

## The Mathematics of Lasers



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



*1d laser:* light bouncing between 2 mirrors

mirrors/confinement

### Resonance

an oscillating mode trapped for a long time in some volume (of light, sound, ...) lifetime  $\tau >> 2\pi/\omega_0$ frequency  $\omega_0$  quality factor  $Q = \omega_0 \tau/2$ energy ~  $e^{-\omega_0 t/Q}$  volume V



### Resonance, Really: Lossless

scalar wave equation

scalar Helmholtz equation

$$\begin{bmatrix} \nabla^2 - \varepsilon * \frac{\partial^2}{\partial t^2} \end{bmatrix} u = \text{sources} \xrightarrow{\text{Fourier}} \begin{bmatrix} \nabla^2 + \varepsilon(\mathbf{x}, \omega) \omega^2 \end{bmatrix} u = s(\mathbf{x}, \omega)$$
  
time-harmonic  
 $u \sim e^{-i\omega t}$   
Maxwell "permittivity"  $\varepsilon$ 





## Resonance, Really: Lossy



outgoing radiation boundary condition [ = limiting-absorption principle:  $\varepsilon + i0^+$ ]

> Im  $\omega$ (G analytic for Im  $\omega > 0$ ) Re  $\omega$   $\times \times \times \times \times \times \times$ resonances = poles in Green's function below (*close to*) real axis

## Resonance, Really: "Leaky Modes"



 $Q = 2\gamma_0 / \omega_0$ 

## Linear Gain

#### stimulated emission [wikipedia]



gain created by pumping electrons to population inversion: = more electrons in excited state

 $N_1$  = ground state pop.  $N_2$  = excited state pop. inversion:  $D = N_2 - N_1 > 0$ 

$$u \sim e^{-i\omega t} \quad \left[\nabla^2 + \varepsilon \omega^2\right] u = s(\mathbf{x}, \omega)$$

gain (exponential *growth* in time): Im  $\varepsilon < 0$  (for  $\omega > 0$ ) Im  $\varepsilon \sim -D$ 

## Nonlinear Gain: Cannot grow forever!

$$u \sim e^{-i\omega t} \quad \left[\nabla^2 + \varepsilon \omega^2\right] u = s(\mathbf{x}, \omega)$$

gain (exponential *growth* in time): Im  $\varepsilon < 0$  (for  $\omega > 0$ )

Im  $\varepsilon \sim -D$ 

gain created by pumping electrons to population inversion: = many electrons in excited state

 $N_1$  = ground state pop.  $N_2$  = excited state pop.  $D = N_2 - N_1 > 0$ 

*u* (electric field) grows exponentially in time... but eventually, the stimulated emission *depletes* the excited states  $\Rightarrow D$  decreases with  $u ~ (1/|u|^2) ...$  "hole burning"

## Passive cavity (linear loss)



### Pump $\Rightarrow$ Gain: nonlinear in field strength





### The steady state



Loss

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

- thresholds
- field emission patterns
- output intensity
- frequencies

of steady-state operation

[ if there is a steady state ...not true if other resonances too close ]

### What's new in laser theory

slide: D. Stone



Lamb

Scully

Haken

mel for

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

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

Direct numerical solutions in space and time impractical in 3d, hard in 2d

SALT [Tureci, Stone (2006)]: steady-state ab-initio lasing theory

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

Only inputs are the gain medium ... quantitative agreement with brute-force

### Motivation: Modern micro/nano lasers <sup>slide:</sup> D. Stone **Complex microcavities: micro-disks,micro-toroids, deformed disks (ARCs), PC defect mode, random...**

(b)



Wavelength (nm)

Gain and scattering

## Semiclassical theory

1. Maxwell equations (classical)  $-\nabla \times \nabla \times (\mathbf{E}^+) - \varepsilon_c \ddot{\mathbf{E}}^+ = \frac{1}{\varepsilon_0} \ddot{\mathbf{P}}^+$  electric field  $E^+ \sim e^{-i\omega t}$  $E = \operatorname{Re} E^+$ 

cavity dielectric

polarization of gain atoms



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

cavity dielectric

polarization of twolevel gain atoms

2. Damped oscillations of electrons in atoms (quantum)

polarization:  $\dot{\mathbf{P}}^+ = (-i\omega_a - \gamma_\perp)\mathbf{P}^+ + \frac{1}{i\hbar}\mathbf{E}^+D$ 

atomic frequency

population inversion (drives oscillation)





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

brute-force Maxwell–Bloch FDTD (finite-difference time-domain) 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 ... supercomputer-scale in 3d ... and systematic design is impractical

### Advantage: timescales!

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

- hard for numerics
- good for analysis

### Ansatz of *M* steady-state modes

$$\mathbf{E}^{+} = \sum_{m=1}^{M} \mathbf{E}_{m}(\mathbf{x})e^{-i\omega_{m}t}$$
$$\mathbf{P}^{+} = \sum_{m=1}^{M} \mathbf{P}_{m}(\mathbf{x})e^{-i\omega_{m}t}$$

...validity checked a posteriori

## Stationary-inversion approximation

key assumption:

 $\gamma_{\perp}, \Delta \omega >> \gamma_{\parallel}$ 

valid for  $< 100 \mu$ m microlasers

"rotating-wave approximation"
 fast oscillations average out to zero
 ... all oscillations are fast compared to γ<sub>||</sub>

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

... leads to:

# $\dot{D} \approx 0$

### stationary-inversion approximation SIE

[ neglecting terms ~ fast rates /  $\gamma_{\parallel}$  ]

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

$$\begin{array}{l} \mathbf{before} \\ \mathbf{before} \\$$

Still nontrivial to solve: equation is nonlinear in both

eigenvalue  $\omega_m \leftarrow$  easier

eigenvector  $\mathbf{E}_m \leftarrow$  harder

## first way to solve SALT: 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

### Comparison of SALT and Maxwell-Bloch: intensities <sup>D. Stone</sup>

slide:



### "Realistic" application to novel lasers

slide: D. Stone

Chua, Chong, ADS, Soljacic, Bravo-Abad, Opt. Express 2010



"Strong interactions in multimode random lasers", H. Tureci, L. Ge, S. Rotter, ADS; Science, 320,643 (2008) – random lasing is "conventional"

**2D Random Lasers** 



### 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. huge basis = huge storage, time in 2d and 3d

# Common pattern for theoretical models

- 1. purely analytical solutions (handful of cases)
- 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 (FDFD) $\nabla \times \nabla \times \mathbf{E}_m = \omega_m^2 \varepsilon_m(\omega_m, \{\mathbf{E}_\nu\}) \mathbf{E}_m$



degrees of freedom:

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

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

### →"just" solve

... but is it reasonable to solve 10<sup>4</sup>–10<sup>7</sup> coupled nonlinear equations?

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  $\mathbf{E}_m$ , easy to solve)

### (omitted details)

... sparse solvers for Newton steps ... eliminating spurious  $E_m=0$  solutions

... linear solvers for passive modes (Im  $\omega$  < 0 poles) ... watch for thresholds of additional modes ... *a posteriori* stability check

### Benchmark comparison with previous 1d results



~5 CPU minutes

... much easier to optimize simple FDFD code!

### Mode-switching lasers in 2d

mode-switching behavior in microdisk laser (solid = Newton, dotted = Bessel basis) 4 mode 1 3  $\ell = 8$ mode 2 $\ell = 7$  $\mathbf{2}$ 1 0.10 0.150.200.25Pump parameter d

Internal intensity of  $\Psi$ 

field profile of mode 1





## From Newton to Anderson

[Wonseok Shin et al, manuscript in preparation (2018)]

Problem: Newton's method requires you to rip your existing optimized Maxwell solver to shreds and re-assemble it into the SALT Jacobian matrix

> ... IEl<sup>2</sup> terms mean you need to write in terms of real matrices of real/imaginary parts

Solution: combine an existing ω-domain *linear* Ax=b (Maxwell/Helmholtz) solver with Anderson acceleration (1965) of a carefully chosen fixed-point equation f(x) = x [Walker & Ni (2011): essentially ~ GMRES Newton] = black-box linear solver + derivative-free updates for the nonlinearity ~ 2–3x more iterations than Newton (10–30 vs. 5–10).

### Full 3d calculation

full-vector simulation of 1.5lasing defect mode in photonic crystal slab Internal intensity of Ψ z1.0y~ 50 x 50 x 30 pixel xcomputational cell: 10 CPU minutes on a laptop 0.5with SALT + Newton's method

0.0

0.05

0.10

Pump parameter d

0.15

### Today's menu

- Laser basics
- The SALT nonlinear eigenproblem
- Noise, linear-response theory, & linewidths

## Lasers: Quick Review

laser = lossy optical resonance + nonlinear gain



## Lasers: Quick Review

laser = lossy optical resonance + nonlinear gain

toy "van der Pol" oscillator model of single-mode laser [e.g. Lax (1967)]:



### Laser noise:



random (quantum/thermal) currents "kick" the laser mode ⇒ Brownian phase drift = finite linewidth

## Microscopic current fluctuations



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

Fields carry:

- Momentum ⇒ Casimir forces
- Energy  $\Rightarrow$  thermal radiation

In a laser: J = random forcing = phase drift

= nonzero laser linewidth

## Toy Laser + Noise

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

lowest-order stochastic ODE:

$$\frac{da_{1}}{dt} \approx C_{11} \left( \left| a_{1}^{0} \right|^{2} - \left| a_{1} \right|^{2} \right) a_{1} + f_{1}(t) \qquad \text{tricky part: getting } f \& C$$
random
forcing
$$\limearize:$$

$$a_{1} = \left[ a_{1}^{0} + \delta_{1}(t) \right] e^{i\varphi_{1}(t)}$$

$$\Rightarrow \dots \Rightarrow \langle \varphi^{2} \rangle = Rt$$
Brownian (Wiener) phase
$$\overset{\delta \text{ fluctuations } \Rightarrow}{\omega_{1}}$$

### Linewidth formulas: a long history

$$\begin{split} \Gamma &= \frac{\hbar\omega_0\gamma_c^2}{2P} \cdot \frac{N_2}{N_2 - N_1} \cdot \left| \frac{\int_{\mathbf{C}} dx |\mathbf{E}_{\mathbf{c}}|^2}{\int_{\mathbf{C}} dx \mathbf{E}_{\mathbf{c}}^2} \right|^2 \cdot \left( \frac{\gamma_{\perp}}{\gamma_{\perp} + \frac{\gamma_c}{2}} \right)^2 \left( 1 + \alpha^2 \right) \\ & \mathbf{ST} \qquad \mathbf{I} \qquad \mathbf{P} \qquad \mathbf{B} \qquad \mathbf{\alpha} \end{split}$$

- Schawlow-Townes ('58) inverse power 1/P scaling
- Incomplete inversion ('67) due to partial inversion
- Petermann ('79) enhancement for lossy cavities
- **Bad-cavity** ('67) reduction due to dispersion
- $\circ$  **\alpha**-factor ('82) coupling of intensity/phase fluctuations

... all make approximations invalid for  $\mu$ -scale lasers...



chaotic cavity



photonic crystal



random laser

### Starting point:

### Maxwell–Bloch

electric field 
$$\nabla \times \nabla \times \mathbf{E} - \frac{\varepsilon_c}{c^2} \ddot{\mathbf{E}} = \frac{4\pi}{c^2} \left[ \ddot{\mathbf{P}}^+ + (\ddot{\mathbf{P}}^+)^* \right]$$
  
gain  $\dot{\mathbf{P}}^+ = -(i\omega_a + \gamma_\perp)\mathbf{P}^+ + \frac{g^2}{i\hbar}\mathbf{E}D$   
population  $\dot{D} = \gamma_{\parallel}(D_0 - D) - \frac{2}{i\hbar}\mathbf{E} \cdot \left[ (\mathbf{P}^*)^+ - \mathbf{P}^+ \right]$ 

[Arecchi & Bonifacio, 1965]

Starting point:

### Langevin Maxwell-Bloch

electric field 
$$\nabla \times \nabla \times \mathbf{E} - \frac{\varepsilon_c}{c^2} \ddot{\mathbf{E}} = \frac{4\pi}{c^2} \left[ \ddot{\mathbf{P}}^+ + (\ddot{\mathbf{P}}^+)^* \right] - \frac{4\pi}{c} \dot{\mathbf{J}}$$
  
gain  $\dot{\mathbf{P}}^+ = -(i\omega_a + \gamma_\perp)\mathbf{P}^+ + \frac{g^2}{i\hbar}\mathbf{E}D$  noise noise population  $\dot{D} = \gamma_{\parallel}(D_0 - D) - \frac{2}{i\hbar}\mathbf{E} \cdot \left[ (\mathbf{P}^*)^+ - \mathbf{P}^+ \right]$   
[Arecchi & Bonifacio, 1965]

Noise correlations: fluctuation–dissipation theorem at T < 0

$$\langle J_i(\omega, x) J_j^*(\omega, x') \rangle = \frac{\omega}{\pi} \delta_{ij} \delta(x - x') \left[ \frac{\hbar \omega}{2} \coth\left(\frac{\hbar \omega}{2kT}\right) \right] \operatorname{Im} \varepsilon(x)$$

[Callen & Welton, 1957]

# The Noisy-SALT linewidth

Maxwell perturbation theory

ODE linearization +

closed-form integration

[Pick et al., PRA 91, 063806 (2015)]

Starting point: Langevin MB. (with **SALT** + **FDT**)

> Dynamical eqs. for lasing mode amplitudes (oscillator eqs.)

formulas for multimode **linewidths** & RO side peaks

## Oscillator equations

Noise-free SALT: 
$$\mathbf{E}(\mathbf{x},t) = \sum_{\mu} \mathbf{E}_{\mu}(\mathbf{x}) a_{\mu 0} e^{-i\omega_{\mu}t}$$
 SALT modes  
Noisy N-SALT:  $\mathbf{E}(\mathbf{x},t) = \sum_{\mu} \mathbf{E}_{\mu}(\mathbf{x}) a_{\mu}(t) e^{-i\omega_{\mu}t}$  SALT modes  
Simple limit: Single-mode "class A" lasers  
 $\frac{da_1}{dt} = C_{11} \left( a_{10}^2 - |a_1|^2 \right) a_1 + f_1$  often derived  
instantaneous restoring force often derived [Lax (1967)]

Most general dynamical equations (class A+B lasers)

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

time-delayed, spatially inhomogeneous restoring force

Solving the oscillator equations  

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

Expand mode amplitudes around steady state:  $a_{\mu} = (a_{\mu 0} + \delta_{\mu}) \exp(i\varphi_{\mu})$  [small noise = linearize in  $\delta_{\mu}$ ]

**•Miracle #1:** can solve analytically for  $\langle \phi_{\mu} \phi_{\nu} \rangle$  correlation function, which gives linewidths.

•Miracle #2:  $\gamma(x)$  exactly cancels and gives same answer as instantaneous model! The simple "class A" model is correct for "class B!"

### Single-mode linewidth formula [Pick et al., PRA 91, 063806 (2015)]



$$\Gamma = \frac{h\omega_0\gamma_0^2}{2P} \cdot \widetilde{n}_{\rm sp} \cdot \widetilde{K} \cdot \widetilde{B} \cdot (1+\widetilde{\alpha}^2)$$
  
ST I P B Q

$$\frac{\int dx \left[\frac{1}{2} \coth(\frac{\hbar\omega\beta}{2}) - \frac{1}{2}\right] \mathrm{Im}\varepsilon |\mathbf{E}_{0}|^{2}}{\int_{\mathrm{P}} dx \, \mathrm{Im} \, \varepsilon \, |\mathbf{E}_{0}|^{2}} \operatorname{Im}\varepsilon |\mathbf{E}_{0}|^{2} \operatorname{Incomplete inversion} \left[ \operatorname{Im} \left[ \frac{-i\omega_{0}^{2} \int \frac{\partial\varepsilon}{\partial|a|^{2}} \mathbf{E}_{0}^{2}}{\int \frac{\partial}{\partial\omega} (\omega^{2}\varepsilon) \mathbf{E}_{0}^{2}} \right] / \operatorname{Re} \left[ \frac{-i\omega_{0}^{2} \int \frac{\partial\varepsilon}{\partial|a|^{2}} \mathbf{E}_{0}^{2}}{\int \frac{\partial}{\partial\omega} (\omega^{2}\varepsilon) \mathbf{E}_{0}^{2}} \right] \\
\mathbb{O} \operatorname{C} \operatorname{factor} \operatorname{factor} \operatorname{C} \operatorname{factor} \operatorname{facto} \operatorname{factor} \operatorname{fac$$

### Brute-force validation

A. Cerjan et al., *Opt. Exp.* 23, 28316 (2015)

Brute-force simulations of Langevin–Maxwell–Bloch show excellent agreement with N-SALT linewidth formula



Only N-SALT captures all relevant physics in MB