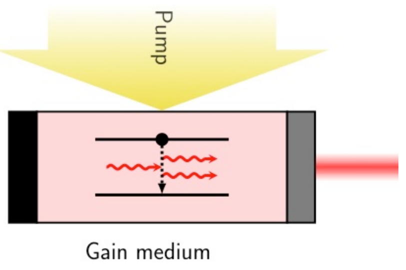
An efficient solution method for the Steady-state Ab-initio Laser Theory

Sofi Esterhazy[1], Matthias Liertzer[2], J. Markus Melenk[1], Stefan Rotter[2]
[1]Institute for Analysis and Scientific Computing, Vienna University of Technology, Vienna, Austria, EU
[2]Institute for Theoretical Physics, Vienna University of Technology, Vienna, Austria, EU

Introduction

- How to simulate a laser?
- Maxwell-Bloch equations
  - Semi-classical description
  - Set of nonlinear coupled, time-dependent PDEs
  - Long time-integration required for the steady-state regime



- Multi-periodic, time-harmonic ansatz more efficient:

$$E(\mathbf{x},t)=\sum_{\mu} u_\mu(\mathbf{x})e^{-ik_\mu t}$$

  - Super-position of a finite number of **active modes** $\{u_\mu, k_\mu\}$ with $k_\mu \in \mathbb{R}$

Steady-state Ab-initio Laser Theory [1]

PDE System

Find $\{u_\mu, k_\mu\}_{\mu=1}^M$ such that

$$\Big[\Delta + k_\mu^2 \varepsilon_\mu\left(\mathbf{x}, \{u_\nu, k_\nu\}_{\nu=1}^M\right)\Big]\, u_\mu(\mathbf{x}) = 0$$

$$\lim_{|\mathbf{x}|\to\infty} \left(\partial_n u_\mu(\mathbf{x}) - ik_\mu u_\mu(\mathbf{x})\right) = 0$$

$$\Im(k_\mu) = 0$$

- Set of M nonlinear coupled **Helmholtz equations** for the M active laser modes
- Nonlinear coupling through the complex-valued **dielectric function**

$$\varepsilon_\mu\left(\mathbf{x}, \{k_\nu, u_\nu\}\right) = \varepsilon_c(\mathbf{x}) + \varepsilon_g^\mu\left(\mathbf{x}, \{k_\nu, u_\nu\}\right)$$

- **Passive contribution** from cavity configuration:

$$\varepsilon_c(\mathbf{x}) = n^2(\mathbf{x})$$

- **Active contribution** refers to pump-induced amplification:

$$\varepsilon_g^\mu\left(\mathbf{x}, \{k_\nu, u_\nu\}\right) = \gamma(k_\mu) D\left(\mathbf{x}, \{k_\nu, u_\nu\}\right)$$

  - Susceptibility and gain curve:

$$\gamma(k_\mu) := \frac{\gamma_\perp}{k_\mu - k_a + i\gamma_\perp}, \qquad \Gamma(k) := |\gamma(k)|^2$$

  with $\gamma_\perp, k_a \in \mathbb{R}$ the gain width and frequency at the center of the gain

  - Population inversion:

$$D\left(\mathbf{x}, \{k_\nu, u_\nu\}\right) = D_0(\mathbf{x}, d)\Big[1 + \sum_{\nu=1}^{M} \Gamma(k_\nu)|u_\nu(\mathbf{x})|^2\Big]^{-1}$$

  with $D_0(\mathbf{x}, d)$ the external pump profile

Solution strategy

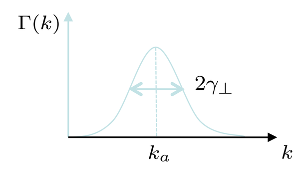
- Path-following technique in which the pump parameter d is increased continuously

Below threshold

- $0 < d < d_1$: no active modes, only **inactive modes**

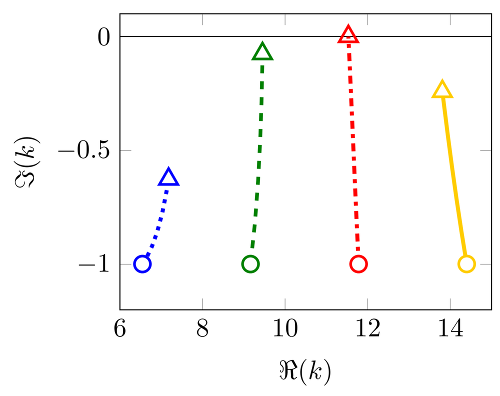
$$\left[\Delta + k_n^2\left(\varepsilon_c(\mathbf{x}) + \gamma(k_n)D_0(\mathbf{x}, d)\right)\right] u_n(\mathbf{x}) = 0$$

  - Spurious solutions at $k = k_a - \gamma_\perp$
  - Frequency-restricted gain curve
  - Eigenvalues k_n of interest within bounded domain



Contour integral method

- The resulting equation has only eigenpairs with eigenvalues in the negative complex plane, i.e. $\Im(k_n) < 0$
- When increasing the pump these eigenvalues move "upwards" to the real axis
- As soon as the imaginary part of one of the eigenvalues becomes positive, the corresponding laser mode must have been activated, and we proceed with the **nonlinear system**



- Initial data at threshold d_1: (u_1, k_1) with $k_1 \in \mathbb{R}$

Above threshold

- $d_1 < d < d_2$: one active mode
- SALT system reduces to one **nonlinear PDE**:

$$\Big[\Delta + k^2\Big(\varepsilon_c(\mathbf{x}) + \gamma(k)\frac{D_0(\mathbf{x}, d)}{1 + \Gamma(k)|u(\mathbf{x})|^2}\Big)\Big]u(\mathbf{x}) = 0$$

Newton method

- Verification of new mode activation
  - Insert solution (u_1^*, k_1^*) into denominator and omit the condition $\Im(k) = 0$

$$\Big[\Delta + k_n^2\Big(\varepsilon_c(\mathbf{x}) + \gamma(k_n)\frac{D_0(\mathbf{x}, d)}{1 + \Gamma(k_1^*)|u_1^*(\mathbf{x})|^2}\Big)\Big]u_n(\mathbf{x}) = 0$$

Contour integral method

- In analogy to the linear case we include an additional laser mode as soon as the imaginary part of one of the eigenvalues becomes positive
- $d_2 < d < d_3$: two active modes

$$\Big[\Delta + k_\mu^2\Big(\varepsilon_c(\mathbf{x}) + \gamma(k_\mu)\frac{D_0(\mathbf{x}, d)}{1 + \sum_\nu \Gamma(k_\nu)|u_\nu(\mathbf{x})|^2}\Big)\Big]u_\mu(\mathbf{x}) = 0$$

$$\Big[\Delta + k_n^2\Big(\varepsilon_c(\mathbf{x}) + \gamma(k_n)\frac{D_0(\mathbf{x}, d)}{1 + \sum_\nu \Gamma(k_\nu^*)|u_\nu^*(\mathbf{x})|^2}\Big)\Big]u_n(\mathbf{x}) = 0$$

- For higher numbers of modes: analogous procedure

FEM Discretization

- Matrix formulation:

$$\left[-\mathbf{L} + ik_\mu\mathbf{R} + k_\mu^2\mathbf{M}^{\varepsilon_c} + k_\mu^2\gamma(k_\mu)\,\mathbf{Q}(X)\right]\mathbf{u}_\mu = 0$$

  for $\mu = 1, \ldots, M$ with $X := (X_1, \ldots, X_M)$ and $X_\mu := (k_\mu, \mathbf{u}_\mu) \in \mathbb{R} \times \mathbb{C}^N$

- $\mathbf{L} := \left(\int_\Omega \nabla\varphi_i \nabla\varphi_j dx\right)_{i,j}$, $\mathbf{R} := \left(\int_{\partial\Omega} \varphi_i\varphi_j d\sigma_x\right)_{i,j}$
- $\mathbf{M}^{\varepsilon_c} := \left(\int_\Omega \varepsilon_c(x)\varphi_i\varphi_j dx\right)_{i,j}$
- $\mathbf{Q}(X) := \left(\int_\Omega \frac{D_0(x,d)\varphi_i(x)\varphi_j(x)}{1 + \sum_\nu \Gamma(k_\nu)|\sum_l u_l^\nu \varphi_l(x)|^2} dx\right)_{i,j}$

Contour Integral Method [2]

- Nonlinear EVP of the form $\mathbf{T}(k)\mathbf{u} = 0$
- The roots of the operator $\mathbf{T}$ are the poles of the inverse

$$\mathbf{T}^{-1}(k) = \sum \frac{1}{k - \lambda_n} v_n w_n^H + R(k)$$

  with λ_n being the eigenvalues, v_n, w_n being the left and right eigenvectors and R being a holomorphic remainder

- Via Residue Theorem

$$A_0 := \frac{1}{2\pi i}\int_{\mathcal{C}} \mathbf{T}^{-1}(z)dz = \sum_n v_n w_n^H = VW^H$$

$$A_1 := \frac{1}{2\pi i}\int_{\mathcal{C}} z\mathbf{T}^{-1}(z)dz = \sum_n \lambda_n v_n w_n^H = V\Lambda W^H$$

- Use reduced SVD $A_0 = V_l \Sigma_l W_l^H$ with l being the number of eigenvalues inside the contour
- Λ similar to $B := V_l^H A_1 W_l \Sigma_l^{-1} \in \mathbb{C}^{l\times l}$
- Projection method avoids computing the inverse of the sparse matrix $\mathbf{T}$
- Trapezoidal rule for exponential convergence

Newton-Raphson method

- Initial guess from previous pump step
- Jacobian can be calculated analytically
- Additional stability conditions needed
  - u_μ phase invariant solutions
  - Exclusion of trivial zero solutions

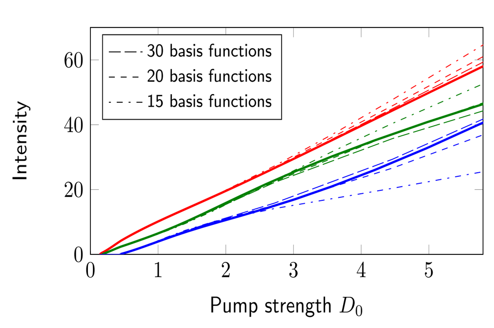
Conclusions

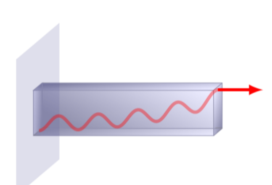
- Efficient method for the steady-state solutions of the time-dependent Maxwell-Bloch equations
- FEM for geometric flexibility in applications
- Stable computation with Newton method
- Contour integral method suitable for verification of mode activation
- For details see [3]

Numerical results and physical applications

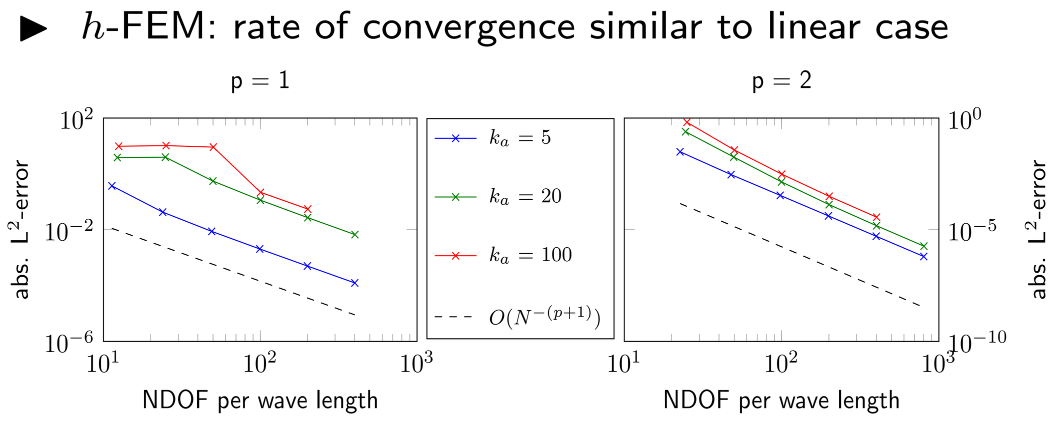
Convergence

- Comparison with constant flux method [1]:





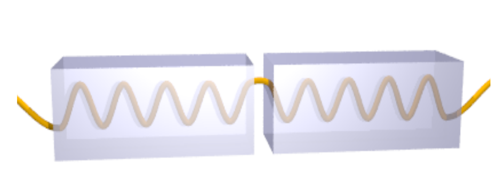
- h-FEM: rate of convergence similar to linear case

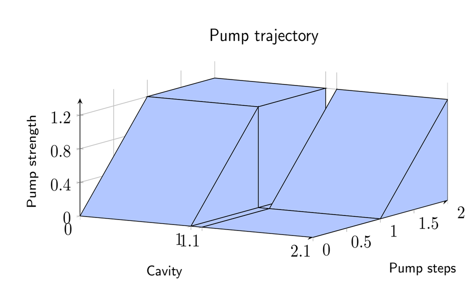


- Robust and powerful numerical implementation

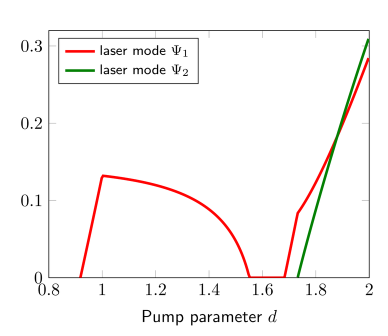
Two cavity laser

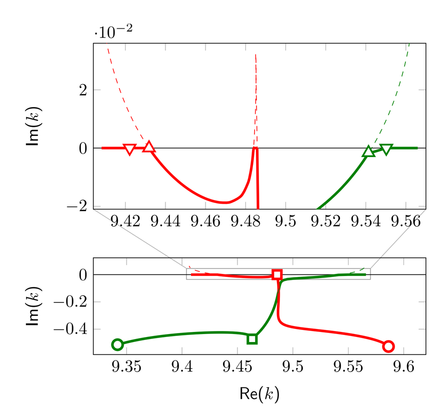
- Cavity and pump configuration:





- Laser shut-off due to exceptional point in the SALT operator [4]:





- Flexible and successful method for a wide range of complex applications

References

[1] H. E. Türeci, A. D. Stone, L. Ge, S. Rotter and R. J. Tandy, Nonlinearity 22 (2009)

[2] W.-J. Beyn, Lin. Alg. Appl. 436, 10 (2012)

[3] S. Esterhazy, D. Liu, M. Liertzer, A. D. Stone, J. M. Melenk, S. Johnson and S. Rotter, PRA, to be submitted

[4] M. Liertzer, L. Ge, A. Cerjan, A. D. Stone and S. Rotter, PRL 108, 173901 (2012)