

The Mathematics of Lasers from Nonlinear Eigenproblems to Linear Noise



Steven G. Johnson MIT Applied Mathematics



Adi Pick (Harvard), David Liu (MIT),

Sofi Esterhazy, M. Liertzer, K. Makris, M. Melenck, S. Rotter (Vienna), Alexander Cerjan & A. Doug Stone (Yale), Li Ge (CUNY), Yidong Chong (NTU)

What is a laser?

- a laser is a resonant cavity...
- with a gain medium...
- pumped by external power source
 population inversion → stimulated emission



mirrors/confinement

Resonance





How Resonance? need mechanism to trap light for long time



[llnl.gov]



metallic cavities: good for microwave, dissipative for infrared



photonic bandgaps (complete or partial + index-guiding)



[Xu & Lipson (2005)]

ring/disc/sphere resonators:
a waveguide bent in circle,
bending loss ~ exp(-radius)

[Akahane, Nature 425, 944 (2003)]



(planar Si slab)



Pump \Rightarrow Gain: nonlinear in field strength













The steady state Gain pump = 0.7Mode intensity Loss

goals of laser theory: for a given laser, determine:

1) thresholds
 2) field emission patterns
 3) output intensity
 4) frequencies

of steady-state operation

[if there is a steady state]

What's new in SALT? Why ab initio?



Lamb

Scully

Haken

mel for

Basic semiclassical theory from early 60's and much of quantum theory

No general method for accurate solution of the equations for arbitrary resonator including non-linearity, openness, multi-mode

Direct numerical solutions in space and time impractical

SALT: direct solution for the multimode steady-state including openness, gain saturation and spatial hole-burning, arbitrary geometry

Ab Initio: Only inputs are constants describing the gain medium, quantitative agreement with brute force simulations

Motivation: Modern micro/nano lasers Complex microcavities: micro-disks,micro-toroids, deformed disks (ARCs), PC defect mode, random...



Semiclassical theory

1. Maxwell's equations (classical) $-\nabla \times \nabla \times (\mathbf{E}^+) - \varepsilon_c \ddot{\mathbf{E}}^+ = \frac{1}{\varepsilon_0} \ddot{\mathbf{P}}^+$

cavity dielectric

polarization of gain atoms





 γ_{\perp} and γ_{\parallel} phenomenological relaxation rates (from collisions, etc)

Maxwell–Bloch equations

• fully time-dependent, multiple unknown fields, nonlinear (Haken, Lamb, 1963)

$$-\nabla \times \nabla \times (\mathbf{E}^{+}) - \varepsilon_{c} \ddot{\mathbf{E}}^{+} = \frac{1}{\varepsilon_{0}} \ddot{\mathbf{P}}^{+}$$
Polarization
induces inversion
$$\dot{\mathbf{P}}^{+} = (-i\omega_{a} - \gamma_{\perp})\mathbf{P}^{+} + \frac{1}{i\hbar}\mathbf{E}^{+}D$$
$$\overset{\text{Polarization}}{\longrightarrow}$$
$$\dot{D} = \gamma_{\parallel}(D_{0} - D) - \frac{2}{i\hbar}[\mathbf{E}^{+} \cdot (\mathbf{P}^{+})^{*} - \mathbf{P}^{+} \cdot (\mathbf{E}^{+})^{*}]$$

Maxwell–Bloch FDTD simulations very expensive but doable



Bermel et. al. (PRB 2006)

Problem: timescales!

 $\gamma_{\parallel} \ll \gamma_{\perp} \ll \omega_a$

FDTD takes very long time to converge to steady state

Solving Maxwell–Bloch for just one set of lasing parameters is expensive and slow, let alone design

Advantage: timescales!

$$\frac{\gamma_{\parallel}}{\gamma_{\perp}} \ll 1, \ \frac{\gamma_{\perp}}{\omega_a} \ll 1$$

- hard for numerics
- good for analysis

Ansatz of steady-state modes



Two key approximations

$$\frac{\gamma_{\parallel}}{\gamma_{\perp}} \ll 1, \ \frac{\gamma_{\perp}}{\omega_a} \ll 1$$

1. "rotating-wave approximation" fast oscillation average out to zero; all oscillations fast compared to inversion

$$\dot{D} = \gamma_{\parallel}(D_0 - D) - rac{2}{i\hbar} [\mathbf{E}^+ \cdot (\mathbf{P}^+)^* - \mathbf{P}^+ \cdot (\mathbf{E}^+)^*]$$

... leads to...

$\dot{D} \approx 0$

2. stationary-inversion approximation

$$\begin{aligned} \mathbf{before} & & = \mathbf{f}_{c} \mathbf{E}^{+} = \frac{1}{\varepsilon_{0}} \mathbf{P}^{+} \\ \dot{\mathbf{P}}^{+} = (-i\omega_{a} - \gamma_{\perp})\mathbf{P}^{+} + \frac{g^{2}}{i\hbar} \mathbf{E}^{+} D \\ \dot{D} = \gamma_{\parallel}(D_{0} - D) - \frac{2}{i\hbar} [\mathbf{E}^{+} \cdot (\mathbf{P}^{+})^{*} - \mathbf{P}^{+} \cdot (\mathbf{E}^{+})^{*}] \end{aligned}$$

$$\begin{aligned} \mathbf{after:} \\ \mathbf{Steady-State Ab-Initio} \\ \mathbf{Lasing Theory,} \\ \mathbf{SALT''} \\ (Tureci, Stone, 2006) \\ \nabla \times \nabla \times \mathbf{E}_{m} = \boldsymbol{\omega}_{m}^{2} \boldsymbol{\varepsilon}_{m} \mathbf{E}_{m} \\ \nabla \times \nabla \times \mathbf{E}_{m} = \boldsymbol{\omega}_{m}^{2} \boldsymbol{\varepsilon}_{m} \mathbf{E}_{m} \\ \varepsilon_{m}(\mathbf{x}) = \varepsilon_{c}(\mathbf{x}) + \frac{\gamma_{\perp}}{\omega_{m} - \omega_{a} + i\gamma_{\perp}} \left[\frac{D_{0}(\mathbf{x})}{1 + \sum \left| \frac{\gamma_{\perp}}{\omega_{\nu} - \omega_{a} + i\gamma_{\perp}} \mathbf{E}_{\nu} \right|^{2}} \right] \end{aligned}$$

Still nontrivial to solve: equation is nonlinear in both

eigenvalue $\omega_m \leftarrow$ easier

eigenvector \mathbf{E}_m \leftarrow harder

Constant-flux "CF" basis method

Tureci, Stone, PRA 2006 (same paper that introduced SALT)

$$\mathbf{E}_m(\mathbf{x}) = \sum_{n=1}^N c_{mn} \mathbf{F}_n(\mathbf{x})$$

solutions to *linear* problem at threshold

$$\mathbb{T}(\omega_m, c_{mn})c_{mn} = 0$$

problem still nonlinear, but very small dimensionality

Example of SALT results using CF hasis method



Ge et al. (PRA 2010)

CF basis method not scalable

- 1. far above threshold, expansion efficiency decreases, need more basis functions
- 2. in most cases basis functions need to be obtained numerically
- 3. storage in 2d and 3d

Common pattern for theories in physics

- 1. purely analytic solutions (handful of cases)
- 2. specialized basis (problem-dependent and hard to scale to arbitrary systems)
- 3. generic grid/mesh, discretize

SALT was here

Can we solve the equations of SALT (which are nonlinear) on a grid **without an intermediate basis?**

Finite-difference discretization

$$\nabla \times \nabla \times \mathbf{E}_m = \omega_m^2 \varepsilon_m(\omega_m, \{\mathbf{E}_\nu\}) \mathbf{E}_m$$



degrees of freedom:

 \mathbf{E}_m at every point on (Yee) grid $m = 1, 2, \dots \#$ modes

 $\nabla \times \nabla \times \rightarrow$ finite differences

 \rightarrow "just" solve

... but is it reasonable to solve 10⁴–10⁷ coupled nonlinear equations?

Yes! Newton: $\mathbf{f}(\mathbf{v}) = 0$ $\mathbf{v}_{guess} \rightarrow \mathbf{v}_{guess} - \left(\frac{\partial \mathbf{f}}{\partial \mathbf{v}}\right)^{-1} \mathbf{f}$ $\mathbf{v} = \begin{pmatrix} \mathbf{E}_m \\ \omega_m \end{pmatrix}, \ \mathbf{f} = \begin{pmatrix} \begin{bmatrix} -\nabla \times \nabla \times + \omega_m^2 \varepsilon_m \end{bmatrix} \mathbf{E}_m \\ \mathbf{E}_m(\mathbf{x}_0) \end{pmatrix}$

key fact #1:

Newton's method converges very quickly when we have a good initial guess (near the actual answer)

key fact # 2: we *have* a good initial guess (at threshold, the problem is linear in \mathbb{E}_m , easy to solve) The linear problem is sparse!

$$\frac{\partial \mathbf{f}}{\partial \mathbf{v}} = \text{Jacobian } \dots \text{ sparse}$$
$$\frac{\partial \mathbf{f}}{\partial \mathbf{v}} \delta \mathbf{v} \approx -\mathbf{f}(\mathbf{v}_{\text{guess}})$$
$$Ax = b$$

A sparse = good solvers ex: Matlab "\", PETSc

$$\mathbf{f}(\mathbf{v}) = 0$$

must have same number of equations as unknowns

1. frequency ω_m is unknown, and

2. amplitude as separate unknown(to eliminate the trivial E=0 solution)

 $\mathbf{E}_m(\mathbf{x}) = a_m \mathbf{E}_m^{\mathrm{normalized}}(\mathbf{x})$

$$\mathbf{f}(\mathbf{v}) = 0$$

must have same number of equations as unknowns

1. frequency ω_m is unknown, and

2. amplitude as separate unknown(to eliminate the trivial E=0 solution)

 $\mathbf{E}_m(\mathbf{x}) = a_m \mathbf{E}_m^{\mathrm{normalized}}(\mathbf{x})$

two extra unknowns, two extra equations, Jacobian matrix stays square

normalization and phase fixing (real and imaginary parts give two equations)

 $\hat{\mathbf{n}} \cdot \mathbf{E}_m^{\text{normalized}}(\mathbf{x}_0) = 1$



Newton converges quadratically given good initial guess

Benchmark comparison with previous 1d results



Confirmation of known 2d results



field profile of mode 1



Demonstration of 3d calculation



Pump parameter d

Lasers: Quick Review

laser = lossy optical resonance + nonlinear gain



Lasers: Quick Review

laser = lossy optical resonance + nonlinear gain

toy TCMT model of single-mode laser:



Laser noise:



random (quantum/thermal) currents "kick" the laser mode

⇒ Brownian phase drift = finite linewidth

Johnson–Nyquist Noise [1926]

(no relation to me)

random current I from thermal noise:

$$I \rightarrow -$$

mean $\langle I^2 \rangle \approx 4kT \times (1/R) \times (bandwidth)$

Generalization: the Fluctuation–Dissipation Theorem

$$\left\langle J_{i}(\omega, \mathbf{x}) J_{j}^{*}(\omega, \mathbf{x}') \right\rangle \xrightarrow{\text{ZP + Bose-Einstein}}_{= \omega \text{Im } \varepsilon} \underbrace{\frac{\text{conductivity}}{\text{Im } \varepsilon}}_{= \omega \text{Im } \varepsilon} \\ = \frac{1}{\pi} \delta_{ij} \delta(\mathbf{x} - \mathbf{x}') \left[\frac{\hbar \omega}{2} \coth\left(\frac{\hbar \omega}{2kT}\right) \right] \overbrace{\sigma(\omega, \mathbf{x})}^{\text{conductivity}}$$

→ kT for high T (classical thermal fluctuations) → $\hbar\omega/2$ for low T (quantum zero-point fluctuations)

[Callen & Welton, 1951]

Consequences of current fluctuations



Fluctuating currents **J** produce fluctuating electromagnetic fields.

Fields carry:

- Momentum ⇒ Casimir forces
- Energy \Rightarrow thermal radiation

In a laser: $\mathbf{J} =$ random forcing

- = phase drift
- = nonzero laser linewidth

Toy TCMT Laser + Noise

[= nonlinear "van der Pol" oscillator, similar to e.g. Lax (1967)]

lowest-order stochastic ODE:



Laser linewidth theory: Long history

Long history of laser-linewidth theory:

- Gordon ('55), Schawlow–Townes ('58): linewidth ~ 1/P
- Petermann ('79): correction for lossy cavities (complex **E**)
- Henry ('82, '86): nonlinear phase/amplitude coupling enhancement
- Elsasser ('85), Kruger ('90): 2-mode nonlinear linewidth interactions
- generalizations: dispersion, incomplete inversion, nonuniform...

Almost always in 1d, only considering a few corrections at a time... (e.g. dispersion but not Henry, only homogeneous inversion...)

• Chong (2013): S-matrix combination of many previous corrections (but not Henry factor or inhomogeneous inversion) ... showed that corrections are intermingled in general cavities

Can we solve the full 3d inhomogeneous problem?

Laser theory troubles:

Until recently, it's been almost impossible to solve for laser modes > threshold in complex microcavities (not 1d-like).

difficulty: optical timescale << electron relaxation timescale

Why bother with linewidth theory if we can't solve *without* noise?

SALT: steady-state ab-initio lasing theory = analytical separation of optical/electronic timescales [Türeci, Stone, and Collier (2006)]

SALT: "ordinary" EM eigenproblem for lasing modes

$$\nabla \times \nabla \times \mathbf{E}_m = \boldsymbol{\omega}_m^2 \boldsymbol{\varepsilon}_m \mathbf{E}_m$$

with nonlinear permittivity ε :

$$\varepsilon_m = \varepsilon_c(\mathbf{x}) + \frac{\gamma_0}{\omega_m - \omega_0 + i\gamma_0} \frac{D_0(\mathbf{x}, d)}{1 + \sum_n \left| a_n \frac{\gamma_0}{\omega_n - \omega_0 + i\gamma_0} \mathbf{E}_n \right|^2}$$

(Lorentzian gain spectrum, mode amplitudes a_n)

Limitation: until recently, SALT only solvable in 1d & simple 2d

New SALT Solvers

= accurate laser modes in new geometries

[Esterhazy, Liu, Liertzer, Cerjan, Ge, Makris, Stone, Melenk, Johnson, Rotter, arXiv:1312.2488 (2013)]



Ab-initio laser-linewidth starting point

The Fluctuation–Dissipation Theorem (FDT)

 $\left\langle J_{i}(\omega, \mathbf{x}) J_{j}^{*}(\omega, \mathbf{x}') \right\rangle \qquad [Callen \& Welton, 1951]$ $= \frac{1}{\pi} \delta_{ij} \delta(\mathbf{x} - \mathbf{x}') \left[\frac{\hbar \omega}{2} \coth\left(\frac{\hbar \omega}{2kT}\right) \right] \overset{\text{conductivity} = \omega \operatorname{Im} \varepsilon}{\sigma(\omega, \mathbf{x})}$

In a gain medium, $\sigma < 0$ and $T \le 0^-$ ($T < 0^-$ = incomplete inversion)

... these small currents randomly "kick" the SALT lasing modes \Rightarrow random (Brownian) phase drift \Rightarrow linewidth

[related starting point, albeit in greatly simplified 1d media, used by Henry (1986)]

Real TCMT equations

[2-level gain medium, timescale >> optical]

Maxwell-Bloch equations:

$$\nabla \times \nabla \times \mathbf{E} + \epsilon_c \, \ddot{\mathbf{E}} = -\ddot{\mathbf{P}} + \mathbf{F} \qquad \text{electric field} \\ \dot{\mathbf{P}} = -i(\omega_a - i\gamma_{\perp})\mathbf{P} - i\gamma_{\perp}\mathbf{E}D \qquad \text{polarization density} \\ \dot{D} = -\gamma_{\parallel} \left(D_p - D + \frac{i}{2} (\mathbf{E} \cdot \mathbf{P}^* - \mathbf{E}^* \cdot \mathbf{P}) \right) \qquad \text{inversion population}$$

+ rotating-wave approx. (lasing modes dominate) ... lots of algebra ...

$$\dot{a}_{\mu} = \sum_{\nu} \left[\int dx \, c_{\mu\nu}(x) \, \gamma(x) \int_{-\infty}^{t} dt' e^{-\gamma(x)(t-t')} \left(a_{\nu0}^{2} - |a_{\nu}(t')|^{2} \right) \right] a_{\mu} + f_{\mu}$$

= non-instantaneous, multi-mode nonlinear gain

TCMT coefficients

[2-level gain medium, timescale >> optical]

$$\dot{a}_{\mu} = \sum_{\nu} \left[\int dx \, c_{\mu\nu}(x) \, \gamma(x) \int_{-\infty}^{t} dt' e^{-\gamma(x)(t-t')} \left(a_{\nu 0}^{2} - |a_{\nu}(t')|^{2} \right) \right] a_{\mu} + f_{\mu}$$

$$c_{\mu\nu} = \frac{-i\omega_{\mu}^{2} \frac{\partial \epsilon(\omega_{\mu})}{\partial |a_{\nu}|^{2}} E_{\mu}^{2}}{\int dx \frac{\partial}{\partial \omega} (\omega^{2} \epsilon) E_{\mu}^{2}}$$

(essentially = 1^{st} order perturbation theory for $\partial \omega / \partial |a|^2$)

currents = forcing
$$\mathbf{F} = d\mathbf{J}/dt \Rightarrow f_{\mu} = \frac{i\int dx E_{\mu}F_{\mu}}{\int dx \frac{\partial}{\partial\omega}(\omega^2 \epsilon)E^2}$$

New 1-mode Linewidth Γ Formula

correct TCMT \Rightarrow plug in FDT $\Rightarrow \langle f^2 \rangle \Rightarrow$ solve stochastic ODEs...

 $\Gamma = \frac{\hbar\omega_{0}}{P} \cdot \frac{\omega_{0}^{2} \iint dx dx' \left(\epsilon''(x)|\mathbf{E}_{0}(x)|^{2}\right) \left(\epsilon''(x')|\mathbf{E}_{0}(x')|^{2}\right) \coth\left(\frac{\hbar\omega_{0}\beta(x)}{2}\right)}{\left|\int dx \mathbf{E}_{0}^{2} \left(\epsilon + \frac{\omega_{0}}{2} \frac{\partial\epsilon}{\partial\omega_{0}}\right)\right|^{2}} \cdot (1 + \tilde{\alpha}^{2})$ generalizedHenry α -factor

Schawlow–Townes inverse scaling with radiated power P_1

~ generalized Petermann factor (including "bad cavity" correction for dispersion), including incomplete inversion

New predictions:

• Fun fact: "toy" instantaneous nonlinearity gives same Γ !

- Correction from inhomogeneous incomplete inversion (... in general, all corrections are intermingled ...)
- "Bad-cavity" (high-leakage) correction to Henry α factor



• Closed-form generalization to arbitrary multimode lasers

in progress...

- Validation against solution of full Maxwell–Bloch equations + thermodynamic noise (in 1d) — A. Cerjan (Yale)
- Design a laser (e.g. with "exceptional points") where new corrections are much larger
- Additional corrections

[e.g. amplified spontaneous emission (ASE) for "passive" modes just below their lasing thresholds; also "colored" noise correction for broad linewidth)

• New SALT models (e.g. semiconductor lasers...) ⇒ new linewidth formulas



Thanks!

Adi Pick (Harvard)



David Liu (MIT)





Stefan Rotter (Vienna Univ. Tech.)



& Sofi Esterhazy, M. Liertzer, K. Makris, M. Melenck





Douglas & Dr. Alex Cerjan (Yale)



Li Ge (CUNY)



Prof. Yidong Chong (NTU)