Microscopic models for engineering of optoelectronic devices

SAND2013-4446P

Weng W. Chow

Sandia National Laboratories, Albuquerque, New Mexico, USA

1) What is a microscopic model and what is not?
2) How to set one up (e.g. quantum-dot laser)
3) What it tells us (about expt and beyond expt)
4) Other examples ...

Thanks to:

Sandia's Energy Frontier Research Center (EFRC), DOE-Basic Energy Sciences
Sonderforschungsbereich (SFB) 787

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Microscopic versus not microscopic

Radiation field:

$$\nabla \cdot \vec{D} = 0 \qquad \nabla \times \vec{E} = -\frac{\partial \vec{B}}{dt}$$

$$\nabla \cdot \vec{B} = 0 \qquad \nabla \times \vec{H} = -\frac{\partial \vec{D}}{dt}$$

Constitutive relations:

$$D = \varepsilon E \qquad B = \mu_0 H$$

$$\overbrace{\varepsilon_r(x, y, z)\vec{E}} + \vec{P}$$

Put in by hand = not microscopic

Calculated with quantum mechanics
= microscopic

Put in by hand:

Linewidth enhancement factor

$$P = -i\frac{\varepsilon_0 nc}{2\omega}G(1 - i\alpha)E$$

polarization

Gain

Example: semiconductor laser

$|E|e^{-i\varphi}$

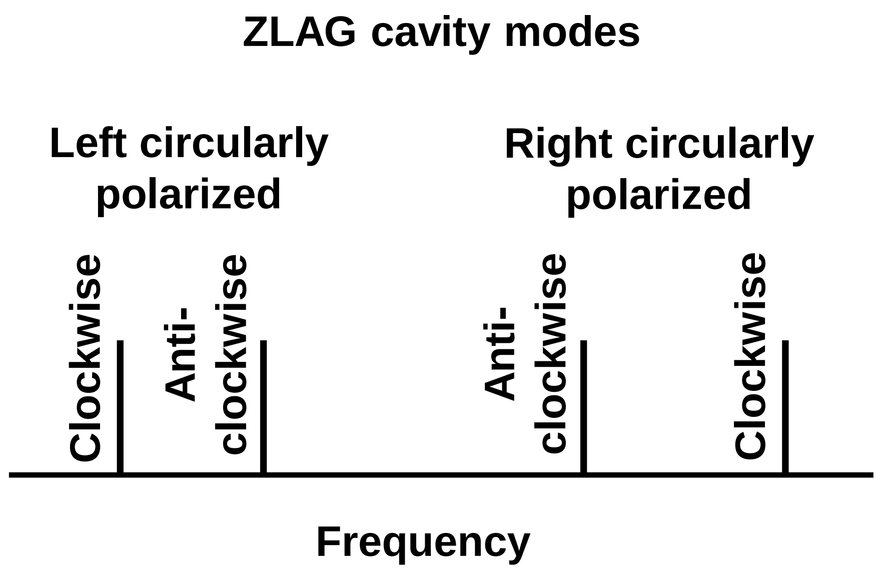
$$\frac{dE}{dt} = -\gamma_c E + (1 - i\alpha)\Gamma A(N - N_{tr})E$$

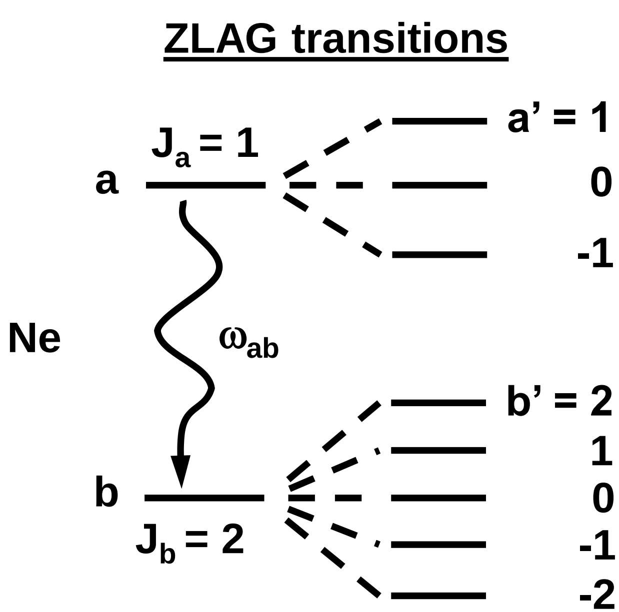
$$\frac{dN}{dt} = \frac{J}{ed} - \gamma_{nr}N - \frac{\varepsilon_b}{\hbar\omega}\Gamma A(N - N_{tr})|E|^2$$

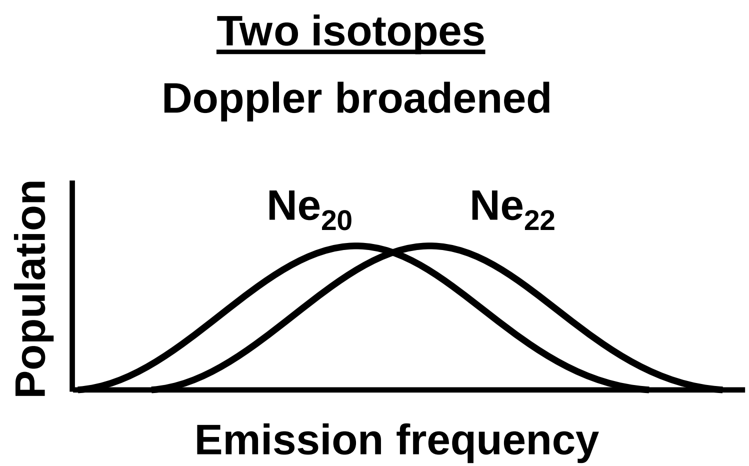
R. Lang and K Kobayashi, JQE (1980) on laser feedback instabilities > 1700 citations

Rose, Lindberg, Chow, Koch and Sargent, JQE (1992) microscopic theory & feedback: 11 citations

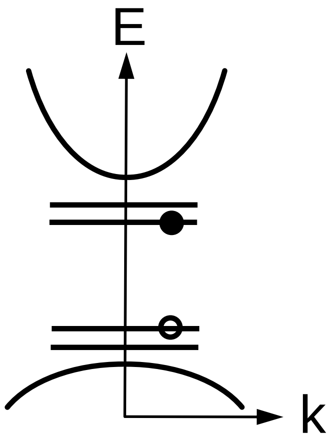
An early microscopic model: ZLAG







Microscopic model for semiconductors



Laser Field

$$H_{c-p} = -\sum_k \left(\wp_k a_k^\dagger b_{-k}^\dagger + \wp_k^* b_{-k} a_k\right) E(z,t)$$

Electronic structure

Interacting electron- hole plasma

$$H_0 = \sum_k \left(\varepsilon_{ek} a_k^\dagger a_k + \varepsilon_{hk} b_{-k}^\dagger b_{-k}\right)$$

Carrier-carrier interaction:

$$H_{c-c} = \frac{1}{2}\sum_{n,m,r,s} W_{nm}^{rs} a_r^\dagger a_s^\dagger a_m a_n + \frac{1}{2}\sum_{n,m,r,s} b_r^\dagger b_s^\dagger b_m b_n - \sum_{n,m,r,s} W_{nm}^{rs} a_r^\dagger b_s^\dagger b_m a_n$$

Carrier-phonon interaction:

$$H_{c-pn} = \sum_{n,q} \hbar G_q a_{n+q}^\dagger a_n \left(b_q + b_{-q}^\dagger\right)$$

$$\int d^3r\, d^3r' \phi_r^*(r)\phi_r^*(r') \frac{e^2}{4\pi\varepsilon_b |r - r'|} \phi_m(r')\phi_n(r)$$

$$\boxed{H = H_0 + H_{c-p} + H_{c-c} + H_{c-pn}}$$

Example: quantum-dot laser

Quantum dots

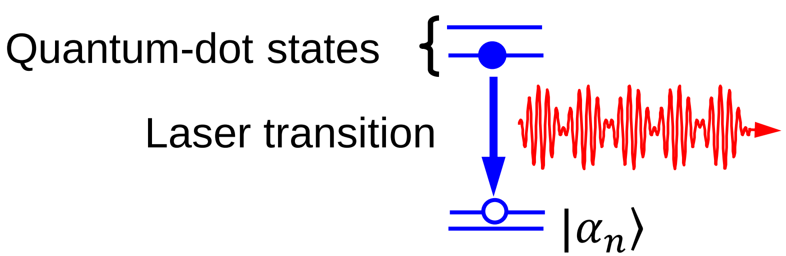
$$\frac{dp_{\alpha_n\beta_n}}{dt} = -i(\omega_{\alpha_n\beta_n} - \omega)p_{\alpha_n\beta_n} - i\Omega_{\alpha_n\beta_n}(n_{e\alpha_n} + n_{h\beta_n} - 1) - \gamma p_{\alpha_n\beta_n}$$

$$\frac{dn_{e\alpha_n}}{dt} = (ip^*_{\alpha_n\beta_n}\Omega_{\alpha_n\beta_n} + c.c.) - \gamma^d_{nr} n_{e\alpha_n}$$

Similar equation for holes

Laser field

$$\frac{dE}{dt} = -\gamma_c E + \underbrace{\frac{i\omega\Gamma}{\varepsilon_b}\frac{N_d}{h}\sum_n \sum_{\alpha_n\beta_n} \mu^*_{\alpha_n\beta_n} p_{\alpha_n\beta_n}}_{\text{Replaces } (1 - i\alpha)\Gamma A(N - N_{tr})E}$$



Example: quantum-dot laser

Quantum dots

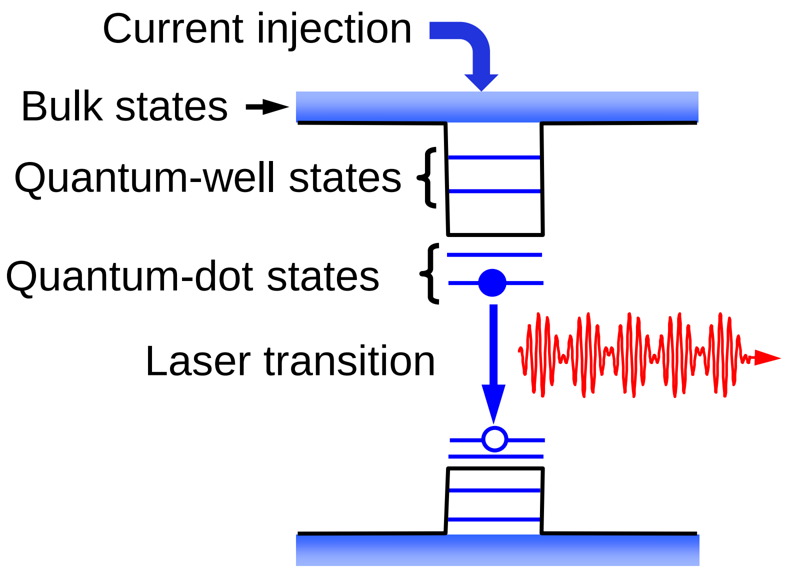
$$\frac{dp_{\alpha_n\beta_n}}{dt} = -i(\omega_{\alpha_n\beta_n} - \omega)p_{\alpha_n\beta_n} - i\Omega_{\alpha_n\beta_n}\left(n_{e\alpha_n} + n_{h\beta_n} - 1\right) - \gamma p_{\alpha_n\beta_n}$$

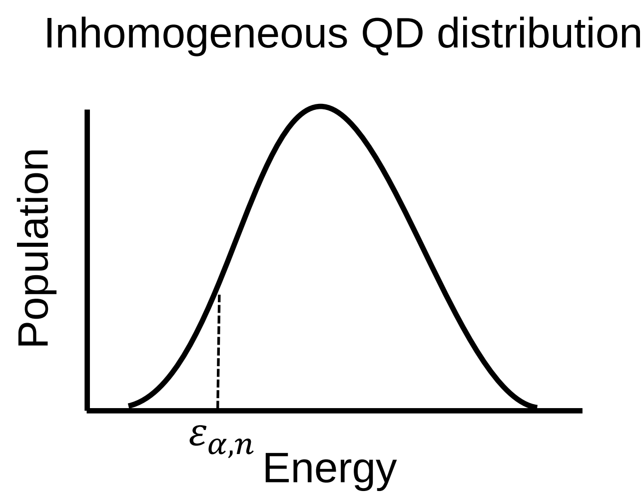
$$\frac{dn_{e\alpha_n}}{dt} = \left(ip^*_{\alpha_n\beta_n}\Omega_{\alpha_n\beta_n} + c.c.\right) - \gamma^d_{nr}n_{e\alpha_n}$$

⇨ ***Similar equation for holes***

Laser field

$$\frac{dE}{dt} = -\gamma_c E + \underbrace{\frac{i\omega\Gamma}{\varepsilon_b}\frac{N_d}{h}\sum_n \sum_{\alpha_n\beta_n} \mu^*_{\alpha_n\beta_n} p_{\alpha_n\beta_n}}_{\text{Replaces } (1-i\alpha)\Gamma A(N-N_{tr})E}$$





Example: quantum-dot laser

Quantum dots

$$\frac{dp_{\alpha_n\beta_n}}{dt} = -i(\omega_{\alpha_n\beta_n} - \omega)p_{\alpha_n\beta_n} - i\Omega_{\alpha_n\beta_n}(n_{e\alpha_n} + n_{h\beta_n} - 1) - \gamma p_{\alpha_n\beta_n}$$

$$\frac{dn_{e\alpha_n}}{dt} = (ip^*_{\alpha_n\beta_n}\Omega_{\alpha_n\beta_n} + c.c.) - \gamma^d_{nr} n_{e\alpha_n}$$

$$-\gamma^{(3)}_{c-c}\left[n_{e\alpha_n} - f\left(\varepsilon_{e\alpha_n}, \mu_e^{(3p)}, T_{3p}\right)\right]$$

⇨ ***Similar equation for holes***

Laser field

$$\frac{dE}{dt} = -\gamma_c E + \frac{i\omega\Gamma}{\varepsilon_b}\frac{N_d}{h}\sum_n \sum_{\alpha_n\beta_n} \mu^*_{\alpha_n\beta_n} p_{\alpha_n\beta_n}$$

Quantum well

Plasma temperature *Lattice temperature*

$$\frac{dn_{\sigma k_\perp}}{dt} = -\gamma^{(2)}_{c-c}\left[n_{\sigma k_\perp} - f\left(\varepsilon_{\sigma k_\perp}, \mu_\sigma^{(2p)}, T_{2p}\right)\right] - \gamma^{(2)}_{c-p}\left[n_{\sigma k_\perp} - f\left(\varepsilon_{\sigma k_\perp}, \mu_\sigma^{(2l)}, T_l\right)\right]$$

$$-\gamma^{(3)}_{c-c}\left[n_{\sigma k_\perp} - f\left(\varepsilon_{\sigma k_\perp}, \mu_\sigma^{(3p)}, T_{3p}\right)\right]$$

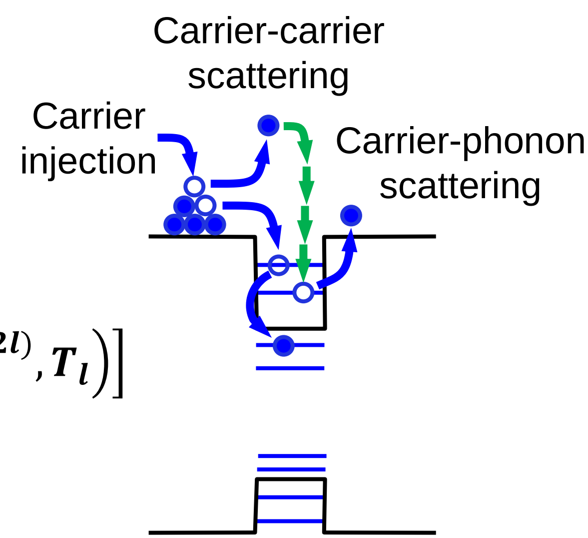
Among QD, QW and bulk

Bulk

$$\frac{dn_{\sigma k}}{dt} = \frac{J}{eV_b N_{p,\sigma}} f(\varepsilon_{\sigma k}, \mu_\sigma^p, T_l)(1 - n_{\sigma k}) - \gamma^b_{nr} n_{\sigma k}$$

$$-\gamma^{(2)}_{c-c}\left[n_{\sigma k} - f\left(\varepsilon_{\sigma k}, \mu_\sigma^{(2p)}, T_{2p}\right)\right] - \gamma^{(2)}_{c-p}\left[n_{\sigma k} - f\left(\varepsilon_{\sigma k}, \mu_\sigma^{(2l)}, T_l\right)\right]$$

$$-\gamma^{(3)}_{c-c}\left[n_{\sigma k} - f\left(\varepsilon_{\sigma k}, \mu_\sigma^{(3p)}, T_{3p}\right)\right]$$



Example: quantum-dot laser

Quantum dots

$$\frac{dp_{\alpha_n\beta_n}}{dt} = -i(\omega_{\alpha_n\beta_n} - \omega)p_{\alpha_n\beta_n} - i\Omega_{\alpha_n\beta_n}(n_{e\alpha_n} + n_{h\beta_n} - 1) - \gamma p_{\alpha_n\beta_n}$$

$$\frac{dn_{e\alpha_n}}{dt} = (ip^*_{\alpha_n\beta_n}\Omega_{\alpha_n\beta_n} + c.c.) - \gamma^d_{nr} n_{e\alpha_n}$$
$$-\gamma^{(3)}_{c-c}\left[n_{e\alpha_n} - f\left(\varepsilon_{e\alpha_n}, \mu^{(3p)}_e, T_{3p}\right)\right] - \gamma^{(3)}_{c-p}\left[n_{e\alpha_n} - f\left(\varepsilon_{e\alpha_n}, \mu^{(3l)}_e, T_l\right)\right]$$

Similar equation for holes

Laser field

$$\frac{dE}{dt} = -\gamma_c E + \frac{i\omega\Gamma}{\varepsilon_b}\frac{N_d}{h}\sum_n \sum_{\alpha_n\beta_n} \mu^*_{\alpha_n\beta_n} p_{\alpha_n\beta_n}$$

Quantum well

Plasma temperature

Lattice temperature

$$\frac{dn_{\sigma k_\perp}}{dt} = -\gamma^{(2)}_{c-c}\left[n_{\sigma k_\perp} - f\left(\varepsilon_{\sigma k_\perp}, \mu^{(2p)}_\sigma, T_{2p}\right)\right] - \gamma^{(2)}_{c-p}\left[n_{\sigma k_\perp} - f\left(\varepsilon_{\sigma k_\perp}, \mu^{(2l)}_\sigma, T_l\right)\right]$$
$$-\gamma^{(3)}_{c-c}\left[n_{\sigma k_\perp} - f\left(\varepsilon_{\sigma k_\perp}, \mu^{(3p)}_\sigma, T_{3p}\right)\right] - \gamma^{(3)}_{c-p}\left[n_{\sigma k_\perp} - f\left(\varepsilon_{\sigma k_\perp}, \mu^{(3l)}_\sigma, T_l\right)\right] - \gamma^{qw}_{nr} n_{\sigma k_\perp}$$

Among QD, QW and bulk

Bulk

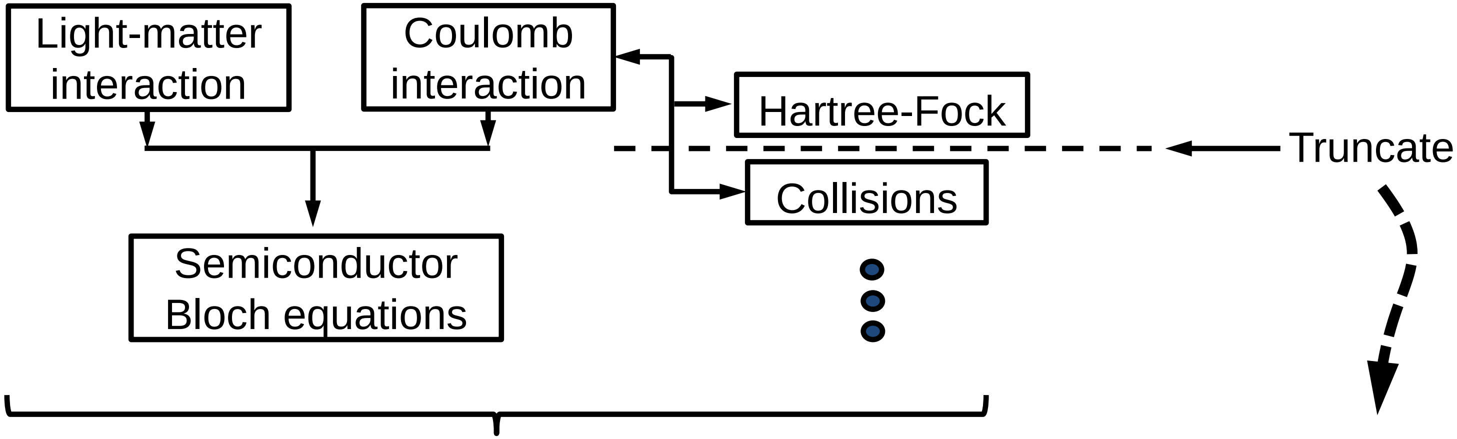
$$\frac{dn_{\sigma k}}{dt} = \frac{J}{eV_b N_{p,\sigma}} f(\varepsilon_{\sigma k}, \mu^p_\sigma, T_l)(1 - n_{\sigma k}) - \gamma^b_{nr} n_{\sigma k}$$
$$-\gamma^{(2)}_{c-c}\left[n_{\sigma k} - f\left(\varepsilon_{\sigma k}, \mu^{(2p)}_\sigma, T_{2p}\right)\right] - \gamma^{(2)}_{c-p}\left[n_{\sigma k} - f\left(\varepsilon_{\sigma k}, \mu^{(2l)}_\sigma, T_l\right)\right]$$
$$-\gamma^{(3)}_{c-c}\left[n_{\sigma k} - f\left(\varepsilon_{\sigma k}, \mu^{(3p)}_\sigma, T_{3p}\right)\right] - \gamma^{(3)}_{c-p}\left[n_{\sigma k} - f\left(\varepsilon_{\sigma k}, \mu^{(3l)}_\sigma, T_l\right)\right]$$

Chow and Koch, IEEE Journ. Quantum Electron. 41, 495 (2005)

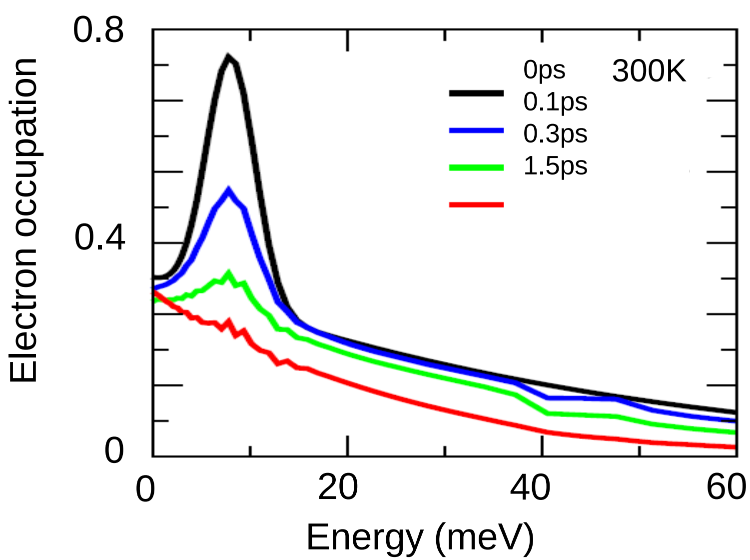
ZLAG

$\vec{n}\vec{\mu}\vec{\rho}\vec{\sigma}$	$d_{\vec{\mu}}$	$d_{\vec{\rho}}$	$d_{\vec{\sigma}}$	Integral Type	$d_{\vec{n}}$	$p_{\vec{n}}$	Transitions	$\theta_{\vec{n}\vec{m}}$
1111	+	+	+	1	+	−	\\\	11
2222	+	+	+	1	+	+	///	22
3333	−	−	−	1	−	−	\\\	33
4444	−	−	−	1	−	+	///	44
1122	+	+	+	1	+	−	//\	12
1221	+	+	+	1	+	−	\//	12
2211	+	+	+	1	+	+	/\\	21
2112	+	+	+	1	+	+	\\/	21
3344	−	−	−	1	−	−	//\	34
3443	−	−	−	1	−	−	\//	34
4433	−	−	−	1	−	+	/\\	43
4334	−	−	−	1	−	+	\\/	43
1133	+	−	−	3	+	−	\\\	13
1331	−	−	+	2	+	−	\\\	13
3311	−	+	+	3	−	−	\\\	31
3113	+	+	−	2	−	−	\\\	31
2244	+	−	−	3	+	+	///	24
2442	−	−	+	2	+	+	///	24
4422	−	+	+	3	−	+	///	42
4224	+	+	−	2	−	+	///	42
2233	+	−	−	3	+	+	/\\	23
2332	−	−	+	2	+	+	\\/	23
3322	−	+	+	3	−	−	//\	32
3223	+	+	−	2	−	−	\//	32
1144	+	−	−	3	−	−	//\	14
1441	−	−	+	2	−	−	\//	14
4411	−	+	+	3	+	+	/\\	41
4114	−	−	+	2	+	+	\\/	41

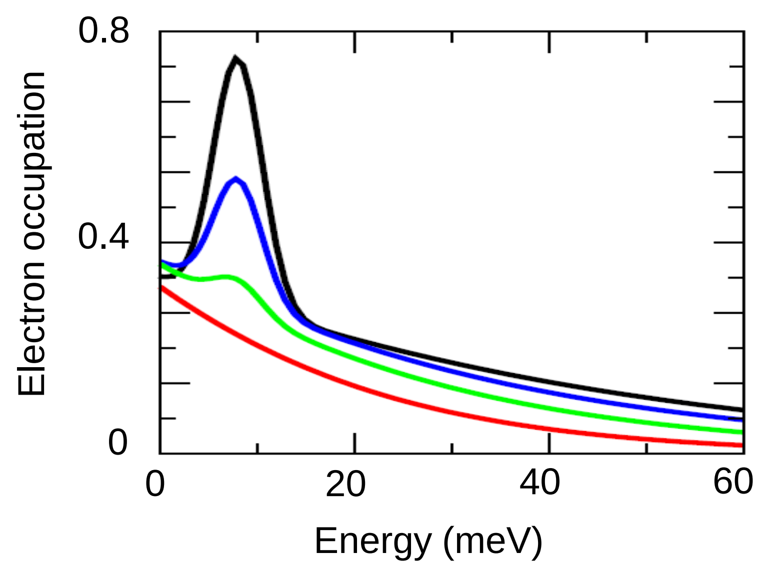
Quantum-kinetic equations vs. our effective-rate approach



2nd Born, Markov

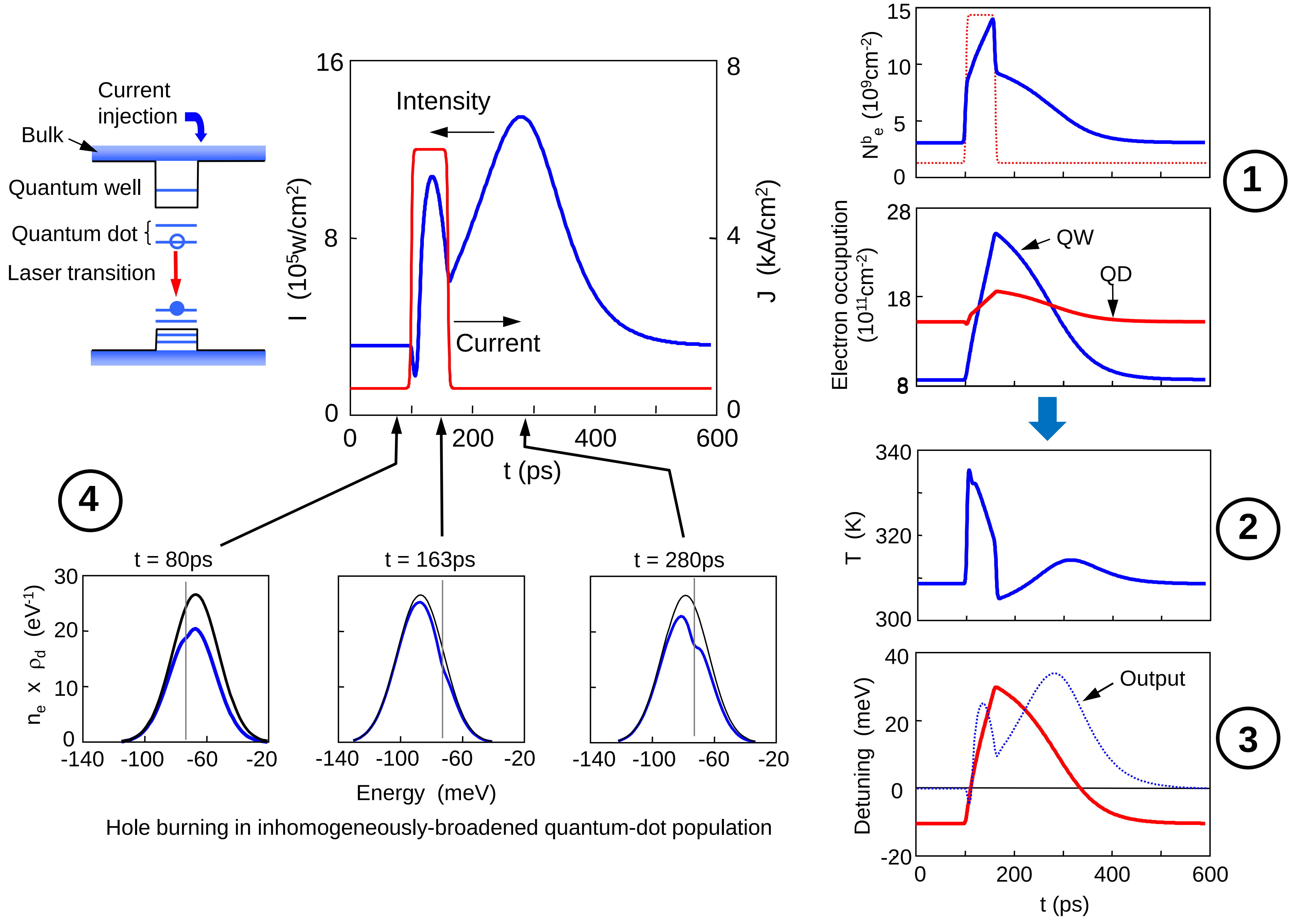


Screened Hartree-Fock & effective relaxation rates

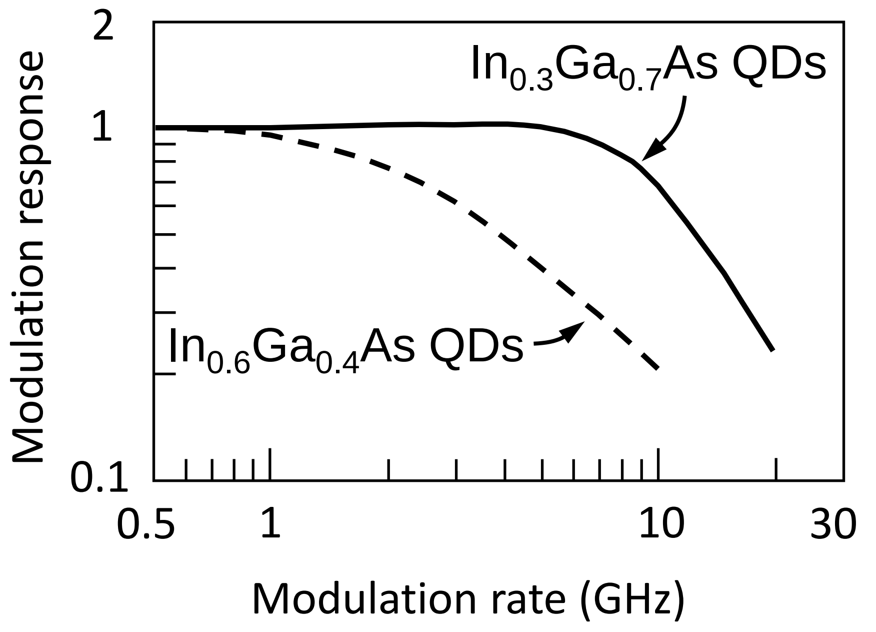


Waldmuller, …, IEEE JQE **42**, 292 (2006)

Nonequilibrium dynamics in a quantum-dot laser



Are quantum dot lasers faster than quantum well ones?



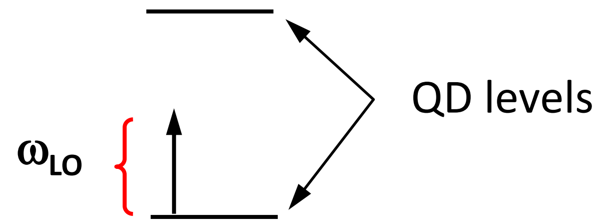
Answer: Not yet. One reason is QD density is too low.

Scattering in quantum dots has to be treated with extra care

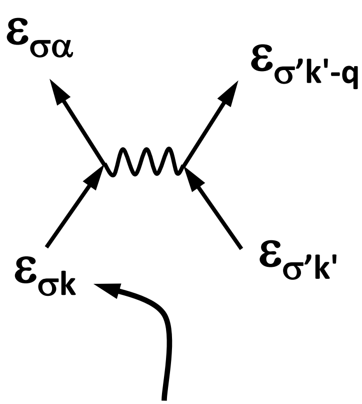
$$\frac{dp_\alpha}{dt} = -i\omega_\alpha p_\alpha - i\Omega_\alpha(n_{e\alpha} + n_{h\alpha} - 1)$$

$$+S_\alpha^{c-c} + S_\alpha^{c-p}$$

(2) Phonon bottleneck problem



(1) Carrier-carrier scattering



Must use renormalized energies
(no Baym-Kadanoff ansatz)

Memory effects important

Schneider, et al, PRB **70**, 235308, 2004

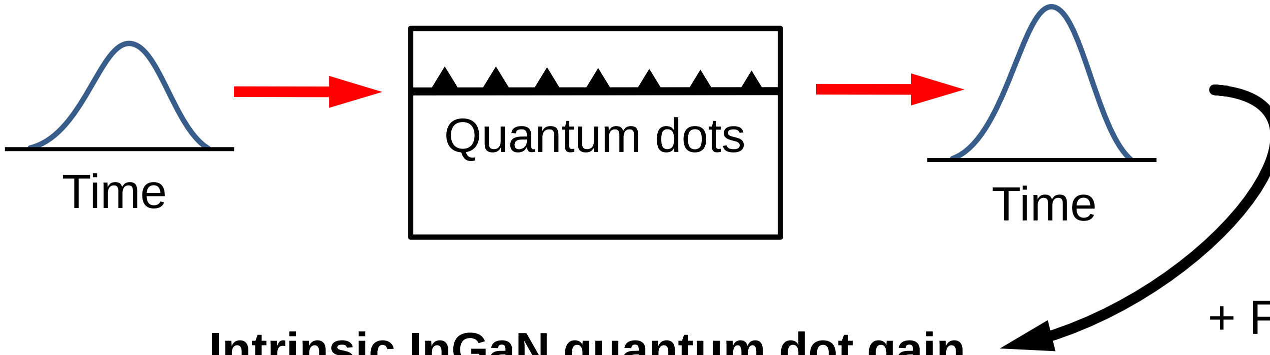
2nd Born treatment overestimates problem

Correct with nonperturbative (polaron) description

Inoshita, Sakaki, PRB 56,4355, 1997

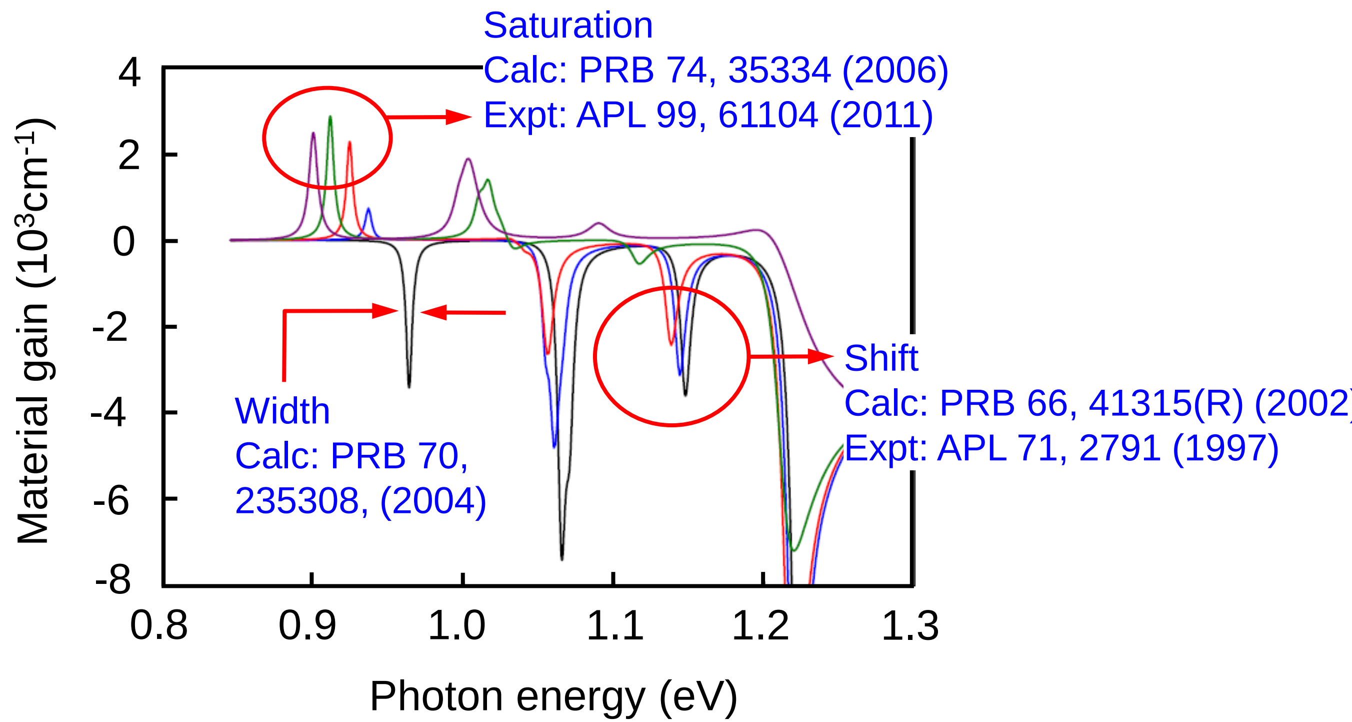
Seebeck et al, PRB 71, 125327, 2005

Quantum dot laser gain



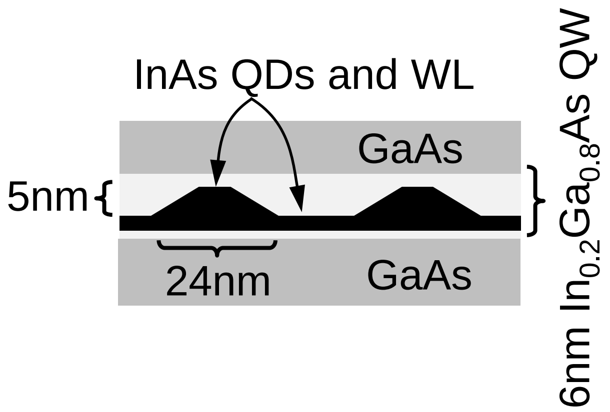
Intrinsic InGaN quantum dot gain

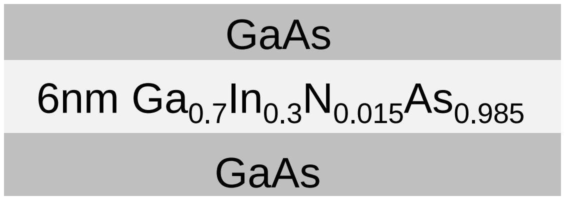
N_{dot}=2x10^{11}cm^{-2}, T=300K, N = 0.1x, 0.5x, 1x,2x,3x10^{12}cm^{-2}

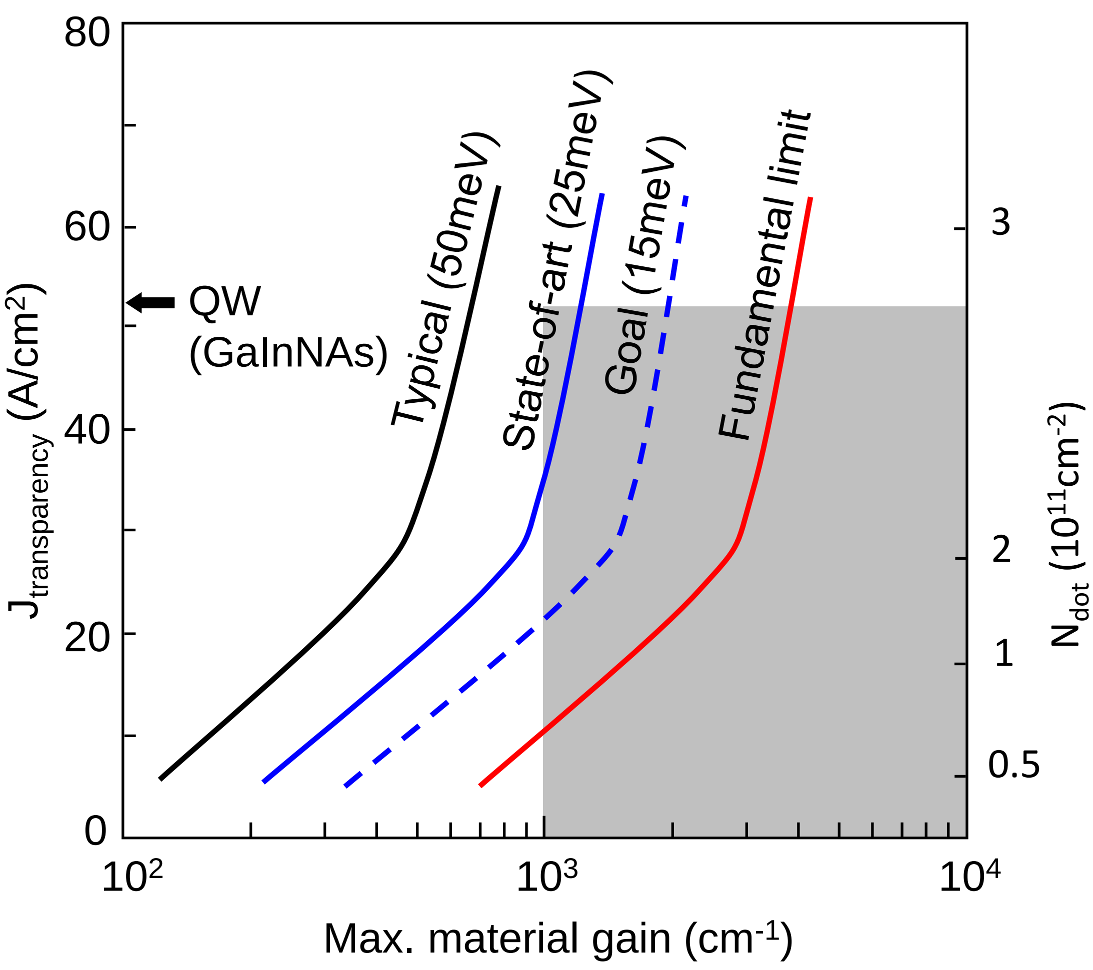


Precise scaling of the axii by rigorous treatment of scattering

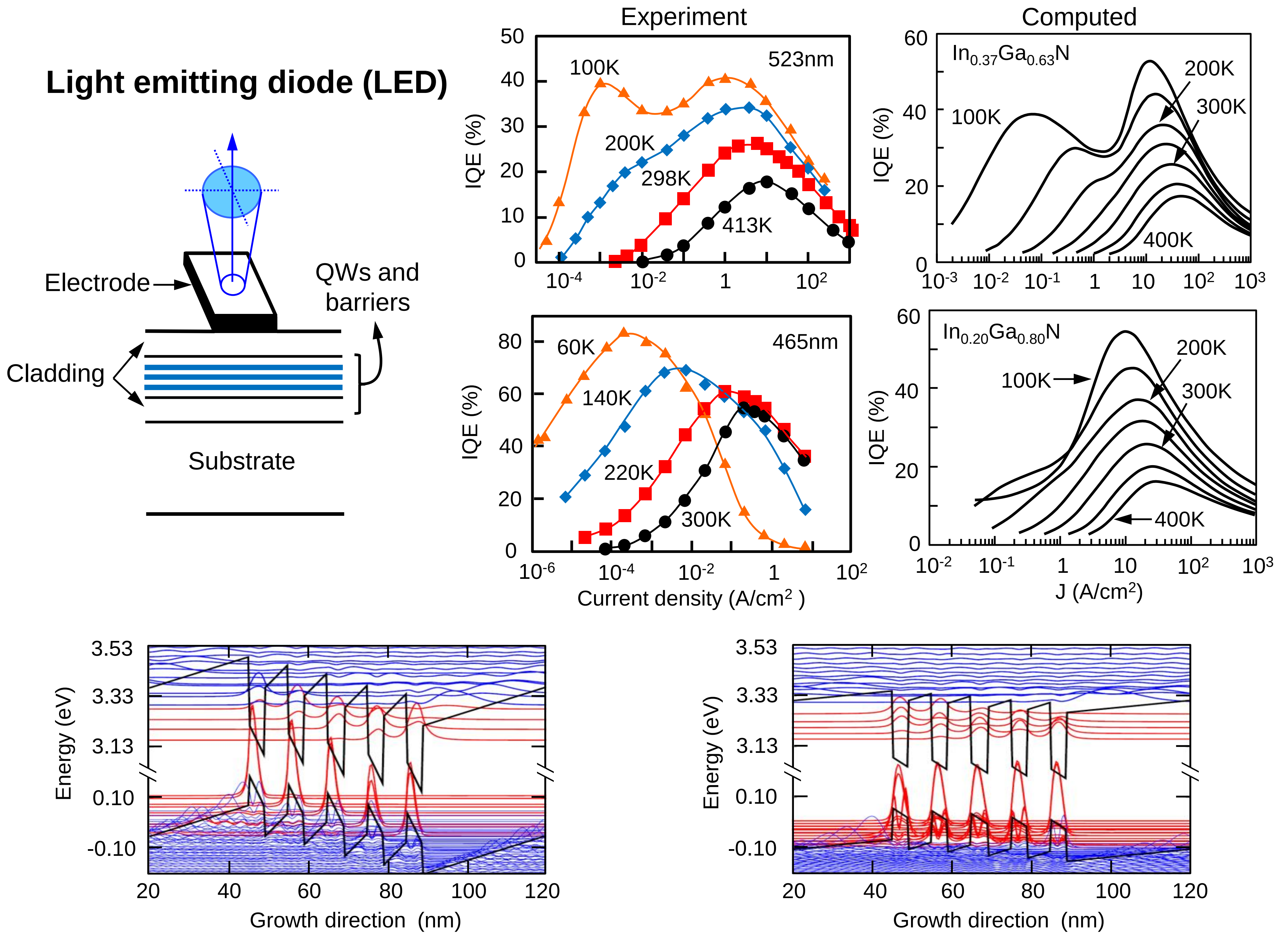
Tradeoff between available gain and required current in a quantum dot gain medium (InAs)





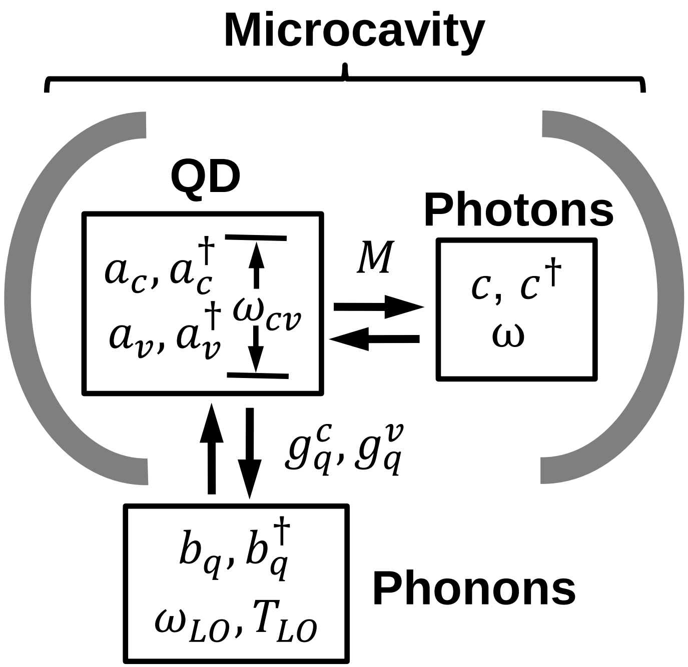


Curves show present status in relation to eventual performance and give guidance on where improvement can be effectively made

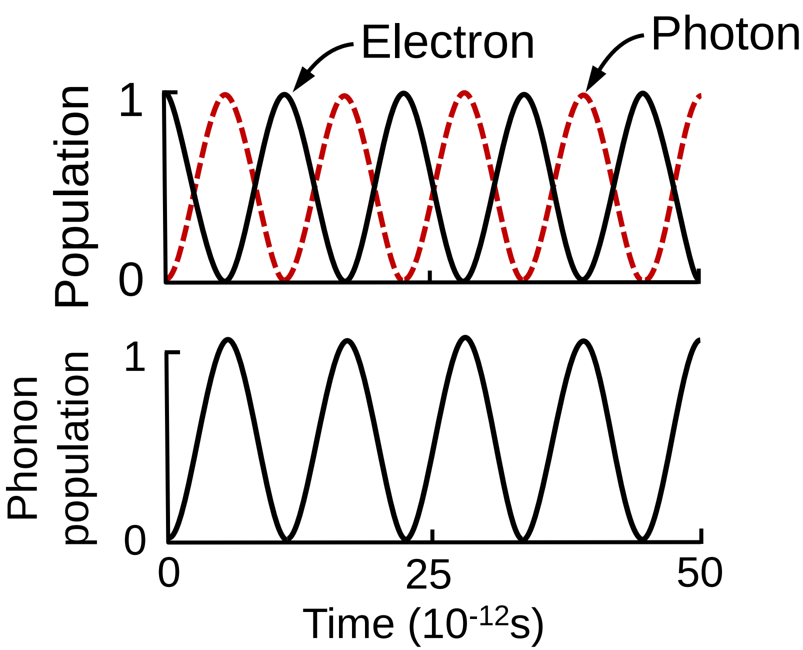


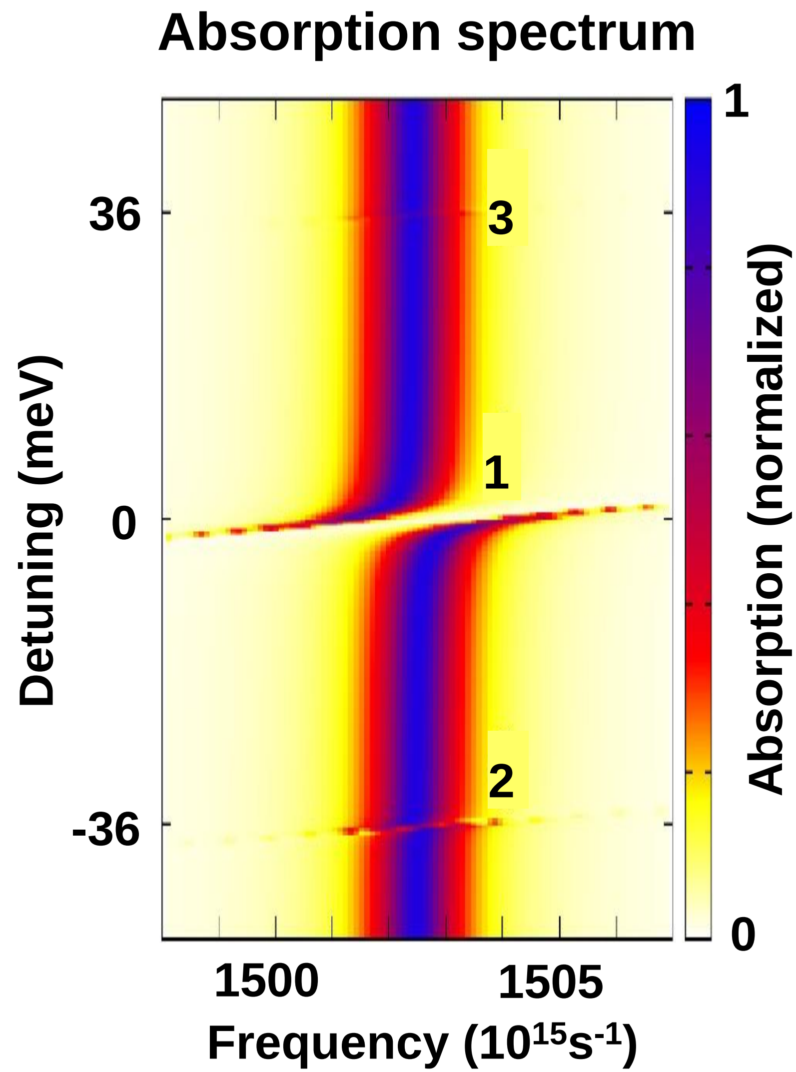
Light emitting diode (LED)
Electrode
QWs and barriers
Cladding
Substrate
Experiment
Computed
523nm
465nm
100K
200K
298K
413K
60K
140K
220K
300K
IQE (%)
Current density (A/cm^2)
$In_{0.37}Ga_{0.63}N$
$In_{0.20}Ga_{0.80}N$
400K
J (A/cm^2)
Energy (eV)
Growth direction (nm)

LO-phonon-assisted Rabi oscillations



Stokes

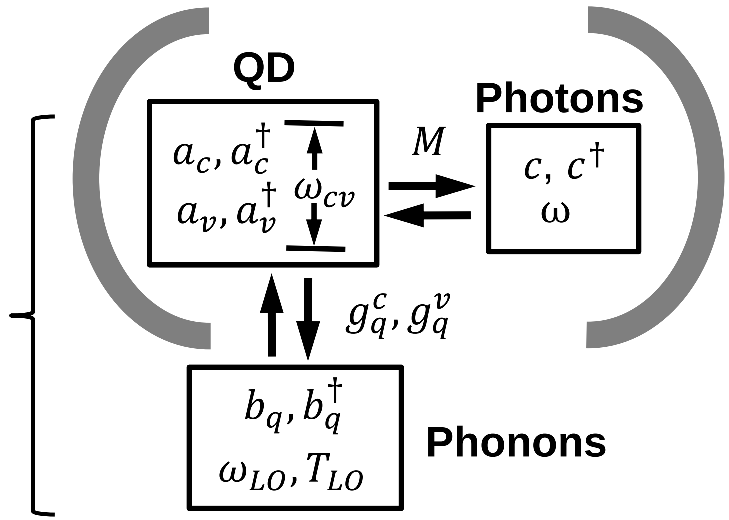


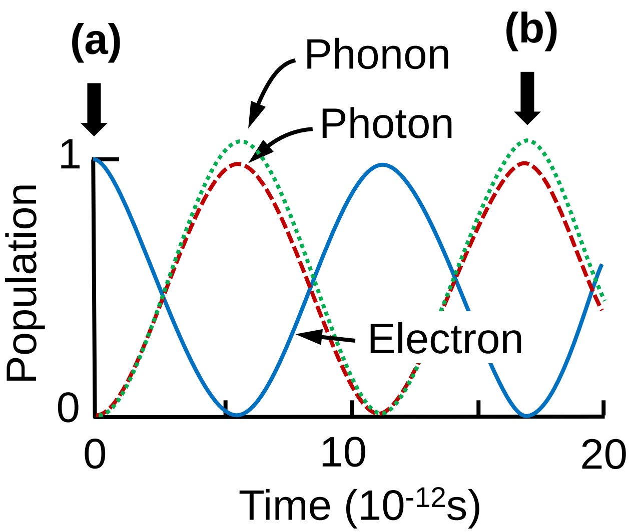


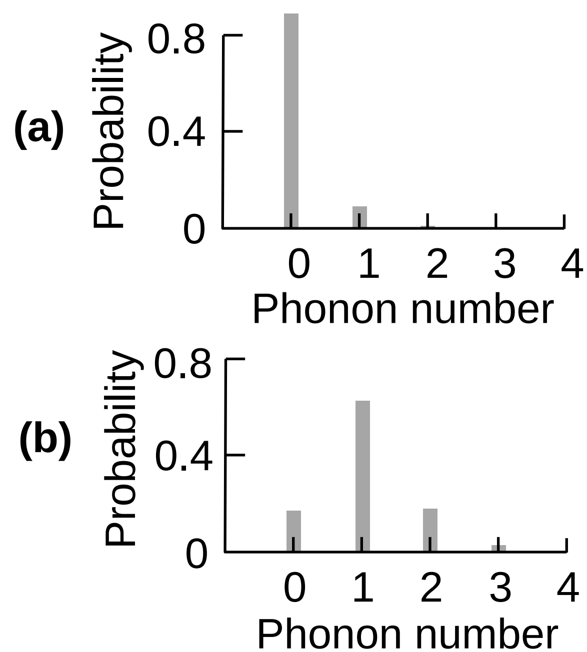
Carmele, Kabuss and Chow, PRB 87, 041305 (R), 2013

Semiconductor QD-microcavity-phonon-bath system

System-bath interaction
-- Beyond 2nd Born
-- With memory effects
-- Tracks phonon statistics







Self-cooled single-photon source?

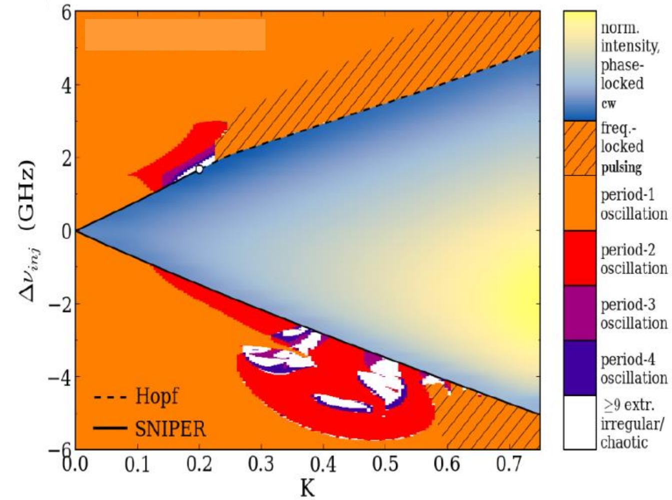
Off-shoots of microscopic optoelectronic model

1) Nonlinear dynamics: Developing new tools for bifurcation analysis

$$\frac{dE}{dt}, \frac{dN}{dt}$$ ⬅ *Present*

$$\left.\begin{array}{c}\dfrac{dn_{\sigma k}}{dt}, \dfrac{dn_{\sigma k_\perp}}{dt}, \dfrac{dn_{e\alpha_n}}{dt} \\ \dfrac{dp_{\alpha_n\beta_n}}{dt}, \dfrac{dE}{dt}\end{array}\right]$$ ⬅ *Would like*

Lingnau, Ludge, Chow, Scholl Phys. Rev. E **86**, 065201 (R), 2012



2) Modeling BEC devices – battery, transistor, oscillator, etc. (with Dana Anderson)

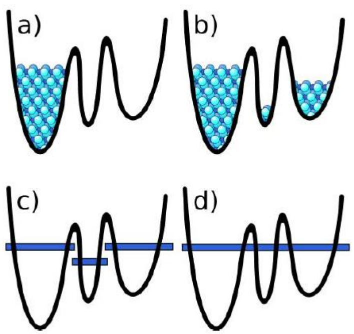


FIG. 1. (Color online) The geometry of a BEC transistor. When the number of atoms in the middle well is small, tunneling from the left into the right well is negligible (a). This is due to the fact that the chemical potential of the middle well does not match that of the two other wells (c). Placing atoms in the middle well increases the chemical potential due to interatomic interactions (d) and enables tunneling then atoms tunnel from the left into the right well. This happens because atom-atom interactions increase the energy of the middle guide (b).

$$\int d^3r \int d^3r' \underbrace{\hat{\psi}^\dagger(r')\hat{\psi}^\dagger(r)} \underbrace{\frac{e^2}{4\pi\varepsilon_b|r-r'|}} \hat{\psi}(r)\hat{\psi}(r)$$

Antisymmetry ➞ symmetric

$$\{c_k, c_{k'}^\dagger\} \rightarrow [a_i, a_j^\dagger]$$

$$\frac{2\pi\hbar^2 a_{sc}}{M}$$

Stickney, Anderson and Zozulya, Phys. Rev. A **75**, 013608, 2007