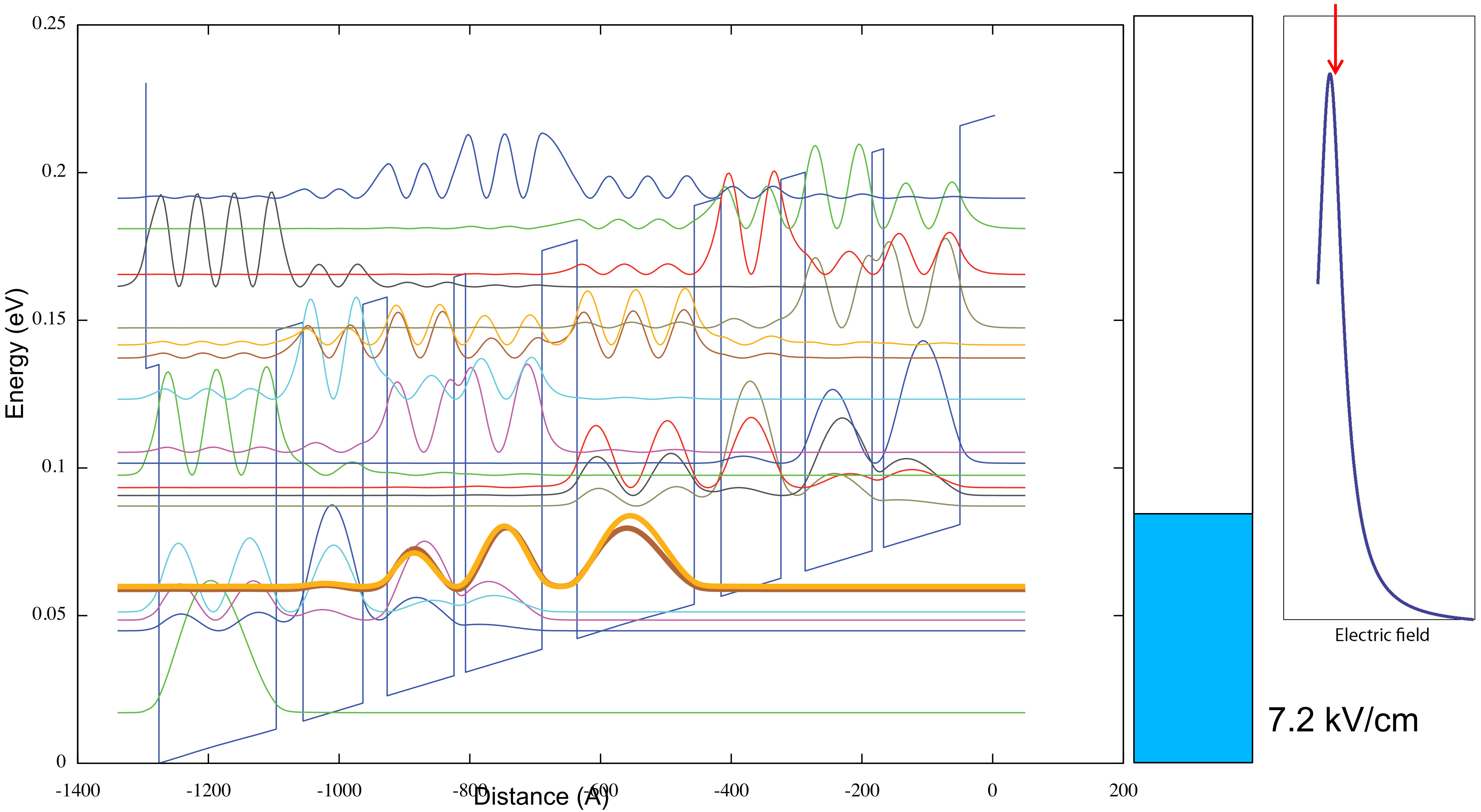


6 kV/cm

Electronic states as a function of bias



Electronic states as a function of bias



Electronic states as a function of bias