Modeling Nonlinear Resonators Comprising Graphene: A Coupled Mode Theory Approach

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Motivation and objectives

**Motivation**

- Exploit graphene’s unique properties in practical nanophotonic resonators
  - Complex linear surface conductivity $\rightarrow$ strongly-confined modes
  - Highly dispersive
  - Highly nonlinear, Kerr-type response $\rightarrow$ low power nonlinear actions
- Expand perturbation theory and coupled mode theory framework to dispersive 2D sheet materials for efficient and accurate simulations

**Objectives**

- Physically model graphene as infinitesimally-thin (2D) material
- Obtain clear design rules for optical bistability in resonant structures
- Propose practical components in NIR and FIR (THz) regimes
Presentation outline

- **Mathematical Framework**
  - Perturbation Theory
  - Energy density in media with imaginary conductivity
  - Coupled Mode Theory
  - Application to optical bistability

- **Graphene Properties**
  - Far-Infrared regime (THz)
  - Near-Infrared regime

- **Resonant Structures**
  - 2D graphene-tube ring resonator (THz)
  - 3D graphene nanoribbon ring resonator (THz)
  - 3D silicon-slot ring resonator incorporating graphene (NIR)

- **Conclusion**
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Mathematical Framework
Perturbation Theory

**Nonlinear frequency shift** (perturbation theory)

Classic form:
\[
\frac{\Delta \omega}{\omega_0} = -\frac{1}{2} \frac{\iint_V (\Delta \tilde{\varepsilon} \mathbf{E}_0) \cdot \mathbf{E}_0^* dV}{\iiint_V \tilde{\varepsilon} \mathbf{E}_0 \cdot \mathbf{E}_0^* dV}
\]

Extended form:
\[
\frac{\Delta \omega}{\omega_0} = -\frac{\iint_V \mathbf{P}_{\text{NL}} \cdot \mathbf{E}_0^* dV - j \frac{1}{\omega_0} \iint_V \mathbf{J}_{\text{NL}} \cdot \mathbf{E}_0^* dV}{\iint_V \varepsilon_0 \frac{\partial \{\omega \tilde{\varepsilon}\}}{\partial \omega} \mathbf{E}_0 \cdot \mathbf{E}_0^* dV + \iint_V \mu_0 \mathbf{H}_0 \cdot \mathbf{H}_0^* dV + \iint_V \frac{\partial \bar{\sigma}_{\text{im}}^{(1)}}{\partial \omega} \mathbf{E}_0 \cdot \mathbf{E}_0^* dV}
\]

[Bravo-Abad, JLT 25, 2539]

[Christopoulos, PRE 94, 062219]

- Polarization nonlinearities
- Current density nonlinearities → Allows for modeling graphene
- Dispersive electric energy
- Extra energy term in media with dispersive complex conductivity
- Magnetic energy in the denominator \((W_e \neq W_m;\text{ next slide})\)
Poynting theorem in the time domain

\[ \langle J(t) \cdot \mathcal{E}(t) \rangle = \frac{1}{2} \sigma_{\text{Re}}^{(1)} \mathcal{E}_0(\omega) \cdot \mathcal{E}_0^*(\omega) + \frac{\partial}{\partial t} \left\{ \frac{1}{4} \partial_{\text{Im}}^{(1)} \partial_{\omega} \mathcal{E}_0(\omega) \cdot \mathcal{E}_0^*(\omega) \right\} \]

- Power loss density
- Stored energy density
- Zero when dispersion is neglected

Physical Remarks

Energy density in media with complex conductivity
Energy density in media with complex conductivity

Poynting theorem in the time domain

\[ \langle J(t) \cdot E(t) \rangle = \frac{1}{2} \bar{\sigma}^{(1)}_{\text{Re}} E_0(\omega) \cdot E_0^*(\omega) + \frac{\partial}{\partial t} \left\{ \frac{1}{4} \frac{\partial \bar{\sigma}^{(1)}_{\text{Im}}}{\partial \omega} E_0(\omega) \cdot E_0^*(\omega) \right\} \]

- Power loss density
- Stored energy density

Zero when dispersion is neglected

Poynting theorem in the frequency domain

\[ - \iiint_V \nabla \cdot S dV = \frac{1}{2} \iiint_V \bar{\sigma}^{(1)}_{\text{Re}} E_0 \cdot E_0^* dV - \]
\[ - j \frac{1}{2} \omega_0 \iiint_V \varepsilon_0 \varepsilon_r E_0 \cdot E_0^* dV + j \frac{1}{2} \omega_0 \iiint_V \mu_0 H_0 \cdot H_0^* dV + j \frac{1}{2} \iiint_V \bar{\sigma}^{(1)}_{\text{Im}} E_0 \cdot E_0^* dV \]
\[ = P_{\text{loss}} + j (-Q_E + Q_H + Q_J) \]

- Reactive power ≠ Dispersive energy (\( Q \neq 2 \omega_0 W \))
- On resonance:
  - \( Q_E = Q_H + Q_J \)
  - \( W_e \neq W_m \) (equality typically taken for granted)
Coupled Mode Theory (CMT)

\[
\frac{da}{dt} = j(\omega_0 + \Delta \omega)a - \left(\frac{1}{\tau_i} + \frac{1}{\tau_e}\right)a + \mu s_i
\]

\[s_t = s_i + \mu a\]

\[\alpha(t)\quad \text{cavity amplitude, } |\alpha|^2 \equiv W_e + W_m + W_j\]

\[\omega_0\quad \text{unperturbed resonance frequency}\]

\[\Delta \omega\quad \text{nonlinear frequency shift}\]

\[\tau\quad \text{photon lifetime, } \tau = 2Q/\omega_0\]

\[\mu\quad \text{coupling coefficient, } \mu = j\sqrt{2/\tau_e}\]

\[s(t)\quad \text{w/g mode amplitude, } |s|^2 \equiv P\]

Steady-state response

\[
\frac{p_{\text{out}}}{p_{\text{in}}} = \frac{(\delta + p_{\text{in}} - p_{\text{out}})^2 + (1 - r_Q)^2}{(\delta + p_{\text{in}} - p_{\text{out}})^2 + (1 + r_Q)^2}
\]

\[\delta = \tau_i(\omega - \omega_0)\quad \text{normalized detuning}\]

\[\delta_{\text{th}} = -\left(1 + r_Q\right)\sqrt{3}\quad \text{detuning threshold for BI}\]

\[r_Q = Q_i/Q_e\quad \text{quality factor ratio}\]

\[p = P/P_0\quad \text{normalized power}\]

\[P_0\quad \text{characteristic power}\]

- Closed-form polynomial equation
- Admits three real positive solutions (optical bistability)
  - \(\delta < \delta_{\text{th}}\) or \(\delta > -\delta_{\text{th}}\)
  - \(P_{\text{in}} > 5P_0\)
- Minimize \(P_0 \propto 1/(Q^2\kappa)\)
- Critical coupling condition, \(r_Q = 1\)

[Tsilipakos, JOSA B 31, 2014]
[Soljacic, PRE 5, 2002]
Application to optical bistability

**Increase in $|\delta|$**

- Higher input power required
- Loop span increases
- Maximum transmission increases
Performance

Application to optical bistability

Increase in $|\delta|$
- Higher input power required
- Loop span increases
- Maximum transmission increases

Decreasing $r_Q$ below 1
- Higher input power required
- $T_{\text{min}}$ increases (loop elevation)
- Loop span increases ($\delta_{\text{th}}$ decreases)

Increase in $|\delta|$

Decreasing $r_Q$ below 1
Application to optical bistability

**Increase in $|\delta|$**
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Graphene Properties
Graphene Properties

Far-Infrared regime (THz)

**Linear Properties**

\[ J_{s,\text{lin}} = \sigma_{\text{intra}}(\omega)E_{0,\parallel} \]

- Only intraband transitions allowed (Drude-like response)
- Complex electrical conductivity \( \sigma_1 = \sigma_{\text{intra}} \)
  - Small \( \text{Re}\{\sigma_1\} \) (low losses)
  - Highly negative \( \text{Im}\{\sigma_1\} \) (plasmonic behavior)
- Strong dispersion

[Falkovsky, Phys. Usp. 178, 887]

**Nonlinear Properties**

\[ J_{s,\text{NL}} = \frac{\sigma_3(\omega)}{4} \left[ 2(E_{0,\parallel} \cdot E_{0,\parallel}^*)E_{0,\parallel} + (E_{0,\parallel} \cdot E_{0,\parallel})E_{0,\parallel}^* \right] \]

- Kerr-type nonlinearity (purely imaginary \( \sigma_3 \))
- \( \sigma_3 = j4.7 \times 10^{-19} \text{ S(m/V)}^2 \) @ 10 THz
- \( n_2^\text{eq} = 2.4 \times 10^{-13} \text{ m}^2/\text{W} \) (self-focusing material)

Near-Infrared regime (NIR)

**Linear Properties**

\[ J_{s, \text{lin}} = \left( \sigma_{\text{intra}}(\omega) + \sigma_{\text{inter}}(\omega) \right) E_{0,\|} \]

- Intraband transitions always allowed
- Interband transitions allowed for \( hf < 2\mu_c \)
- Low loss regime \( \mu_c \approx 0.4 \text{ eV} \) @ \( \lambda = 1.55 \mu\text{m} \) (0.8 eV)
- Mild dispersion

[Hanson, IEEE Trans. Ant. Propag. 56, 064302]

**Nonlinear Properties**

\[ J_{s, \text{NL}} = \frac{\sigma_3(\omega)}{4} \left[ 2(E_{0,\|} \cdot E_{0,\|}^*)E_{0,\|} + (E_{0,\|} \cdot E_{0,\|}^*)E_{0,\|}^* \right] \]

- Kerr-type nonlinearity (purely imaginary \( \sigma_3 \))
- \( n_2^{\text{eq}} = -1 \times 10^{-13} \text{ m}^2/\text{W} \) (defocusing material)
- \( \sigma_3 = -j5.5 \times 10^{-21} \text{ S(m/V)}^2 \) @ 1.55 \( \mu\text{m} \)

[Dremetsika, Opt. Lett. 41, 3281]
[Vermeulen, PRA 6, 044006]
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Resonant Structures
**Resonator Design**

**2D graphene-tube ring resonator (1)**

- Resonator: Infinite graphene tube
- Bus waveguide: Infinite graphene sheet
- Surface Plasmon Polaritons supported at THz
  - Sub-wavelength confinement
  - Low radiation losses
  - Low-power, Kerr-induced bistability

**Nonlinear frequency shift**

\[ \Delta \omega = \left( \frac{\omega_0}{c_0} \right)^3 \kappa_s \frac{\sigma_{3,\text{Im}}^\text{max}}{\varepsilon_0^2} (W_e + W_m + W_j) \]

**Characteristic Power**

\[ P_0 = \frac{\varepsilon_0^2 c_0^3}{2 \omega_0 \sigma_{3,\text{Im}}^\text{max} \kappa_s Q_i^2} \propto \frac{1}{\kappa_s Q_i^2} \]

\( P_0 \) must be minimized for optimum performance

[Christopoulos, PRE 94, 062219]
[Tsilipakos, JLT 34, 1333]
Resonator Design

2D graphene-tube ring resonator (2)

- $\kappa_s \propto 1/R$
- $\kappa_s^{\text{non}} \approx 4\kappa_s^{\text{disp}}$
2D graphene-tube ring resonator (2)

- $\kappa_s \propto 1/R$
- $\kappa_s \text{non} \approx 4\kappa_s \text{disp}$
- $Q_i \propto R$
- $Q_i \text{disp} \approx 2Q_i \text{non}$
Resonator Design

2D graphene-tube ring resonator (2)

- NL feedback parameter $\kappa_s$
  - $\kappa_S \propto 1/R$
  - $\kappa_s^\text{non} \approx 4\kappa_s^\text{disp}$

- Intrinsic $Q$-factor $Q_i$
  - $Q_i \propto R$
  - $Q_i^\text{disp} \approx 2Q_i^\text{non}$

- Char. Power $P_0$ (W/m)
  - $P_0 = 1.32$ W/m
  - $P_0^\text{3D} \approx 20$ $\mu$W
  - $f_0 = 10.021$ THz

- $R = 2$ $\mu$m
- $g = 1.74$ $\mu$m

- $\kappa_s^\text{non} (Q_i^\text{non})^2 = \kappa_s^\text{disp} (Q_i^\text{disp})^2$

- $P_0$ is the same since $\kappa_s^\text{non} (Q_i^\text{non})^2 = \kappa_s^\text{disp} (Q_i^\text{disp})^2$

- Total minimum of $P_0$ for low-power bistability

- Critical coupling [$r_Q = 1$]
Device Performance

2D graphene-tube ring resonator (3)

**CW case**

- CMT
  - \( Q_i^{\text{disp}} \approx 2Q_i^{\text{non}} \Rightarrow \delta^{\text{disp}} = 2\delta^{\text{non}} \)
  - Always include dispersion

- NL-VFEM
  - Two power sweeps (ascending and descending)
  - Initial condition of each step: previous solution
  - Excellent agreement between FEM and CMT

![Graph showing device performance](image-url)
2D graphene-tube ring resonator (3)

**Device Performance**

### CW case

- **CMT**
  - \( Q_i^{\text{disp}} \approx 2Q_i^{\text{non}} \Rightarrow \delta^{\text{disp}} = 2\delta^{\text{non}} \)
  - Always include dispersion

- **NL-VFEM**
  - Two power sweeps (ascending and descending)
  - Initial condition of each step: previous solution
  - Excellent agreement between FEM and CMT

#### Dynamic memory implementation

![Diagram showing power transmission over time with dynamic memory implementation](diagram.png)

- CMT dispersive
- CMT nondispersive
- FEM up-sweep
- FEM down-sweep

- Power (W/m)
- Time (ps)

- 150 ps
Device Performance

3D graphene nanoribbon ring resonator

- Infinite graphene sheet
- Resonator/waveguide:
  - "Written" with $|\sigma_{1,\text{Im}}| < |\sigma'_{1,\text{Im}}|
  - Uneven ground and/or voltage
- Surface Plasmon Polariton supported at THz

- $R = 10.1 \, \mu m$
- $g = 2.20 \, \mu m$
- $Q_i^{\text{non}} = 1048$
- $Q_i^{\text{disp}} = 2080$
- $P_0 = 24 \, \mu W$
- $f_0 = 10 \, \text{THz}$
- $\kappa_s^{\text{non}} = 6.52$
- $\kappa_s^{\text{disp}} = 1.65$

[Vakil and Engheta, Science 332, 1291]
**Device Performance**

**3D silicon-slot ring resonator incorporating graphene**

- Graphene with conductivity $\sigma_1$
- Silica (SiO$_2$)
- Silicon (Si)

- Si-slot platform
  - High confinement
  - Major $E$-field component $\parallel$ to graphene

- Infinite graphene sheet on top

**Device Parameters**

- $R = 3.25 \, \mu m$
- $g = 150 \, nm$
- $P_{0, Kerr} = 6.2 \, mW$
- $\lambda_0 = 1.553 \, \mu m$
- $P_{0,s, Kerr} = 6.1 \, mW$
- $P_{0,b, Kerr} = 1.6 \, W$
Conclusion

Summary

- Strict framework for nonlinear resonators comprising bulk (3D) and/or sheet (2D) dispersive material
- Rigorous design rules for low-power bistability
- Excellent agreement with full-wave simulations
- Practical 3D nanophotonic components in both NIR and FIR (THz) regimes
- Opens the way for switching, memory, and logic applications

To probe further ...

- Incorporate Two Photon Absorption in graphene
- Exploit the framework for multi-channel non-linear actions
  - Two-channel $\chi^{(3)}$ effects: Cross-Phase Modulation, Third Harmonic Generation
  - Three-channel $\chi^{(3)}$ effects: Degenerated Four-Wave Mixing
- Dynamic control via graphene’s free carriers ($\mu_c$ tuning)
Thank you!

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And... there is more

Back up material!
Physical Remarks

Energy density in media with complex conductivity (full proof)

- Poynting vector in time domain: \( \nabla \cdot \mathbf{S} = -\nabla \cdot (\mathbf{E} \times \mathbf{H}) = \mathbf{J} \cdot \mathbf{E} + \frac{\partial \mathbf{D}}{\partial t} \cdot \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} \cdot \mathbf{H} \)

- Second and third terms correspond to stored energy. What about the first term?

- Slow varying envelope: \( \mathcal{F} = \text{Re}\{\mathbf{F}_0 \exp(\pm j\omega_0 t)\} = (\mathbf{F}_0 + \mathbf{F}_0^*)/2 \) \( \mathcal{F} = \{\mathbf{E}, \mathbf{J}\} \)

- Time averaging w.r.t. \( T_0 = 2\pi/\omega_0 \): \( \langle \mathbf{J} \cdot \mathbf{E} \rangle = (\mathbf{E}_0^* \cdot \mathbf{J}_0 + \mathbf{E}_0 \cdot \mathbf{J}_0^*)/4 \)

- Fourier transform on the envelope: \( \mathbf{J}_0(t) = \frac{1}{2\pi} \int \mathbf{j}_0(\omega)e^{j\omega t} \, d\omega \)

- Apply Ohm’s law to the “high” frequency: \( \mathbf{j}_0(\omega) = \bar{\sigma}^{(1)}(\omega + \omega_0)\mathbf{E}_0(\omega) \)

- Expand \( \bar{\sigma}^{(1)} \) in Taylor series:

\[
\bar{\sigma}_{\text{Re}}^{(1)}(\omega + \omega_0) \approx \bar{\sigma}_{\text{Re}}^{(1)}(\omega_0) \\
\bar{\sigma}_{\text{Im}}^{(1)}(\omega + \omega_0) \approx \bar{\sigma}_{\text{Im}}^{(1)}(\omega_0) + \omega \frac{\partial \bar{\sigma}_{\text{Im}}^{(1)}}{\partial \omega} \bigg|_{\omega=\omega_0}
\]

- Inverse Fourier transform on the result

- Finally:

\[
\langle \mathbf{J} \cdot \mathbf{E} \rangle = \frac{1}{2} \bar{\sigma}_{\text{Re}}^{(1)} \mathbf{E}_0 \cdot \mathbf{E}_0^* + \frac{\partial}{\partial t} \left\{ \frac{1}{4} \frac{\partial \bar{\sigma}_{\text{Im}}^{(1)}}{\partial \omega} \mathbf{E}_0 \cdot \mathbf{E}_0^* \right\}
\]

[Landau and Lifshitz, Electrodynamics of continuous media, Elsevier, 1984]
[Christopoulos, PRE 94, 062219]
Correct calculation of $\kappa$

**FEM eigenvalue solution**
- Two degenerated counter-propagating modes
- Standing-wave pattern
- $E(\rho, \varphi) = e^+(\rho, \varphi) + e^-(\rho, \varphi)$
- $H(\rho, \varphi) = h^+(\rho, \varphi) + h^-(\rho, \varphi)$

**FEM propagation solution**
- One single mode propagating (counter)clockwise
- Traveling-wave pattern
- $E(\rho, \varphi) = e^+(\rho, \varphi)$
- $H(\rho, \varphi) = h^+(\rho, \varphi)$

\[
\begin{align*}
\mathbf{e}^\pm(\rho, \varphi) &= [e_{\rho}(\rho)\hat{\rho} \pm j e_{\rho}(\rho)\hat{\Phi}]\exp\{-\mp jm\varphi\} \\
\mathbf{h}^\pm(\rho, \varphi) &= \mp h_z(\rho)\hat{z}\exp\{-\mp jm\varphi\}
\end{align*}
\]

\[
\frac{\kappa_s^{\text{prop}}}{\kappa_s^{\text{eig}}} = \frac{2}{3}
\]
Resonator Design

3D graphene nanoribbon ring resonator

\[ R = 10.1 \, \mu m \]
\[ g = 2.20 \, \mu m \]
\[ P_0 = 24 \, \mu W \]
\[ f_0 = 10 \, \text{THz} \]

Nonlinear feedback parameter

\[
\kappa_S = \left( \frac{c_0}{\omega_0} \right)^4 \frac{\iint_S \sigma_3 \left( 2 |E_{0,\parallel}|^4 + |E_{0,\parallel} \cdot E_{0,\parallel}|^2 \right) dS}{\left[ \iiint_V \varepsilon_r |E_0|^2 dV + \iiint_V \eta_0^2 |H_0|^2 dV + \frac{1}{\varepsilon_0} \iint_S \frac{\partial \sigma_{1,\text{im}}}{\partial \omega} |E_{0,\parallel}|^2 dS \right]^2} \sigma_3^{\text{max}}
\]
Resonator Design

3D silicon-slot ring resonator incorporating graphene

- **Resonator Design**
  - $R = 3.25 \, \mu m$
  - $g = 150 \, \text{nm}$
  - $P_0 = 6.2 \, \text{mW}$
  - $\lambda_0 = 1.553 \, \text{nm}$

**Nonlinear feedback parameters**

- **Silicon $\kappa_b$**
  \[ \kappa_b = \left( \frac{c_0}{\omega_0} \right)^3 \left( \frac{1}{3} \iint_V n^2 n_2 (2 |E_0|^4 + |E_0 \cdot E_0|^2) dV \right) \]
  \[ \left[ \iint_V \varepsilon_r |E_0|^2 dV + \iint_V \eta_0^2 |H_0|^2 dV + \frac{1}{\varepsilon_0} \iint_S \frac{\partial \sigma_{1,\text{Im}}}{\partial \omega} |E_{0,\|}|^2 dS \right]^2 n_2^{\max} \]

- **Graphene with conductivity $\sigma_1$**
  \[ \kappa_s = \left( \frac{c_0}{\omega_0} \right)^4 \left( \frac{2}{\varepsilon_0} \right) \left( \frac{1}{3} \iint_S \sigma_3 \left( 2 |E_{0,\||}|^4 + |E_{0,\||} \cdot E_{0,\||}|^2 \right) dS \right) \]
  \[ \left[ \iint_V \varepsilon_r |E_0|^2 dV + \iint_V \eta_0^2 |H_0|^2 dV + \frac{1}{\varepsilon_0} \iint_S \frac{\partial \sigma_{1,\text{Im}}}{\partial \omega} |E_{0,\|}|^2 dS \right]^2 \sigma_3^{\max} \]

Graphene with conductivity $\sigma_1$
- silica (SiO$_2$)
- silicon (Si)